



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:05 PM BST

PDB ID : 3RSZ
Title : Maltodextran bound basal state conformation of yeast glycogen synthase isoform 2
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2011-05-02
Resolution : 3.01 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) : 1.13
EDS : 2.13.1
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) : 2.13.1

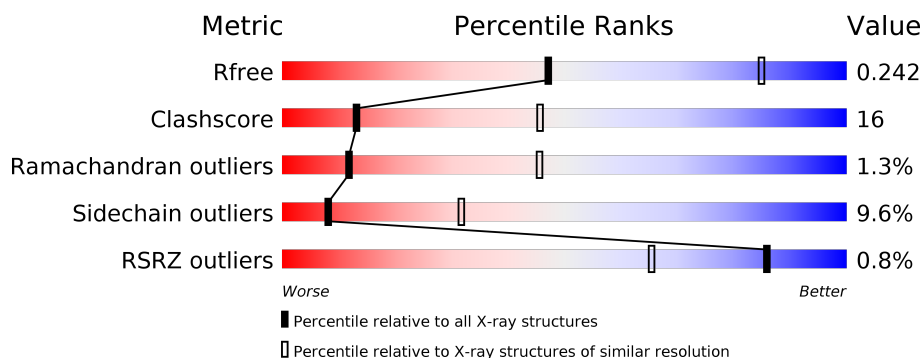
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.





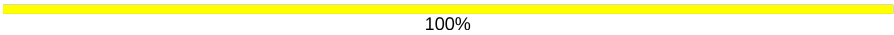

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 $\leq 5\%$. 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	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 54%, yellow 25%, orange 5%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 54% 25% 5% 16% </div> </div>
1	B	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 54%, yellow 26%, orange 5%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 54% 26% • 16% </div> </div>
1	C	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 53%, yellow 27%, orange 5%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 53% 27% 5% 15% </div> </div>
1	D	725	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 54%, yellow 26%, orange 5%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 54% 26% • 15% </div> </div>
2	E	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 40%, grey 60%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 40% 60% </div> </div>
2	F	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	4	 50%50%
3	H	4	 75%25%
3	I	4	 100%
3	J	4	 25%75%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	J	1	-	-	-	X
3	GLC	J	4	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20011 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	B	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	C	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			
1	D	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ARG	engineered mutation	UNP P27472
A	581	ALA	ARG	engineered mutation	UNP P27472
A	583	ALA	ARG	engineered mutation	UNP P27472
B	-19	MET	-	expression tag	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	580	ALA	ARG	engineered mutation	UNP P27472
B	581	ALA	ARG	engineered mutation	UNP P27472
B	583	ALA	ARG	engineered mutation	UNP P27472
C	-19	MET	-	expression tag	UNP P27472
C	-18	GLY	-	expression tag	UNP P27472
C	-17	SER	-	expression tag	UNP P27472
C	-16	SER	-	expression tag	UNP P27472
C	-15	HIS	-	expression tag	UNP P27472
C	-14	HIS	-	expression tag	UNP P27472
C	-13	HIS	-	expression tag	UNP P27472
C	-12	HIS	-	expression tag	UNP P27472
C	-11	HIS	-	expression tag	UNP P27472
C	-10	HIS	-	expression tag	UNP P27472
C	-9	SER	-	expression tag	UNP P27472
C	-8	SER	-	expression tag	UNP P27472
C	-7	GLY	-	expression tag	UNP P27472
C	-6	LEU	-	expression tag	UNP P27472
C	-5	VAL	-	expression tag	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP P27472
C	-3	ARG	-	expression tag	UNP P27472
C	-2	GLY	-	expression tag	UNP P27472
C	-1	SER	-	expression tag	UNP P27472
C	0	HIS	-	expression tag	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	580	ALA	ARG	engineered mutation	UNP P27472
C	581	ALA	ARG	engineered mutation	UNP P27472
C	583	ALA	ARG	engineered mutation	UNP P27472
D	-19	MET	-	expression tag	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression tag	UNP P27472
D	-15	HIS	-	expression tag	UNP P27472
D	-14	HIS	-	expression tag	UNP P27472
D	-13	HIS	-	expression tag	UNP P27472
D	-12	HIS	-	expression tag	UNP P27472
D	-11	HIS	-	expression tag	UNP P27472
D	-10	HIS	-	expression tag	UNP P27472
D	-9	SER	-	expression tag	UNP P27472
D	-8	SER	-	expression tag	UNP P27472
D	-7	GLY	-	expression tag	UNP P27472
D	-6	LEU	-	expression tag	UNP P27472
D	-5	VAL	-	expression tag	UNP P27472
D	-4	PRO	-	expression tag	UNP P27472
D	-3	ARG	-	expression tag	UNP P27472
D	-2	GLY	-	expression tag	UNP P27472
D	-1	SER	-	expression tag	UNP P27472
D	0	HIS	-	expression tag	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	580	ALA	ARG	engineered mutation	UNP P27472
D	581	ALA	ARG	engineered mutation	UNP P27472
D	583	ALA	ARG	engineered mutation	UNP P27472

- Molecule 2 is a protein called Glycogen [starch] synthase isoform 2.

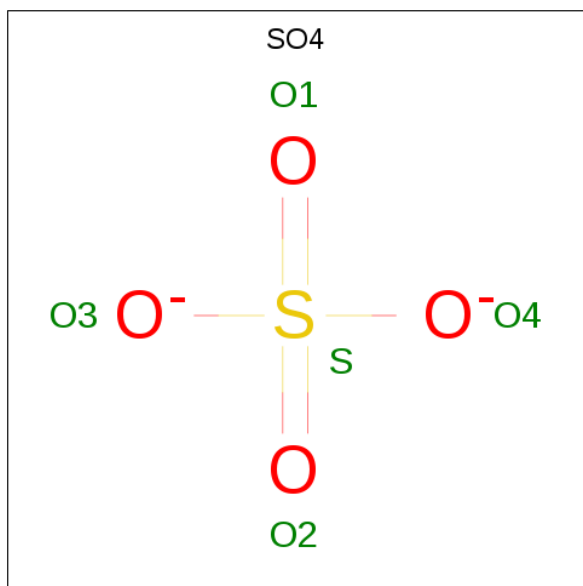
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	1	0	0
			10	6	2	2			
2	F	5	Total	C	N	O	1	0	0
			25	15	5	5			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	4	Total	C	O	0	0	0
			45	24	21			
3	H	4	Total	C	O	0	0	0
			45	24	21			
3	I	4	Total	C	O	0	0	0
			45	24	21			
3	J	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

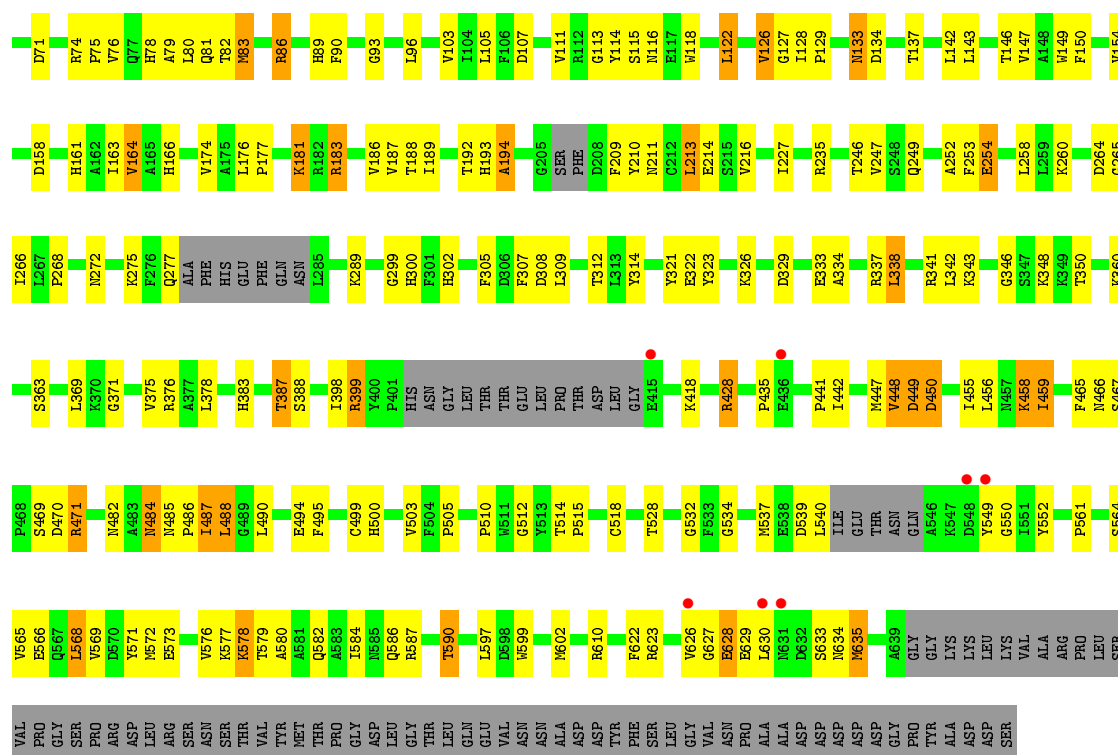


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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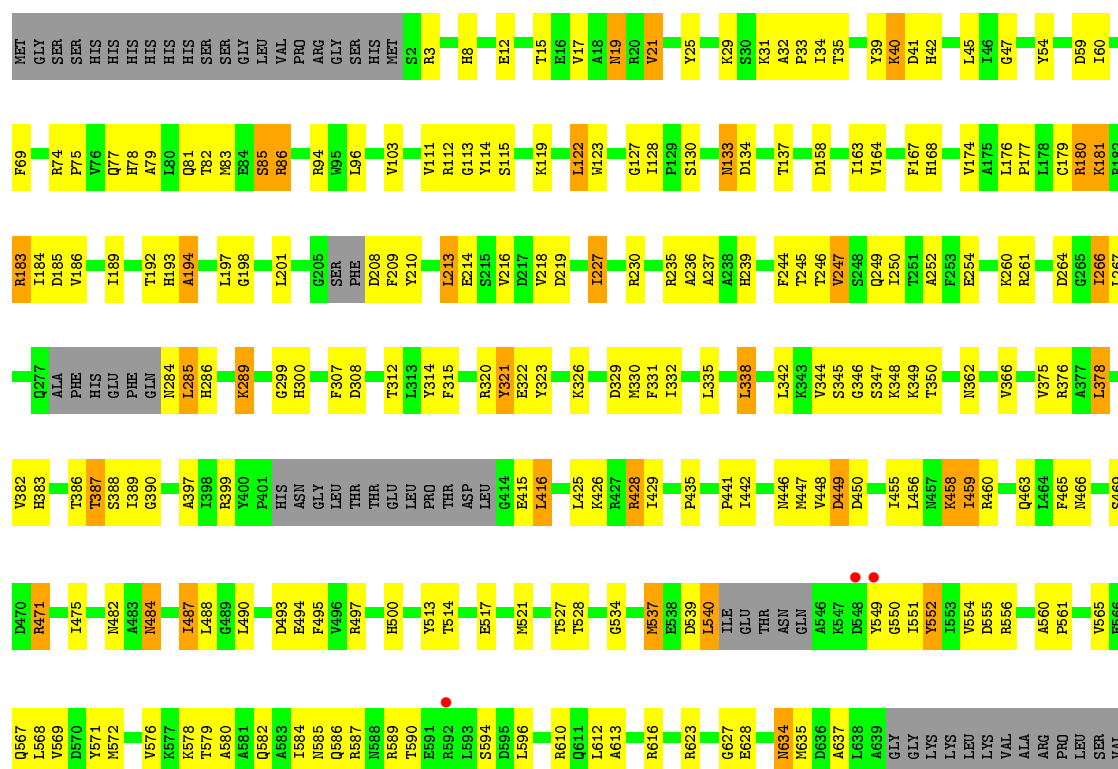
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		



• Molecule 1: Glycogen [starch] synthase isoform 2

Chain C: 53% 27% 5% 15%



PRO	GLY	PRO	GLY	ASP	LEU	ARG	ASP	LEU	ARG	SER	ASN	THR	VAL	TYR	MET	THR	PRO	PRO	GLY	ASP	ASP	LEU	GLY	THR	LEU	GLN	GLU	VAL	ASN	ASN	ALA	ASP	ASP	TYR	PHE	SER	LEU	GLY	VAL	ASN	ASN	PRO	ALA	ALA	ASP	ASP	ASP	ASP	ASP	GLY	PRO	TYR	ALA	ASP	ASP	SER
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• Molecule 1: Glycogen [starch] synthase isoform 2

Chain D: 

THR	VAL	TYR	THR	THR	PRO	GLY	ASP	LEU	GLY	THR	GLN	GLU	VAL	ASN	ASN	ALA	ASP	ASP	TYR	PHE	SER	LEU	VAL	VAL	ASN	PRO	ALA	ALA	ASP	ASP	ASP	ASP	ASP	GLY	PRO	TYR	ALA	LYS	LYS	LEU	LYS	VAL	ALA	ARG	PRO	LEU	SER	VAL	GLY	SER	PRO	ARG	ASP	LEU	ARG	SER	ASN	SER
F575	V576	K577	K578	T579	A580	A581	Q582	A583	I584	N585	Q586	R587	H588	R589	T590	S594	D595	L596	R610	G611	L612	R616	R623	M634	K635	D636	A637	L638	A639	GLY	GLY	LYS	LEU	LYS	VAL	ALA	ARG	PRO	LEU	SER	VAL	PRO	PRO	GLY	SER	ARG	ASP	LEU	ARG	SER	ASN	SER						
T386	T387	S388	I389	R399	Y400	P401	HIS	ASN	GLY	LEU	THR	THR	THR	GLU	LEU	PRO	THR	ASP	G414	E415	L416	L425	K426	R427	R428	I429	L430	I441	I442	M446	M447	V448	D449	D450	I455	L456	K457	K458	I459	R460	Q463	L464	F465	N466	S469	D470	R471	I475	N482									
A483	M484	I487	L488	G489	L490	D493	E494	F495	V496	R497	H500	Y513	T514	E517	M521	T527	T528	G534	M537	E538	D539	L540	I541	GLU	THR	ASN	GLN	A546	K547	D548	Y549	O550	I551	Y552	I553	V554	D555	R556	A560	P561	V565	E566	Q567	L568	V569	D570	Y571	M572										
HIS	GLU	PHE	GLN	L284	L285	H286	F289	G299	H300	F305	D306	F307	D308	T312	L313	Y314	F315	R320	Y321	E322	Y323	K326	D329	M330	F331	I332	L335	L338	L342	K343	V344	S345	G346	S347	K348	T349	T350	N362	V366	V375	D376	A377	L378	V382	H383													
I189	T192	A194	L197	G198	L201	G205	SER	PHE	D208	F209	Y210	L213	E214	S215	V216	D217	V218	D219	I227	R230	R235	A236	A237	A238	E239	F244	T245	T246	V247	Q248	Q249	I250	T251	A252	F253	E254	K260	R261	D264	G265	I266	L267	Q277	ALA	PHE													
H78	A79	L80	Q81	H82	M83	E84	S85	R86	R88	R94	Y95	L96	V103	I104	L105	V111	R112	G113	S115	K119	L122	W123	G127	I128	P129	S130	N133	D134	T137	D158	I163	V164	F167	H168	V174	A175	L176	P177	L178	C179	R180	K181	R182	R183	I184	D185	V186											
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	S2	R3	H8	E12	T15	E16	V17	A18	N19	R20	V21	K31	A32	P33	I34	T35	Y39	K40	D41	H42	L45	L46	G47	Y54	D59	I60	R74	P75	V76	I78	V186								

• Molecule 2: Glycogen [starch] synthase isoform 2

Chain E: 

X3	X4	UNK	UNK	UNK
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• Molecule 2: Glycogen [starch] synthase isoform 2

Chain F: 

There are no outlier residues recorded for this chain.

• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G: 



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  75% 25%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:  100%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.56Å 166.73Å 121.14Å 90.00° 103.25° 90.00°	Depositor
Resolution (Å)	47.56 – 3.01 47.56 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.56-3.01) 98.9 (47.56-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.207 , 0.244 0.200 , 0.242	Depositor DCC
R_{free} test set	3673 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20011	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, SO4

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	0.39	0/5038	0.54	0/6819
1	B	0.39	0/5038	0.54	0/6819
1	C	0.40	0/5050	0.56	0/6835
1	D	0.39	0/5050	0.55	1/6835 (0.0%)
All	All	0.39	0/20176	0.55	1/27308 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	540	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4923	0	4850	165	0
1	B	4923	0	4850	156	0
1	C	4935	0	4859	169	0
1	D	4935	0	4859	168	0
2	E	10	0	4	0	0
2	F	25	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	45	0	39	1	0
3	H	45	0	39	2	0
3	I	45	0	39	0	0
3	J	45	0	39	2	0
4	A	20	0	0	1	0
4	B	20	0	0	0	0
4	C	20	0	0	1	0
4	D	20	0	0	1	0
All	All	20011	0	19585	644	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 16.

All (644) 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:C:539:ASP:O	1:C:540:LEU:HD23	1.57	1.02
1:C:314:TYR:H	1:C:500:HIS:HD2	1.10	0.95
1:D:314:TYR:H	1:D:500:HIS:HD2	1.07	0.93
1:B:235:ARG:HH21	1:B:260:LYS:HG3	1.35	0.91
1:A:235:ARG:HH21	1:A:260:LYS:HG3	1.34	0.90
1:B:442:ILE:HD12	1:B:459:ILE:HD11	1.57	0.86
1:C:549:TYR:O	1:C:590:THR:HG22	1.76	0.86
1:A:390:GLY:HA2	1:C:386:THR:HG21	1.55	0.86
1:B:399:ARG:NH2	1:D:308:ASP:HA	1.91	0.86
1:A:442:ILE:HD12	1:A:459:ILE:HD11	1.57	0.83
1:D:549:TYR:O	1:D:590:THR:HG22	1.79	0.83
1:C:122:LEU:HD13	1:C:128:ILE:HB	1.60	0.83
1:B:399:ARG:HH22	1:D:308:ASP:HA	1.44	0.82
1:D:314:TYR:H	1:D:500:HIS:CD2	1.96	0.82
1:D:122:LEU:HD13	1:D:128:ILE:HB	1.61	0.81
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.64	0.80
1:A:482:ASN:HB3	1:A:484:ASN:HD21	1.47	0.79
1:A:386:THR:HG21	1:C:390:GLY:HA2	1.62	0.79
1:D:448:VAL:O	1:D:449:ASP:HB2	1.83	0.79
1:B:549:TYR:O	1:B:590:THR:HG22	1.83	0.79
1:B:482:ASN:HB3	1:B:484:ASN:HD21	1.47	0.79
1:A:549:TYR:O	1:A:590:THR:HG22	1.83	0.78
1:C:612:LEU:HD21	1:C:616:ARG:HH21	1.47	0.78
1:C:448:VAL:O	1:C:449:ASP:HB2	1.83	0.78
1:D:484:ASN:HD22	1:D:484:ASN:H	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD13	1:A:128:ILE:HB	1.68	0.76
1:C:314:TYR:H	1:C:500:HIS:CD2	1.98	0.76
1:C:484:ASN:H	1:C:484:ASN:HD22	1.33	0.76
1:B:307:PHE:O	1:D:399:ARG:NH2	2.19	0.75
1:B:122:LEU:HD13	1:B:128:ILE:HB	1.68	0.75
1:D:612:LEU:HD21	1:D:616:ARG:HH21	1.50	0.75
1:A:386:THR:HG21	1:C:390:GLY:CA	2.16	0.75
1:B:448:VAL:O	1:B:449:ASP:HB2	1.86	0.75
1:D:550:GLY:HA3	1:D:590:THR:HG22	1.66	0.75
1:A:482:ASN:HB3	1:A:484:ASN:ND2	2.02	0.74
1:C:312:THR:HG22	1:C:350:THR:HB	1.68	0.74
1:C:208:ASP:OD1	1:C:209:PHE:N	2.20	0.74
1:D:312:THR:HG22	1:D:350:THR:HB	1.69	0.74
1:B:12:GLU:HB3	1:B:45:LEU:HD23	1.70	0.74
1:D:314:TYR:N	1:D:500:HIS:HD2	1.85	0.73
1:A:448:VAL:O	1:A:449:ASP:HB2	1.87	0.73
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.70	0.73
1:B:482:ASN:HB3	1:B:484:ASN:ND2	2.02	0.73
1:C:314:TYR:N	1:C:500:HIS:HD2	1.87	0.73
1:D:487:ILE:HG22	1:D:488:LEU:N	2.04	0.73
1:D:208:ASP:OD1	1:D:209:PHE:N	2.21	0.72
1:A:429:ILE:HG12	1:C:397:ALA:HB1	1.70	0.72
1:B:442:ILE:CD1	1:B:459:ILE:HD11	2.19	0.72
1:A:442:ILE:CD1	1:A:459:ILE:HD11	2.19	0.72
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.19	0.72
1:C:383:HIS:O	1:C:387:THR:HG23	1.90	0.71
1:B:487:ILE:HG22	1:B:488:LEU:N	2.05	0.71
1:C:210:TYR:CE1	1:C:250:ILE:HD11	2.25	0.71
1:A:308:ASP:O	1:A:312:THR:HG23	1.91	0.71
1:A:448:VAL:O	1:A:448:VAL:HG12	1.90	0.70
1:C:487:ILE:HG22	1:C:488:LEU:N	2.06	0.70
1:C:213:LEU:O	1:C:216:VAL:HG22	1.91	0.70
1:C:332:ILE:HD13	1:C:459:ILE:HG22	1.73	0.70
1:D:484:ASN:ND2	1:D:484:ASN:H	1.89	0.70
1:B:192:THR:HG22	1:B:246:THR:HG22	1.72	0.70
1:B:448:VAL:O	1:B:448:VAL:HG12	1.90	0.70
1:C:585:ASN:HB3	1:C:589:ARG:NH2	2.06	0.70
1:A:192:THR:HG22	1:A:246:THR:HG22	1.73	0.70
1:A:487:ILE:HG22	1:A:488:LEU:N	2.06	0.70
1:D:332:ILE:HD13	1:D:459:ILE:HG22	1.73	0.70
1:C:484:ASN:ND2	1:C:484:ASN:H	1.88	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:TYR:CE1	1:D:250:ILE:HD11	2.25	0.69
1:B:308:ASP:O	1:B:312:THR:HG23	1.92	0.69
1:D:585:ASN:HB3	1:D:589:ARG:NH2	2.06	0.69
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.21	0.69
1:C:210:TYR:HE1	1:C:250:ILE:HD11	1.56	0.69
1:C:86:ARG:HH11	1:C:86:ARG:HB3	1.58	0.69
1:B:314:TYR:H	1:B:500:HIS:HD2	1.39	0.68
1:D:86:ARG:HB3	1:D:86:ARG:HH11	1.59	0.68
1:B:383:HIS:O	1:B:387:THR:HG23	1.93	0.68
1:C:192:THR:HG22	1:C:246:THR:HG22	1.75	0.68
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.75	0.68
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.76	0.68
1:B:578:LYS:HG3	1:B:582:GLN:HB3	1.76	0.68
1:D:213:LEU:O	1:D:216:VAL:HG22	1.94	0.68
1:D:192:THR:HG22	1:D:246:THR:HG22	1.74	0.67
1:D:382:VAL:O	1:D:386:THR:HG23	1.94	0.67
1:B:447:MET:HG3	1:B:456:LEU:HD11	1.75	0.67
1:A:578:LYS:HG3	1:A:582:GLN:HB3	1.76	0.67
1:C:54:TYR:HE1	1:C:60:ILE:HD11	1.58	0.67
1:D:210:TYR:HE1	1:D:250:ILE:HD11	1.56	0.67
1:A:580:ALA:O	1:A:584:ILE:HG13	1.95	0.67
1:B:323:TYR:OH	1:B:458:LYS:HG3	1.94	0.66
1:D:539:ASP:O	1:D:540:LEU:HD23	1.94	0.66
1:A:314:TYR:H	1:A:500:HIS:HD2	1.42	0.66
1:D:8:HIS:HE1	1:D:39:TYR:OH	1.79	0.66
1:A:383:HIS:O	1:A:387:THR:HG23	1.95	0.66
1:D:425:LEU:O	1:D:429:ILE:HG13	1.95	0.66
1:D:448:VAL:O	1:D:448:VAL:HG12	1.94	0.66
1:A:323:TYR:OH	1:A:458:LYS:HG3	1.95	0.66
1:C:612:LEU:HD21	1:C:616:ARG:NH2	2.11	0.66
1:B:484:ASN:ND2	1:B:484:ASN:H	1.94	0.66
1:B:572:MET:O	1:B:576:VAL:HG23	1.96	0.66
1:A:572:MET:O	1:A:576:VAL:HG23	1.96	0.66
1:D:383:HIS:O	1:D:387:THR:HG23	1.96	0.66
1:A:447:MET:HG3	1:A:456:LEU:HD11	1.77	0.66
1:C:448:VAL:O	1:C:448:VAL:HG12	1.96	0.65
1:D:264:ASP:O	1:D:635:MET:HG3	1.96	0.65
1:C:133:ASN:HD22	1:C:133:ASN:H	1.44	0.65
1:C:264:ASP:O	1:C:635:MET:HG3	1.96	0.65
1:B:264:ASP:O	1:B:635:MET:HG3	1.97	0.65
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:C	1:A:213:LEU:HD12	2.18	0.64
1:B:580:ALA:O	1:B:584:ILE:HG13	1.98	0.64
1:C:634:ASN:ND2	1:C:637:ALA:HB2	2.12	0.64
1:B:213:LEU:C	1:B:213:LEU:HD12	2.18	0.64
1:B:8:HIS:HE1	1:B:39:TYR:OH	1.81	0.64
1:C:382:VAL:O	1:C:386:THR:HG23	1.97	0.64
1:A:264:ASP:O	1:A:635:MET:HG3	1.97	0.64
1:A:390:GLY:CA	1:C:386:THR:HG21	2.26	0.64
1:C:8:HIS:HE1	1:C:39:TYR:OH	1.81	0.64
1:D:634:ASN:ND2	1:D:637:ALA:HB2	2.12	0.64
1:D:12:GLU:HB3	1:D:45:LEU:HD23	1.80	0.63
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.80	0.63
1:D:54:TYR:HE1	1:D:60:ILE:HD11	1.61	0.63
1:D:612:LEU:HD21	1:D:616:ARG:NH2	2.13	0.63
1:C:572:MET:O	1:C:576:VAL:HG23	1.99	0.63
1:C:32:ALA:HB3	1:C:33:PRO:HD3	1.80	0.63
1:A:8:HIS:HE1	1:A:39:TYR:OH	1.81	0.62
1:A:484:ASN:ND2	1:A:484:ASN:H	1.97	0.62
1:B:442:ILE:HB	1:B:459:ILE:HD11	1.82	0.62
1:D:572:MET:O	1:D:576:VAL:HG23	2.00	0.62
1:C:425:LEU:O	1:C:429:ILE:HG13	1.99	0.62
1:B:322:GLU:HB2	1:B:326:LYS:HG2	1.82	0.62
1:C:315:PHE:CE2	1:C:572:MET:HG2	2.35	0.62
1:D:133:ASN:H	1:D:133:ASN:HD22	1.45	0.61
1:B:181:LYS:HD3	1:B:181:LYS:O	2.00	0.61
1:A:550:GLY:HA3	1:A:590:THR:HG22	1.81	0.61
1:C:389:ILE:HG23	1:C:416:LEU:HD13	1.82	0.61
3:J:3:GLC:H62	3:J:4:GLC:O5	2.00	0.61
1:C:218:VAL:HG23	1:C:219:ASP:H	1.65	0.60
1:D:389:ILE:HG23	1:D:416:LEU:HD13	1.83	0.60
1:A:113:GLY:C	1:A:115:SER:H	2.04	0.60
1:C:218:VAL:HG23	1:C:219:ASP:N	2.16	0.60
1:A:322:GLU:HB2	1:A:326:LYS:HG2	1.83	0.60
1:A:442:ILE:HB	1:A:459:ILE:HD11	1.82	0.60
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.83	0.60
1:B:550:GLY:HA3	1:B:590:THR:HG22	1.82	0.60
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.37	0.60
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.84	0.60
1:C:245:THR:OG1	1:C:267:LEU:HD12	2.02	0.60
1:C:338:LEU:HD22	1:C:338:LEU:O	2.02	0.60
1:D:579:THR:HG23	1:D:582:GLN:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ASN:H	1:B:484:ASN:HD22	1.48	0.59
1:B:314:TYR:H	1:B:500:HIS:CD2	2.20	0.59
1:D:245:THR:OG1	1:D:267:LEU:HD12	2.02	0.59
1:B:113:GLY:C	1:B:115:SER:H	2.04	0.59
1:B:573:GLU:HG2	1:B:577:LYS:HE3	1.84	0.59
1:C:579:THR:HG23	1:C:582:GLN:OE1	2.02	0.59
1:B:181:LYS:HD3	1:B:181:LYS:C	2.23	0.59
1:A:573:GLU:HG2	1:A:577:LYS:HE3	1.85	0.59
1:C:330:MET:HG2	1:C:565:VAL:HG22	1.85	0.59
1:A:181:LYS:HD3	1:A:181:LYS:O	2.01	0.59
1:A:181:LYS:HD3	1:A:181:LYS:C	2.23	0.59
1:C:19:ASN:N	1:C:19:ASN:HD22	2.01	0.59
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.85	0.59
1:B:17:VAL:CG2	1:B:47:GLY:HA3	2.32	0.59
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.38	0.58
1:D:315:PHE:CE2	1:D:572:MET:HG2	2.38	0.58
1:D:218:VAL:HG23	1:D:219:ASP:N	2.18	0.58
1:B:442:ILE:HD12	1:B:459:ILE:CD1	2.30	0.58
1:A:442:ILE:HD12	1:A:459:ILE:CD1	2.30	0.58
1:D:19:ASN:HD22	1:D:19:ASN:N	2.01	0.58
1:D:213:LEU:C	1:D:213:LEU:HD12	2.24	0.58
1:A:305:PHE:HZ	1:A:309:LEU:HG	1.69	0.58
1:D:218:VAL:HG23	1:D:219:ASP:H	1.68	0.58
1:D:338:LEU:O	1:D:338:LEU:HD22	2.04	0.58
1:D:79:ALA:O	1:D:83:MET:HG2	2.04	0.58
1:A:484:ASN:H	1:A:484:ASN:HD22	1.52	0.57
1:A:5:LEU:O	1:A:8:HIS:HD2	1.87	0.57
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.38	0.57
1:A:86:ARG:HB3	1:A:86:ARG:HH11	1.68	0.57
1:D:330:MET:HG2	1:D:565:VAL:HG22	1.85	0.57
1:A:174:VAL:O	1:A:177:PRO:HD2	2.03	0.57
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.34	0.57
1:D:20:ARG:NH1	4:D:802:SO4:O3	2.38	0.57
1:C:484:ASN:HD22	1:C:484:ASN:N	2.02	0.57
1:B:59:ASP:HB2	1:B:96:LEU:HD21	1.86	0.57
1:C:79:ALA:O	1:C:83:MET:HG2	2.05	0.57
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.70	0.57
1:C:312:THR:HA	1:C:350:THR:O	2.05	0.57
1:A:490:LEU:HD22	1:A:494:GLU:HB3	1.87	0.57
1:B:5:LEU:O	1:B:8:HIS:HD2	1.87	0.57
1:B:80:LEU:HD22	1:B:90:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ILE:HB	1:C:459:ILE:HD11	1.87	0.57
1:B:143:LEU:O	1:B:147:VAL:HG23	2.04	0.56
1:D:134:ASP:CG	1:D:137:THR:HG23	2.26	0.56
1:D:487:ILE:CG2	1:D:488:LEU:N	2.68	0.56
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.36	0.56
1:B:254:GLU:HG3	1:B:258:LEU:HD12	1.88	0.56
1:B:577:LYS:O	1:B:578:LYS:C	2.42	0.56
1:A:113:GLY:O	1:A:115:SER:N	2.38	0.56
1:A:577:LYS:O	1:A:578:LYS:C	2.44	0.56
1:C:181:LYS:C	1:C:181:LYS:HD3	2.26	0.56
1:A:552:TYR:HD1	1:A:571:TYR:CD2	2.24	0.56
1:B:174:VAL:O	1:B:177:PRO:HD2	2.05	0.56
1:B:552:TYR:HD1	1:B:571:TYR:CD2	2.24	0.56
1:C:134:ASP:CG	1:C:137:THR:HG23	2.26	0.56
1:D:312:THR:HA	1:D:350:THR:O	2.05	0.56
1:A:254:GLU:HG3	1:A:258:LEU:HD12	1.88	0.56
1:B:399:ARG:NH2	1:D:307:PHE:O	2.39	0.56
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.88	0.56
1:A:539:ASP:O	1:A:540:LEU:HD23	2.06	0.55
1:B:113:GLY:O	1:B:115:SER:N	2.39	0.55
1:B:193:HIS:O	1:B:194:ALA:HB2	2.06	0.55
1:C:315:PHE:HE2	1:C:572:MET:HG2	1.71	0.55
1:C:448:VAL:O	1:C:449:ASP:CB	2.54	0.55
1:A:17:VAL:CG2	1:A:47:GLY:HA3	2.36	0.55
1:C:487:ILE:CG2	1:C:488:LEU:N	2.70	0.55
1:D:442:ILE:HB	1:D:459:ILE:HD11	1.88	0.55
1:B:312:THR:HG22	1:B:350:THR:HB	1.89	0.55
1:D:322:GLU:HB2	1:D:326:LYS:HG2	1.89	0.55
1:A:314:TYR:H	1:A:500:HIS:CD2	2.22	0.55
1:B:490:LEU:HD22	1:B:494:GLU:HB3	1.87	0.55
1:B:627:GLY:O	1:B:628:GLU:HB3	2.06	0.55
1:D:181:LYS:HD3	1:D:181:LYS:C	2.27	0.55
1:D:344:VAL:C	1:D:346:GLY:H	2.10	0.55
1:D:484:ASN:N	1:D:484:ASN:HD22	2.03	0.55
1:A:143:LEU:O	1:A:147:VAL:HG23	2.06	0.55
1:A:20:ARG:NH1	4:A:801:SO4:O1	2.40	0.55
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.70	0.55
1:D:448:VAL:O	1:D:449:ASP:CB	2.54	0.55
1:C:213:LEU:HD12	1:C:213:LEU:C	2.27	0.54
1:A:193:HIS:O	1:A:194:ALA:HB2	2.07	0.54
1:A:312:THR:HG22	1:A:350:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.88	0.54
1:A:338:LEU:O	1:A:338:LEU:HD22	2.08	0.54
1:A:487:ILE:CG2	1:A:488:LEU:N	2.71	0.54
1:B:487:ILE:CG2	1:B:488:LEU:N	2.70	0.54
1:A:133:ASN:ND2	1:A:133:ASN:H	2.06	0.54
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.39	0.54
1:B:338:LEU:HD22	1:B:338:LEU:O	2.08	0.53
1:B:61:LEU:HG	1:B:93:GLY:HA2	1.90	0.53
1:A:627:GLY:O	1:A:628:GLU:HB3	2.07	0.53
1:C:322:GLU:HB2	1:C:326:LYS:HG2	1.90	0.53
1:D:299:GLY:HA2	1:D:375:VAL:HG21	1.90	0.53
1:B:539:ASP:O	1:B:540:LEU:HD23	2.09	0.53
1:D:450:ASP:OD1	1:D:460:ARG:NH2	2.41	0.53
1:B:17:VAL:HG21	1:B:47:GLY:HA3	1.91	0.53
1:B:133:ASN:ND2	1:B:133:ASN:H	2.06	0.53
1:D:86:ARG:HB3	1:D:86:ARG:NH1	2.22	0.53
1:C:54:TYR:CE1	1:C:60:ILE:HD11	2.42	0.53
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.41	0.53
1:C:344:VAL:C	1:C:346:GLY:H	2.12	0.53
1:A:61:LEU:HG	1:A:93:GLY:HA2	1.90	0.52
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.92	0.52
1:D:578:LYS:HG3	1:D:582:GLN:HB3	1.92	0.52
1:A:341:ARG:NH2	1:A:566:GLU:OE1	2.41	0.52
3:G:1:GLC:H62	3:G:2:GLC:H5	1.90	0.52
1:A:448:VAL:O	1:A:449:ASP:CB	2.56	0.52
1:B:235:ARG:HH21	1:B:260:LYS:CG	2.16	0.52
1:C:350:THR:OG1	1:C:471:ARG:NH1	2.43	0.52
1:C:86:ARG:HB3	1:C:86:ARG:NH1	2.22	0.52
1:D:21:VAL:HG12	1:D:21:VAL:O	2.09	0.52
1:B:499:CYS:O	1:B:587:ARG:NH2	2.42	0.52
1:C:578:LYS:HG3	1:C:582:GLN:HB3	1.91	0.52
1:A:163:ILE:CG2	1:A:186:VAL:HG12	2.40	0.52
1:A:12:GLU:HG3	1:A:166:HIS:HB3	1.91	0.52
1:D:315:PHE:HE2	1:D:572:MET:HG2	1.75	0.52
1:D:447:MET:HG3	1:D:456:LEU:HD11	1.92	0.52
1:B:579:THR:HG23	1:B:582:GLN:OE1	2.09	0.52
1:C:447:MET:HG3	1:C:456:LEU:HD11	1.92	0.52
1:D:174:VAL:O	1:D:177:PRO:HD2	2.10	0.52
1:B:163:ILE:CG2	1:B:186:VAL:HG12	2.40	0.51
1:C:484:ASN:ND2	1:C:484:ASN:N	2.58	0.51
1:C:285:LEU:HD13	1:C:497:ARG:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:THR:HG23	1:A:582:GLN:OE1	2.10	0.51
1:C:112:ARG:O	1:C:115:SER:HB2	2.10	0.51
1:C:123:TRP:O	1:C:127:GLY:HA2	2.11	0.51
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.46	0.51
1:A:103:VAL:CG1	1:A:105:LEU:HG	2.40	0.51
1:A:490:LEU:HD13	1:A:495:PHE:HA	1.92	0.51
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.91	0.51
1:A:8:HIS:CE1	1:A:39:TYR:OH	2.63	0.51
1:B:447:MET:HG3	1:B:456:LEU:CD1	2.40	0.51
1:D:189:ILE:HD11	1:D:610:ARG:HA	1.92	0.51
1:D:17:VAL:CG2	1:D:47:GLY:HA3	2.41	0.51
1:D:285:LEU:HD13	1:D:497:ARG:HD3	1.91	0.51
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.91	0.51
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.45	0.51
1:A:235:ARG:HH21	1:A:260:LYS:CG	2.16	0.51
1:B:428:ARG:NH1	1:B:428:ARG:HA	2.25	0.51
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.92	0.51
1:C:82:THR:O	1:C:85:SER:HB2	2.10	0.51
1:A:499:CYS:O	1:A:587:ARG:NH2	2.44	0.51
1:B:103:VAL:CG1	1:B:105:LEU:HG	2.40	0.50
1:A:386:THR:CG2	1:C:390:GLY:HA2	2.37	0.50
1:B:268:PRO:HB2	1:B:602:MET:HE1	1.93	0.50
1:B:8:HIS:CE1	1:B:39:TYR:OH	2.63	0.50
1:C:299:GLY:HA2	1:C:375:VAL:HG21	1.93	0.50
1:D:31:LYS:O	1:D:35:THR:HG23	2.12	0.50
1:B:74:ARG:N	1:B:75:PRO:CD	2.74	0.50
1:A:192:THR:CG2	1:A:246:THR:HG22	2.40	0.50
1:B:127:GLY:O	1:B:129:PRO:HD3	2.11	0.50
1:D:484:ASN:ND2	1:D:484:ASN:N	2.59	0.50
1:A:74:ARG:N	1:A:75:PRO:CD	2.74	0.50
1:C:552:TYR:N	1:C:552:TYR:CD2	2.80	0.49
1:A:17:VAL:HG21	1:A:47:GLY:HA3	1.94	0.49
1:B:578:LYS:HG3	1:B:582:GLN:CB	2.42	0.49
1:B:623:ARG:HG3	1:B:628:GLU:O	2.12	0.49
1:B:490:LEU:HD13	1:B:495:PHE:HA	1.95	0.49
1:C:21:VAL:HG12	1:C:21:VAL:O	2.11	0.49
1:A:127:GLY:O	1:A:129:PRO:HD3	2.12	0.49
1:B:503:VAL:O	1:B:505:PRO:HD3	2.12	0.49
1:A:265:GLY:HA3	1:A:635:MET:SD	2.52	0.49
1:B:341:ARG:NH2	1:B:566:GLU:OE1	2.42	0.49
1:C:227:ILE:HD12	1:C:230:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ARG:O	1:D:115:SER:HB2	2.12	0.49
1:D:308:ASP:O	1:D:312:THR:HG23	2.12	0.49
1:D:54:TYR:CE1	1:D:60:ILE:HD11	2.44	0.49
1:A:586:GLN:O	1:A:590:THR:HG23	2.12	0.49
1:B:448:VAL:O	1:B:449:ASP:CB	2.55	0.49
1:B:30:SER:O	1:B:599:TRP:CD1	2.65	0.49
1:A:447:MET:HG3	1:A:456:LEU:CD1	2.42	0.49
1:D:123:TRP:O	1:D:127:GLY:HA2	2.13	0.49
1:B:447:MET:HB2	1:B:450:ASP:OD2	2.12	0.49
1:C:300:HIS:CE1	1:C:475:ILE:CD1	2.96	0.49
1:A:146:THR:O	1:A:149:TRP:HB3	2.13	0.48
1:A:623:ARG:HG3	1:A:628:GLU:O	2.13	0.48
1:C:192:THR:CG2	1:C:246:THR:HG22	2.43	0.48
1:C:181:LYS:HD3	1:C:181:LYS:O	2.12	0.48
1:D:471:ARG:NE	1:D:471:ARG:HA	2.28	0.48
1:A:34:ILE:HA	1:A:34:ILE:HD12	1.73	0.48
1:A:397:ALA:HB1	1:C:429:ILE:HG12	1.95	0.48
1:D:82:THR:O	1:D:85:SER:HB2	2.14	0.48
1:B:442:ILE:CB	1:B:459:ILE:HD11	2.43	0.48
1:C:31:LYS:O	1:C:35:THR:HG23	2.13	0.48
1:D:227:ILE:HD12	1:D:230:ARG:HD2	1.94	0.48
1:D:198:GLY:HA3	1:D:254:GLU:OE1	2.13	0.48
1:D:8:HIS:CE1	1:D:39:TYR:OH	2.64	0.48
1:A:447:MET:HB2	1:A:450:ASP:OD2	2.14	0.48
1:A:623:ARG:HH21	1:A:629:GLU:HB3	1.79	0.48
1:C:471:ARG:NE	1:C:471:ARG:HA	2.28	0.48
1:C:308:ASP:O	1:C:312:THR:HG23	2.13	0.48
1:D:181:LYS:HD3	1:D:181:LYS:O	2.13	0.48
1:A:465:PHE:CE1	3:H:3:GLC:H2	2.49	0.48
1:B:252:ALA:HB2	1:B:266:ILE:HD11	1.96	0.48
1:B:31:LYS:O	1:B:35:THR:HG23	2.13	0.48
1:C:8:HIS:CE1	1:C:39:TYR:OH	2.65	0.48
1:A:442:ILE:CB	1:A:459:ILE:HD11	2.43	0.48
1:C:455:ILE:O	1:C:459:ILE:HG23	2.14	0.48
1:A:31:LYS:O	1:A:35:THR:HG23	2.14	0.47
1:B:272:ASN:O	1:B:275:LYS:HB3	2.14	0.47
1:B:398:ILE:HG23	1:D:305:PHE:HD2	1.79	0.47
1:D:565:VAL:O	1:D:569:VAL:HG23	2.14	0.47
1:B:586:GLN:O	1:B:590:THR:HG23	2.13	0.47
1:D:300:HIS:CE1	1:D:475:ILE:CD1	2.97	0.47
1:A:265:GLY:O	1:A:266:ILE:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:THR:CG2	1:B:246:THR:HG22	2.40	0.47
1:B:265:GLY:HA3	1:B:635:MET:SD	2.53	0.47
1:A:150:PHE:O	1:A:154:VAL:HG23	2.14	0.47
1:C:227:ILE:O	1:C:227:ILE:CG2	2.63	0.47
1:A:272:ASN:O	1:A:275:LYS:HB3	2.15	0.47
1:A:428:ARG:HA	1:A:428:ARG:NH1	2.30	0.47
1:A:578:LYS:HG3	1:A:582:GLN:CB	2.42	0.47
1:C:17:VAL:CG2	1:C:47:GLY:HA3	2.44	0.47
1:C:198:GLY:HA3	1:C:254:GLU:OE1	2.15	0.47
1:C:465:PHE:O	1:C:466:ASN:HB2	2.15	0.47
1:D:192:THR:CG2	1:D:246:THR:HG22	2.42	0.47
1:C:174:VAL:O	1:C:177:PRO:HD2	2.13	0.47
1:C:244:PHE:HD2	1:C:261:ARG:HG2	1.79	0.47
1:D:213:LEU:HD12	1:D:214:GLU:N	2.29	0.47
1:A:510:PRO:O	1:A:532:GLY:HA3	2.15	0.47
1:B:126:VAL:O	1:B:128:ILE:HG13	2.15	0.47
1:C:235:ARG:HH21	1:C:260:LYS:HG3	1.80	0.47
1:A:512:GLY:O	1:A:515:PRO:HD2	2.15	0.47
1:C:113:GLY:C	1:C:115:SER:H	2.17	0.47
1:D:168:HIS:HD2	1:D:193:HIS:NE2	2.13	0.47
1:D:3:ARG:NH1	1:D:185:ASP:OD2	2.41	0.47
1:C:565:VAL:O	1:C:569:VAL:HG23	2.15	0.47
1:D:567:GLN:HG2	1:D:571:TYR:CE1	2.50	0.47
1:B:150:PHE:O	1:B:154:VAL:HG23	2.15	0.47
1:B:528:THR:O	1:B:534:GLY:HA3	2.15	0.47
1:C:168:HIS:HD2	1:C:193:HIS:NE2	2.13	0.47
1:A:113:GLY:C	1:A:115:SER:N	2.68	0.46
1:A:76:VAL:O	1:A:79:ALA:HB3	2.15	0.46
1:D:133:ASN:ND2	1:D:133:ASN:H	2.13	0.46
1:D:362:ASN:HB2	1:D:446:ASN:HB2	1.98	0.46
1:A:81:GLN:O	1:A:82:THR:C	2.53	0.46
1:B:213:LEU:HD21	1:B:253:PHE:CE1	2.50	0.46
1:D:455:ILE:O	1:D:459:ILE:HG23	2.14	0.46
1:C:362:ASN:HB2	1:C:446:ASN:HB2	1.97	0.46
1:C:528:THR:O	1:C:534:GLY:HA3	2.15	0.46
1:A:252:ALA:HB2	1:A:266:ILE:HD11	1.96	0.46
1:A:30:SER:O	1:A:599:TRP:CD1	2.68	0.46
1:A:623:ARG:NH2	1:A:629:GLU:HB3	2.31	0.46
1:B:623:ARG:HH21	1:B:629:GLU:HB3	1.79	0.46
1:C:197:LEU:HD23	1:C:197:LEU:HA	1.77	0.46
1:C:321:TYR:C	1:C:321:TYR:CD1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LYS:HB3	1:C:41:ASP:H	1.57	0.46
1:C:567:GLN:HG2	1:C:571:TYR:CE1	2.50	0.46
1:C:442:ILE:CD1	1:C:459:ILE:HD11	2.46	0.46
1:D:235:ARG:HH21	1:D:260:LYS:HG3	1.80	0.46
1:A:96:LEU:O	1:D:427:ARG:HD2	2.15	0.46
1:B:623:ARG:NH2	1:B:629:GLU:HB3	2.31	0.46
1:D:113:GLY:C	1:D:115:SER:H	2.20	0.46
1:C:586:GLN:O	1:C:590:THR:HG23	2.16	0.46
1:D:285:LEU:HA	1:D:285:LEU:HD23	1.67	0.46
1:D:442:ILE:CD1	1:D:459:ILE:HD11	2.45	0.45
1:D:552:TYR:N	1:D:552:TYR:CD2	2.83	0.45
1:B:398:ILE:HA	1:B:398:ILE:HD12	1.87	0.45
1:B:514:THR:OG1	1:B:515:PRO:HD3	2.16	0.45
1:D:344:VAL:HG12	1:D:345:SER:N	2.31	0.45
1:C:213:LEU:HD12	1:C:214:GLU:N	2.31	0.45
1:A:514:THR:OG1	1:A:515:PRO:HD3	2.17	0.45
1:B:17:VAL:HG22	1:B:47:GLY:HA3	1.96	0.45
1:B:81:GLN:O	1:B:82:THR:C	2.53	0.45
1:A:565:VAL:O	1:A:569:VAL:HG23	2.17	0.45
1:B:512:GLY:O	1:B:515:PRO:HD2	2.17	0.45
1:C:177:PRO:HG3	1:C:236:ALA:HB1	1.97	0.45
1:C:331:PHE:CE2	1:C:335:LEU:HD11	2.52	0.45
1:D:425:LEU:HD23	1:D:425:LEU:HA	1.80	0.45
1:C:490:LEU:HD13	1:C:495:PHE:HA	1.99	0.45
1:D:286:HIS:ND1	1:D:587:ARG:NH2	2.65	0.45
1:D:197:LEU:HA	1:D:197:LEU:HD23	1.78	0.45
1:C:179:CYS:SG	1:C:184:ILE:HD12	2.57	0.45
1:C:252:ALA:HB2	1:C:266:ILE:HD11	1.99	0.45
1:C:342:LEU:HD22	1:C:347:SER:HB3	1.99	0.45
1:D:227:ILE:O	1:D:227:ILE:CG2	2.65	0.45
1:D:244:PHE:HD2	1:D:261:ARG:HG2	1.81	0.45
1:D:528:THR:O	1:D:534:GLY:HA3	2.17	0.45
1:A:268:PRO:HB2	1:A:602:MET:HE1	1.99	0.44
1:A:80:LEU:O	1:A:83:MET:HB2	2.17	0.44
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.82	0.44
1:C:176:LEU:HD12	1:C:237:ALA:HB1	1.99	0.44
1:C:463:GLN:HA	1:C:465:PHE:CE2	2.52	0.44
1:A:213:LEU:HD21	1:A:253:PHE:CE1	2.51	0.44
1:C:428:ARG:NH1	1:C:428:ARG:HA	2.31	0.44
1:D:12:GLU:OE2	1:D:168:HIS:HE1	2.00	0.44
1:D:180:ARG:CG	1:D:180:ARG:HH11	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LEU:HD23	1:C:285:LEU:HA	1.69	0.44
1:A:7:ASN:ND2	1:A:161:HIS:HD2	2.16	0.44
1:A:465:PHE:O	1:A:466:ASN:HB2	2.18	0.44
1:A:467:SER:O	1:A:470:ASP:HB2	2.17	0.44
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.46	0.44
1:B:116:ASN:C	1:B:118:TRP:N	2.69	0.44
1:B:146:THR:O	1:B:149:TRP:HB3	2.18	0.44
1:B:485:ASN:HA	1:B:486:PRO:HD3	1.87	0.44
1:A:307:PHE:HD1	1:A:312:THR:HG21	1.83	0.44
1:A:4:ASP:OD2	1:A:7:ASN:HB3	2.18	0.44
1:B:4:ASP:OD2	1:B:7:ASN:HB3	2.17	0.44
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.40	0.44
1:A:235:ARG:NH2	1:A:260:LYS:HG3	2.17	0.44
1:D:321:TYR:CD1	1:D:321:TYR:C	2.91	0.44
1:B:467:SER:O	1:B:470:ASP:HB2	2.18	0.44
1:C:34:ILE:HD12	1:C:34:ILE:HA	1.62	0.44
1:C:74:ARG:HG3	1:C:78:HIS:CE1	2.53	0.44
1:D:252:ALA:HB2	1:D:266:ILE:HD11	2.00	0.44
1:D:586:GLN:O	1:D:590:THR:HG23	2.18	0.44
1:B:360:LYS:HB3	1:B:448:VAL:HB	2.00	0.43
1:D:463:GLN:HA	1:D:465:PHE:CE2	2.52	0.43
1:A:176:LEU:HD21	1:A:188:THR:HB	1.99	0.43
1:A:487:ILE:HG22	1:A:488:LEU:HB2	2.00	0.43
1:A:528:THR:O	1:A:534:GLY:HA3	2.17	0.43
1:D:490:LEU:HD22	1:D:494:GLU:HB3	2.00	0.43
1:D:74:ARG:HG3	1:D:78:HIS:CE1	2.53	0.43
1:A:19:ASN:N	1:A:19:ASN:HD22	2.16	0.43
1:D:177:PRO:HG3	1:D:236:ALA:HB1	1.98	0.43
1:A:7:ASN:ND2	1:A:161:HIS:CD2	2.86	0.43
1:B:265:GLY:O	1:B:266:ILE:HD13	2.18	0.43
1:C:12:GLU:OE2	1:C:168:HIS:HE1	2.01	0.43
1:D:179:CYS:SG	1:D:184:ILE:HD12	2.58	0.43
1:D:580:ALA:O	1:D:584:ILE:HG13	2.18	0.43
1:B:465:PHE:O	1:B:466:ASN:HB2	2.19	0.43
1:B:80:LEU:O	1:B:83:MET:HB2	2.19	0.43
1:C:286:HIS:ND1	1:C:587:ARG:NH2	2.65	0.43
1:C:344:VAL:HG12	1:C:345:SER:N	2.32	0.43
1:C:29:LYS:HE2	4:C:801:SO4:O3	2.18	0.43
1:D:540:LEU:HD13	1:D:596:LEU:CD1	2.48	0.43
1:A:503:VAL:O	1:A:505:PRO:HD3	2.19	0.43
1:C:458:LYS:O	1:C:458:LYS:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:LEU:HD22	1:C:494:GLU:HB3	1.99	0.43
1:D:331:PHE:CE2	1:D:335:LEU:HD11	2.53	0.43
1:A:164:VAL:HA	1:A:187:VAL:HG23	2.00	0.43
1:A:360:LYS:HB3	1:A:448:VAL:HB	2.00	0.43
1:C:235:ARG:HG2	1:C:239:HIS:CD2	2.54	0.43
1:D:575:PHE:O	1:D:578:LYS:HB2	2.19	0.43
1:D:74:ARG:N	1:D:75:PRO:CD	2.82	0.43
1:A:96:LEU:CD1	1:D:430:LEU:HD12	2.49	0.43
1:C:183:ARG:HB2	1:C:183:ARG:HE	1.54	0.43
1:B:7:ASN:ND2	1:B:161:HIS:HD2	2.17	0.43
1:B:302:HIS:CD2	1:B:371:GLY:HA2	2.54	0.43
1:C:554:VAL:HG12	1:C:555:ASP:O	2.18	0.43
1:D:342:LEU:HD22	1:D:347:SER:HB3	2.01	0.43
1:A:3:ARG:NH2	1:A:158:ASP:O	2.51	0.43
1:A:537:MET:HE2	1:A:597:LEU:HD21	2.00	0.43
1:B:487:ILE:HG22	1:B:488:LEU:HB2	2.00	0.43
1:C:75:PRO:CB	1:C:158:ASP:HB2	2.49	0.43
1:D:482:ASN:HB3	1:D:484:ASN:ND2	2.34	0.43
1:D:490:LEU:HD13	1:D:495:PHE:HA	2.01	0.43
1:B:164:VAL:HA	1:B:187:VAL:HG23	2.01	0.42
1:B:227:ILE:CG2	1:B:227:ILE:O	2.67	0.42
1:C:517:GLU:O	1:C:521:MET:HG3	2.19	0.42
1:C:610:ARG:O	1:C:613:ALA:HB3	2.18	0.42
1:C:623:ARG:HB2	1:C:623:ARG:HE	1.67	0.42
1:D:176:LEU:HD12	1:D:237:ALA:HB1	2.01	0.42
1:D:300:HIS:HE1	1:D:441:PRO:O	2.02	0.42
1:A:173:GLY:O	1:A:176:LEU:HB2	2.18	0.42
1:A:209:PHE:O	1:A:211:ASN:N	2.52	0.42
1:A:299:GLY:HA2	1:A:375:VAL:HG21	2.00	0.42
1:B:34:ILE:HA	1:B:34:ILE:HD12	1.73	0.42
1:B:471:ARG:HA	1:B:471:ARG:NE	2.34	0.42
1:C:560:ALA:HB1	1:C:561:PRO:HD2	2.01	0.42
1:A:515:PRO:O	1:A:518:CYS:HB3	2.19	0.42
1:B:442:ILE:HD11	3:J:2:GLC:H2	2.00	0.42
1:C:180:ARG:CG	1:C:180:ARG:HH11	2.31	0.42
1:C:321:TYR:O	1:C:321:TYR:CD1	2.72	0.42
1:C:537:MET:HG3	1:C:551:ILE:CD1	2.49	0.42
1:D:40:LYS:HB3	1:D:41:ASP:H	1.60	0.42
1:B:176:LEU:HD21	1:B:188:THR:HB	2.00	0.42
1:C:214:GLU:H	1:C:214:GLU:HG2	1.55	0.42
1:C:416:LEU:HD23	1:C:416:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:GLY:HA3	1:C:590:THR:HG21	1.99	0.42
1:C:552:TYR:HD1	1:C:571:TYR:CD2	2.38	0.42
1:D:266:ILE:HD13	1:D:266:ILE:HA	1.78	0.42
1:A:208:ASP:OD1	1:A:209:PHE:N	2.49	0.42
1:A:302:HIS:CD2	1:A:371:GLY:HA2	2.54	0.42
1:C:74:ARG:N	1:C:75:PRO:CD	2.83	0.42
1:D:537:MET:HG3	1:D:551:ILE:CD1	2.49	0.42
1:D:560:ALA:HB1	1:D:561:PRO:HD2	2.01	0.42
1:A:74:ARG:HG3	1:A:78:HIS:CE1	2.55	0.42
1:C:201:LEU:HA	1:C:201:LEU:HD23	1.88	0.42
1:C:527:THR:HG21	1:C:534:GLY:HA2	2.01	0.42
1:D:342:LEU:HA	1:D:342:LEU:HD23	1.94	0.42
1:D:552:TYR:HD1	1:D:571:TYR:CD2	2.38	0.42
1:B:300:HIS:HE1	1:B:441:PRO:O	2.01	0.42
1:C:580:ALA:O	1:C:584:ILE:HG13	2.19	0.42
1:D:554:VAL:HG12	1:D:555:ASP:O	2.19	0.42
1:A:116:ASN:C	1:A:118:TRP:N	2.73	0.42
1:B:7:ASN:ND2	1:B:161:HIS:CD2	2.87	0.42
1:B:266:ILE:HG22	1:B:268:PRO:HD3	2.00	0.42
1:C:300:HIS:HE1	1:C:441:PRO:O	2.03	0.42
1:D:320:ARG:HB3	1:D:322:GLU:HG3	2.02	0.42
1:B:134:ASP:CG	1:B:137:THR:HG23	2.40	0.42
1:B:565:VAL:O	1:B:569:VAL:HG23	2.20	0.42
1:D:428:ARG:NH1	1:D:428:ARG:HA	2.34	0.42
1:D:75:PRO:CB	1:D:158:ASP:HB2	2.50	0.42
1:A:465:PHE:CZ	3:H:3:GLC:H2	2.54	0.42
1:A:89:HIS:O	1:A:107:ASP:CB	2.68	0.42
1:B:623:ARG:HG3	1:B:628:GLU:C	2.40	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.88	0.41
1:B:113:GLY:C	1:B:115:SER:N	2.68	0.41
1:B:49:LEU:HD11	1:B:54:TYR:CG	2.55	0.41
1:C:167:PHE:CD2	1:C:176:LEU:HD21	2.54	0.41
1:D:183:ARG:HB2	1:D:183:ARG:HE	1.53	0.41
1:A:17:VAL:HG22	1:A:47:GLY:HA3	2.01	0.41
1:D:465:PHE:O	1:D:466:ASN:HB2	2.19	0.41
1:A:49:LEU:HD11	1:A:54:TYR:CG	2.54	0.41
1:A:71:ASP:O	1:A:74:ARG:HB2	2.21	0.41
1:C:133:ASN:H	1:C:133:ASN:ND2	2.13	0.41
1:C:320:ARG:HB3	1:C:322:GLU:HG3	2.01	0.41
1:D:349:LYS:O	1:D:471:ARG:HG3	2.20	0.41
1:A:16:GLU:OE1	1:A:22:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:HIS:HE1	1:A:441:PRO:O	2.03	0.41
1:A:31:LYS:HZ3	1:A:35:THR:HG21	1.85	0.41
1:B:89:HIS:O	1:B:107:ASP:CB	2.68	0.41
1:B:115:SER:O	1:B:118:TRP:HB2	2.21	0.41
1:B:116:ASN:C	1:B:118:TRP:H	2.24	0.41
1:B:134:ASP:OD1	1:B:137:THR:HG23	2.20	0.41
1:B:343:LYS:O	1:B:346:GLY:N	2.47	0.41
1:C:482:ASN:HB3	1:C:484:ASN:ND2	2.35	0.41
1:D:235:ARG:HG2	1:D:239:HIS:CD2	2.54	0.41
1:D:527:THR:HG21	1:D:534:GLY:HA2	2.02	0.41
1:D:579:THR:H	1:D:582:GLN:HB2	1.85	0.41
1:A:227:ILE:CG2	1:A:227:ILE:O	2.68	0.41
1:B:266:ILE:HD13	1:B:266:ILE:HA	1.81	0.41
1:B:334:ALA:CB	1:B:568:LEU:HD13	2.50	0.41
1:B:299:GLY:HA2	1:B:375:VAL:HG21	2.02	0.41
1:D:34:ILE:HD12	1:D:34:ILE:HA	1.62	0.41
1:C:247:VAL:HA	1:C:267:LEU:O	2.21	0.41
1:D:193:HIS:O	1:D:194:ALA:HB2	2.20	0.41
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.55	0.41
1:D:77:GLN:O	1:D:81:GLN:HG3	2.21	0.41
1:A:334:ALA:CB	1:A:568:LEU:HD13	2.50	0.41
1:A:164:VAL:HB	1:A:187:VAL:HG23	2.03	0.41
1:A:539:ASP:O	1:A:540:LEU:CD2	2.69	0.41
1:A:622:PHE:CE1	1:A:626:VAL:HG21	2.56	0.41
1:B:337:ARG:O	1:B:341:ARG:HG3	2.20	0.41
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.86	0.41
1:B:76:VAL:O	1:B:79:ALA:HB3	2.21	0.41
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.55	0.41
1:C:77:GLN:O	1:C:81:GLN:HG3	2.21	0.41
1:D:180:ARG:HG3	1:D:180:ARG:NH1	2.36	0.41
1:D:344:VAL:C	1:D:346:GLY:N	2.73	0.41
1:A:369:LEU:HD23	1:A:487:ILE:HD13	2.03	0.41
1:A:623:ARG:HG3	1:A:628:GLU:C	2.40	0.41
1:C:307:PHE:CD1	1:C:312:THR:HG21	2.56	0.41
1:C:331:PHE:O	1:C:335:LEU:HD12	2.21	0.41
1:C:342:LEU:HD22	1:C:347:SER:CB	2.51	0.41
1:D:103:VAL:CG1	1:D:105:LEU:HG	2.51	0.41
1:D:487:ILE:HG22	1:D:488:LEU:H	1.84	0.41
1:D:550:GLY:HA3	1:D:590:THR:HG21	2.01	0.41
1:A:471:ARG:HA	1:A:471:ARG:NE	2.36	0.41
1:A:485:ASN:HA	1:A:486:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HD23	1:A:487:ILE:CD1	2.50	0.41
1:B:369:LEU:HD23	1:B:487:ILE:CD1	2.50	0.41
1:D:416:LEU:HA	1:D:416:LEU:HD23	1.90	0.41
1:A:126:VAL:O	1:A:128:ILE:HG13	2.21	0.41
1:A:17:VAL:HG12	1:A:45:LEU:HB3	2.02	0.41
1:A:369:LEU:HA	1:A:369:LEU:HD23	1.82	0.41
1:B:537:MET:HE2	1:B:597:LEU:HD21	2.02	0.41
1:B:626:VAL:HG11	1:B:630:LEU:HD12	2.02	0.41
1:C:344:VAL:C	1:C:346:GLY:N	2.73	0.41
1:A:213:LEU:CD1	1:A:213:LEU:C	2.89	0.40
1:A:626:VAL:HG11	1:A:630:LEU:HD12	2.01	0.40
1:B:209:PHE:O	1:B:211:ASN:N	2.53	0.40
1:B:3:ARG:NH2	1:B:158:ASP:O	2.53	0.40
1:B:74:ARG:HG3	1:B:78:HIS:CE1	2.55	0.40
1:C:560:ALA:HB1	1:C:561:PRO:CD	2.51	0.40
1:D:331:PHE:O	1:D:335:LEU:HD12	2.21	0.40
1:D:487:ILE:HD12	1:D:487:ILE:HA	1.83	0.40
1:A:397:ALA:HB3	1:C:378:LEU:HD11	2.02	0.40
1:B:142:LEU:HA	1:B:142:LEU:HD23	1.87	0.40
1:B:17:VAL:HG12	1:B:45:LEU:HB3	2.03	0.40
1:B:622:PHE:CE1	1:B:626:VAL:HG21	2.57	0.40
1:C:349:LYS:O	1:C:471:ARG:HG3	2.21	0.40
1:D:134:ASP:OD2	1:D:137:THR:HG23	2.21	0.40
1:D:167:PHE:CD2	1:D:176:LEU:HD21	2.55	0.40
1:D:517:GLU:O	1:D:521:MET:HG3	2.20	0.40
1:B:333:GLU:OE2	1:B:337:ARG:HD2	2.21	0.40
1:C:627:GLY:O	1:C:628:GLU:HB3	2.20	0.40
1:D:17:VAL:HG22	1:D:47:GLY:HA3	2.02	0.40
1:A:399:ARG:NH2	1:C:308:ASP:HA	2.36	0.40
1:B:510:PRO:O	1:B:532:GLY:HA3	2.22	0.40
1:B:515:PRO:O	1:B:518:CYS:HB3	2.21	0.40
1:B:561:PRO:O	1:B:564:SER:HB2	2.21	0.40
1:B:71:ASP:O	1:B:74:ARG:HB2	2.21	0.40
1:C:193:HIS:O	1:C:194:ALA:HB2	2.21	0.40
1:C:25:TYR:CD2	1:C:25:TYR:C	2.94	0.40
1:C:289:LYS:N	1:C:289:LYS:HD2	2.36	0.40
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.76	0.40
1:D:623:ARG:HE	1:D:623:ARG:HB2	1.68	0.40
1:A:266:ILE:HG22	1:A:268:PRO:HD3	2.03	0.40
1:A:73:MET:C	1:A:75:PRO:HD2	2.41	0.40
1:B:17:VAL:CG1	1:B:45:LEU:HB3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:PHE:CD2	1:C:77:GLN:HB2	2.57	0.40
1:D:201:LEU:HA	1:D:201:LEU:HD23	1.88	0.40
1:D:307:PHE:CD1	1:D:312:THR:HG21	2.56	0.40
1:D:560:ALA:HB1	1:D:561:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	601/725 (83%)	535 (89%)	56 (9%)	10 (2%)	9	39
1	B	601/725 (83%)	542 (90%)	49 (8%)	10 (2%)	9	39
1	C	603/725 (83%)	550 (91%)	46 (8%)	7 (1%)	13	48
1	D	603/725 (83%)	548 (91%)	50 (8%)	5 (1%)	19	57
All	All	2408/2900 (83%)	2175 (90%)	201 (8%)	32 (1%)	12	45

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	TYR
1	A	449	ASP
1	B	114	TYR
1	B	449	ASP
1	C	285	LEU
1	C	415	GLU
1	C	449	ASP
1	D	285	LEU
1	D	415	GLU
1	D	449	ASP
1	A	194	ALA

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Mol	Chain	Res	Type
1	B	194	ALA
1	C	194	ALA
1	A	183	ARG
1	A	578	LYS
1	A	628	GLU
1	B	126	VAL
1	B	210	TYR
1	B	578	LYS
1	B	628	GLU
1	D	194	ALA
1	A	126	VAL
1	A	210	TYR
1	B	183	ARG
1	C	114	TYR
1	D	21	VAL
1	A	435	PRO
1	C	21	VAL
1	B	435	PRO
1	A	448	VAL
1	C	435	PRO
1	B	448	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	526/622 (85%)	478 (91%)	48 (9%)	9	34
1	B	526/622 (85%)	477 (91%)	49 (9%)	9	33
1	C	527/622 (85%)	474 (90%)	53 (10%)	7	29
1	D	527/622 (85%)	475 (90%)	52 (10%)	8	30
All	All	2106/2488 (85%)	1904 (90%)	202 (10%)	8	32

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	16	GLU
1	A	17	VAL
1	A	19	ASN
1	A	34	ILE
1	A	35	THR
1	A	40	LYS
1	A	42	HIS
1	A	83	MET
1	A	86	ARG
1	A	111	VAL
1	A	122	LEU
1	A	133	ASN
1	A	164	VAL
1	A	181	LYS
1	A	183	ARG
1	A	213	LEU
1	A	216	VAL
1	A	247	VAL
1	A	249	GLN
1	A	254	GLU
1	A	289	LYS
1	A	321	TYR
1	A	338	LEU
1	A	348	LYS
1	A	363	SER
1	A	376	ARG
1	A	378	LEU
1	A	387	THR
1	A	388	SER
1	A	399	ARG
1	A	418	LYS
1	A	426	LYS
1	A	428	ARG
1	A	450	ASP
1	A	455	ILE
1	A	458	LYS
1	A	459	ILE
1	A	469	SER
1	A	471	ARG
1	A	484	ASN
1	A	487	ILE
1	A	488	LEU

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Mol	Chain	Res	Type
1	A	568	LEU
1	A	590	THR
1	A	633	SER
1	A	634	ASN
1	A	635	MET
1	B	15	THR
1	B	16	GLU
1	B	17	VAL
1	B	19	ASN
1	B	34	ILE
1	B	35	THR
1	B	40	LYS
1	B	42	HIS
1	B	83	MET
1	B	86	ARG
1	B	111	VAL
1	B	122	LEU
1	B	133	ASN
1	B	164	VAL
1	B	181	LYS
1	B	183	ARG
1	B	213	LEU
1	B	214	GLU
1	B	216	VAL
1	B	247	VAL
1	B	249	GLN
1	B	254	GLU
1	B	277	GLN
1	B	289	LYS
1	B	321	TYR
1	B	338	LEU
1	B	348	LYS
1	B	363	SER
1	B	376	ARG
1	B	378	LEU
1	B	387	THR
1	B	388	SER
1	B	399	ARG
1	B	418	LYS
1	B	428	ARG
1	B	450	ASP
1	B	455	ILE

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Mol	Chain	Res	Type
1	B	458	LYS
1	B	459	ILE
1	B	469	SER
1	B	471	ARG
1	B	484	ASN
1	B	487	ILE
1	B	488	LEU
1	B	568	LEU
1	B	590	THR
1	B	633	SER
1	B	634	ASN
1	B	635	MET
1	C	15	THR
1	C	19	ASN
1	C	40	LYS
1	C	42	HIS
1	C	85	SER
1	C	86	ARG
1	C	94	ARG
1	C	103	VAL
1	C	111	VAL
1	C	119	LYS
1	C	122	LEU
1	C	130	SER
1	C	133	ASN
1	C	164	VAL
1	C	180	ARG
1	C	181	LYS
1	C	183	ARG
1	C	213	LEU
1	C	227	ILE
1	C	247	VAL
1	C	249	GLN
1	C	266	ILE
1	C	284	ASN
1	C	289	LYS
1	C	321	TYR
1	C	338	LEU
1	C	348	LYS
1	C	366	VAL
1	C	376	ARG
1	C	378	LEU

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Mol	Chain	Res	Type
1	C	387	THR
1	C	388	SER
1	C	399	ARG
1	C	416	LEU
1	C	426	LYS
1	C	428	ARG
1	C	458	LYS
1	C	459	ILE
1	C	469	SER
1	C	471	ARG
1	C	484	ASN
1	C	487	ILE
1	C	493	ASP
1	C	513	TYR
1	C	514	THR
1	C	537	MET
1	C	540	LEU
1	C	552	TYR
1	C	556	ARG
1	C	568	LEU
1	C	594	SER
1	C	596	LEU
1	C	634	ASN
1	D	15	THR
1	D	19	ASN
1	D	40	LYS
1	D	42	HIS
1	D	85	SER
1	D	86	ARG
1	D	94	ARG
1	D	103	VAL
1	D	111	VAL
1	D	119	LYS
1	D	122	LEU
1	D	130	SER
1	D	133	ASN
1	D	164	VAL
1	D	180	ARG
1	D	181	LYS
1	D	183	ARG
1	D	213	LEU
1	D	227	ILE

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Mol	Chain	Res	Type
1	D	247	VAL
1	D	249	GLN
1	D	266	ILE
1	D	284	ASN
1	D	289	LYS
1	D	321	TYR
1	D	338	LEU
1	D	348	LYS
1	D	366	VAL
1	D	376	ARG
1	D	378	LEU
1	D	387	THR
1	D	388	SER
1	D	399	ARG
1	D	416	LEU
1	D	426	LYS
1	D	428	ARG
1	D	458	LYS
1	D	459	ILE
1	D	469	SER
1	D	471	ARG
1	D	484	ASN
1	D	487	ILE
1	D	493	ASP
1	D	513	TYR
1	D	514	THR
1	D	537	MET
1	D	552	TYR
1	D	556	ARG
1	D	568	LEU
1	D	594	SER
1	D	596	LEU
1	D	634	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	ASN
1	A	8	HIS
1	A	19	ASN
1	A	78	HIS

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	156	HIS
1	A	168	HIS
1	A	239	HIS
1	A	300	HIS
1	A	484	ASN
1	A	500	HIS
1	A	567	GLN
1	A	621	GLN
1	A	634	ASN
1	B	6	GLN
1	B	7	ASN
1	B	8	HIS
1	B	78	HIS
1	B	133	ASN
1	B	168	HIS
1	B	239	HIS
1	B	249	GLN
1	B	300	HIS
1	B	484	ASN
1	B	500	HIS
1	B	567	GLN
1	B	621	GLN
1	B	634	ASN
1	C	6	GLN
1	C	7	ASN
1	C	8	HIS
1	C	19	ASN
1	C	78	HIS
1	C	81	GLN
1	C	133	ASN
1	C	168	HIS
1	C	239	HIS
1	C	300	HIS
1	C	484	ASN
1	C	500	HIS
1	C	621	GLN
1	C	634	ASN
1	D	6	GLN
1	D	7	ASN
1	D	8	HIS
1	D	19	ASN

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Mol	Chain	Res	Type
1	D	78	HIS
1	D	81	GLN
1	D	133	ASN
1	D	168	HIS
1	D	239	HIS
1	D	300	HIS
1	D	484	ASN
1	D	500	HIS
1	D	621	GLN
1	D	634	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 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	GLC	G	1	3	12,12,12	0.79	0	17,17,17	1.06	1 (5%)
3	GLC	G	2	3	11,11,12	0.84	0	15,15,17	1.84	5 (33%)
3	GLC	G	3	3	11,11,12	1.38	1 (9%)	15,15,17	2.67	6 (40%)
3	GLC	G	4	3	11,11,12	1.21	1 (9%)	15,15,17	2.09	5 (33%)
3	GLC	H	1	3	12,12,12	1.11	1 (8%)	17,17,17	1.64	3 (17%)
3	GLC	H	2	3	11,11,12	0.80	0	15,15,17	2.02	6 (40%)
3	GLC	H	3	3	11,11,12	0.93	0	15,15,17	1.88	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	H	4	3	11,11,12	0.84	0	15,15,17	1.72	4 (26%)
3	GLC	I	1	3	12,12,12	0.78	0	17,17,17	1.17	1 (5%)
3	GLC	I	2	3	11,11,12	0.81	0	15,15,17	1.50	3 (20%)
3	GLC	I	3	3	11,11,12	0.82	0	15,15,17	2.26	5 (33%)
3	GLC	I	4	3	11,11,12	0.92	0	15,15,17	1.83	4 (26%)
3	GLC	J	1	3	12,12,12	0.85	0	17,17,17	1.33	1 (5%)
3	GLC	J	2	3	11,11,12	0.91	0	15,15,17	1.60	4 (26%)
3	GLC	J	3	3	11,11,12	1.18	1 (9%)	15,15,17	2.17	5 (33%)
3	GLC	J	4	3	11,11,12	0.83	0	15,15,17	1.91	6 (40%)

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	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	GLC	G	2	3	-	0/2/19/22	0/1/1/1
3	GLC	G	3	3	-	1/2/19/22	0/1/1/1
3	GLC	G	4	3	-	0/2/19/22	0/1/1/1
3	GLC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
3	GLC	H	3	3	-	0/2/19/22	0/1/1/1
3	GLC	H	4	3	-	2/2/19/22	0/1/1/1
3	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
3	GLC	I	3	3	-	0/2/19/22	0/1/1/1
3	GLC	I	4	3	-	0/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	3	3	-	0/2/19/22	0/1/1/1
3	GLC	J	4	3	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4	GLC	O5-C1	3.09	1.48	1.43
3	G	3	GLC	C4-C5	3.00	1.59	1.53
3	H	1	GLC	O4-C4	2.53	1.48	1.43
3	J	3	GLC	O5-C1	2.18	1.47	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	GLC	O4-C4-C5	6.21	124.71	109.30
3	I	3	GLC	O4-C4-C5	5.02	121.75	109.30
3	H	3	GLC	O5-C5-C6	4.90	114.89	107.20
3	G	4	GLC	C6-C5-C4	-4.65	102.12	113.00
3	J	3	GLC	C1-C2-C3	4.29	114.94	109.67
3	H	4	GLC	C1-O5-C5	-4.20	106.50	112.19
3	G	3	GLC	O5-C1-C2	-4.14	104.39	110.77
3	H	2	GLC	O5-C1-C2	-3.98	104.63	110.77
3	G	3	GLC	O5-C5-C6	3.90	113.31	107.20
3	J	2	GLC	O4-C4-C5	3.89	118.95	109.30
3	G	2	GLC	O5-C5-C6	3.87	113.27	107.20
3	G	3	GLC	O4-C4-C3	-3.81	101.54	110.35
3	I	3	GLC	O5-C1-C2	-3.79	104.92	110.77
3	I	4	GLC	O5-C5-C6	-3.64	101.49	107.20
3	H	2	GLC	O4-C4-C5	3.59	118.21	109.30
3	J	3	GLC	C2-C3-C4	-3.52	104.80	110.89
3	J	3	GLC	O4-C4-C5	3.49	117.96	109.30
3	G	4	GLC	C2-C3-C4	-3.36	105.08	110.89
3	I	2	GLC	C3-C4-C5	-3.35	104.27	110.24
3	I	4	GLC	C2-C3-C4	-3.35	105.11	110.89
3	J	3	GLC	O5-C1-C2	-3.26	105.74	110.77
3	H	1	GLC	O4-C4-C5	3.25	117.37	109.30
3	I	3	GLC	O5-C5-C6	3.25	112.29	107.20
3	H	2	GLC	C1-C2-C3	3.22	113.62	109.67
3	I	3	GLC	C1-C2-C3	3.16	113.55	109.67
3	J	3	GLC	O4-C4-C3	-3.12	103.14	110.35
3	I	3	GLC	O4-C4-C3	-3.08	103.23	110.35
3	H	1	GLC	O5-C5-C6	3.07	114.07	106.44
3	G	3	GLC	O3-C3-C4	-3.06	103.28	110.35
3	H	3	GLC	O4-C4-C3	-3.05	103.29	110.35
3	J	4	GLC	O5-C1-C2	-3.03	106.10	110.77
3	J	4	GLC	C1-O5-C5	2.99	116.24	112.19
3	G	4	GLC	O2-C2-C1	-2.93	103.15	109.15
3	I	2	GLC	O4-C4-C5	2.87	116.42	109.30
3	G	2	GLC	O4-C4-C5	2.84	116.34	109.30
3	J	4	GLC	C1-C2-C3	2.82	113.13	109.67
3	G	2	GLC	C6-C5-C4	-2.75	106.57	113.00
3	J	2	GLC	O4-C4-C3	-2.62	104.28	110.35
3	J	4	GLC	O5-C5-C6	2.62	111.31	107.20
3	H	2	GLC	O4-C4-C3	-2.58	104.37	110.35
3	G	4	GLC	O5-C1-C2	-2.57	106.80	110.77
3	I	1	GLC	C6-C5-C4	-2.56	107.01	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	GLC	C2-C3-C4	-2.53	106.51	110.89
3	G	4	GLC	O5-C5-C6	-2.52	103.25	107.20
3	I	4	GLC	C6-C5-C4	-2.38	107.43	113.00
3	J	2	GLC	O5-C5-C6	2.37	110.92	107.20
3	G	2	GLC	C3-C4-C5	-2.36	106.04	110.24
3	J	2	GLC	O5-C1-C2	-2.32	107.18	110.77
3	I	2	GLC	O5-C5-C6	2.32	110.84	107.20
3	H	1	GLC	O1-C1-C2	2.32	115.55	109.03
3	H	2	GLC	O5-C5-C6	2.29	110.80	107.20
3	H	4	GLC	C3-C4-C5	-2.26	106.21	110.24
3	G	2	GLC	O5-C1-C2	-2.22	107.35	110.77
3	H	4	GLC	C2-C3-C4	-2.21	107.07	110.89
3	I	4	GLC	O5-C1-C2	-2.16	107.44	110.77
3	H	4	GLC	O5-C5-C4	2.15	116.06	110.83
3	H	2	GLC	C2-C3-C4	-2.10	107.26	110.89
3	G	3	GLC	C6-C5-C4	2.06	117.84	113.00
3	G	1	GLC	C6-C5-C4	-2.04	108.22	113.00
3	J	4	GLC	O4-C4-C3	2.04	115.06	110.35
3	J	1	GLC	O5-C5-C6	2.01	111.44	106.44
3	J	4	GLC	C2-C3-C4	-2.01	107.42	110.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	4	GLC	O5-C5-C6-O6
3	G	3	GLC	O5-C5-C6-O6
3	H	4	GLC	C4-C5-C6-O6

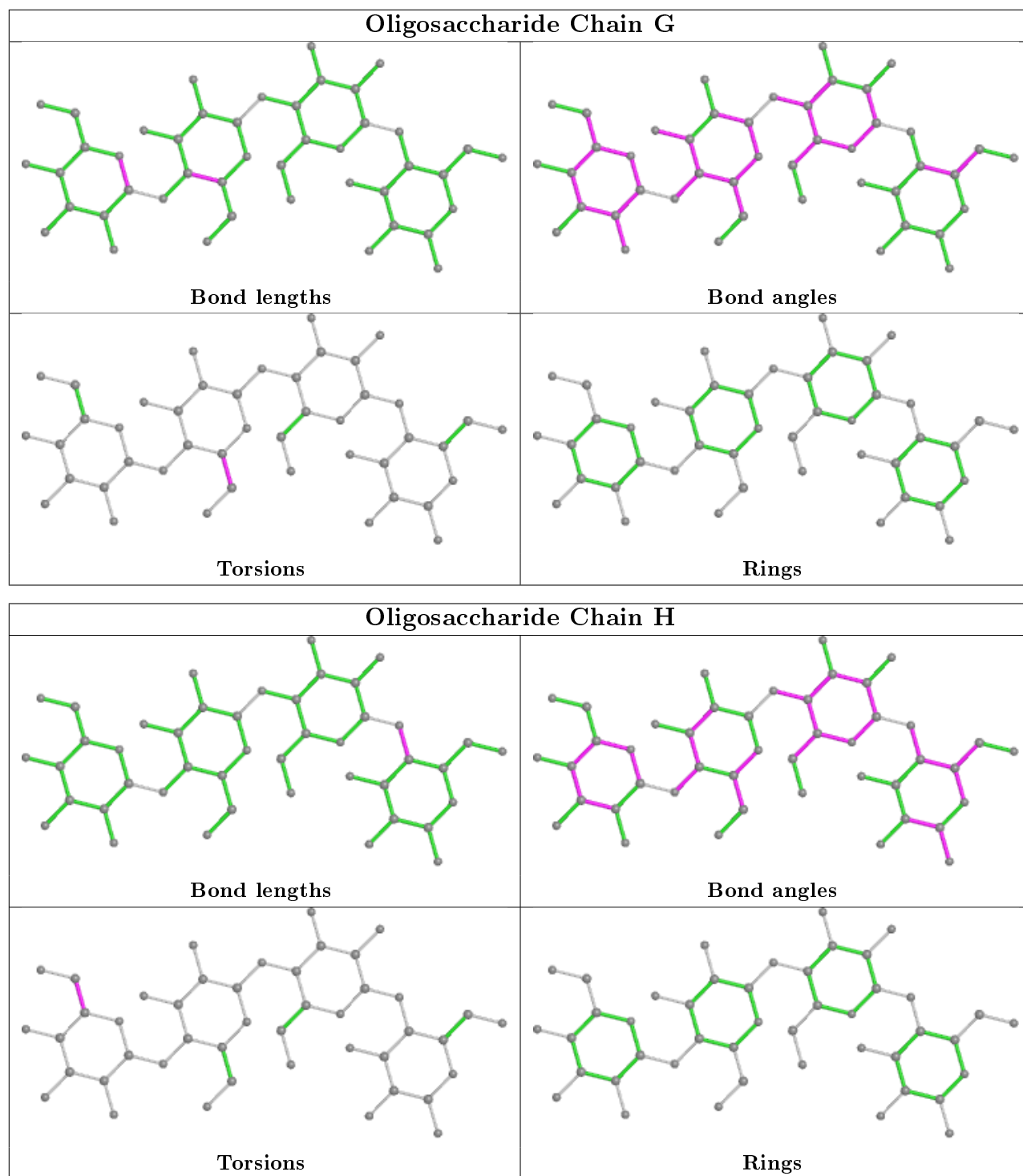
There are no ring outliers.

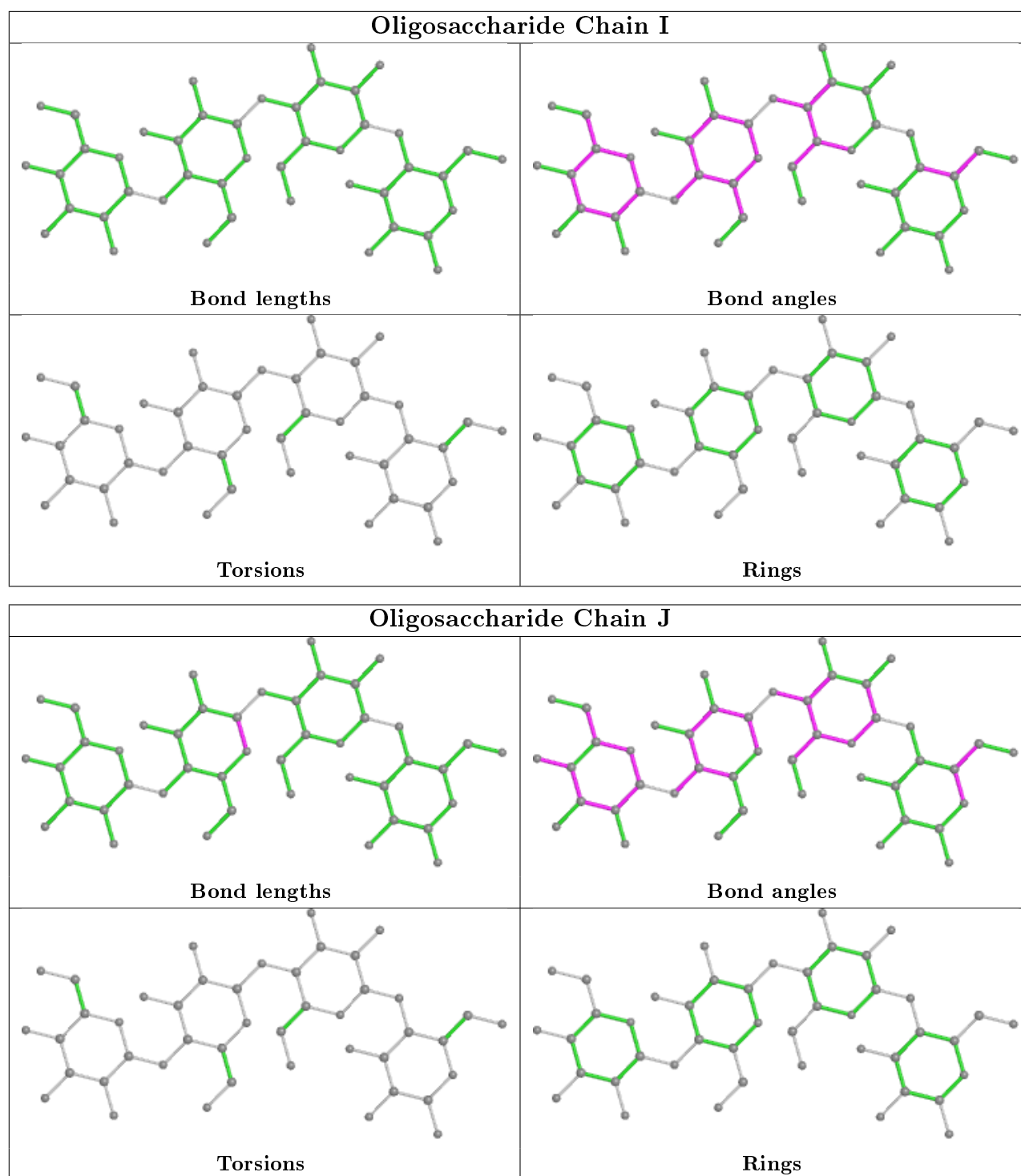
6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	4	GLC	1	0
3	G	2	GLC	1	0
3	H	3	GLC	2	0
3	J	3	GLC	1	0
3	G	1	GLC	1	0
3	J	2	GLC	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](#)

16 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	$\# Z > 2$
4	SO4	D	801	-	4,4,4	0.33	0	6,6,6	0.41	0
4	SO4	B	801	-	4,4,4	0.16	0	6,6,6	0.26	0
4	SO4	C	706	-	4,4,4	0.18	0	6,6,6	0.27	0
4	SO4	C	804	-	4,4,4	0.13	0	6,6,6	0.20	0
4	SO4	D	804	-	4,4,4	0.13	0	6,6,6	0.24	0
4	SO4	A	804	-	4,4,4	0.15	0	6,6,6	0.20	0
4	SO4	B	804	-	4,4,4	0.12	0	6,6,6	0.11	0
4	SO4	D	803	-	4,4,4	0.16	0	6,6,6	0.18	0
4	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.13	0
4	SO4	B	706	-	4,4,4	0.20	0	6,6,6	0.22	0
4	SO4	C	801	-	4,4,4	0.19	0	6,6,6	0.08	0
4	SO4	B	802	-	4,4,4	0.34	0	6,6,6	0.29	0
4	SO4	A	803	-	4,4,4	0.19	0	6,6,6	0.21	0
4	SO4	D	802	-	4,4,4	0.15	0	6,6,6	0.21	0
4	SO4	A	802	-	4,4,4	0.23	0	6,6,6	0.41	0
4	SO4	C	803	-	4,4,4	0.18	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	SO4	1	0
4	C	801	SO4	1	0
4	D	802	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	611/725 (84%)	-0.18	7 (1%)	80 56	56, 79, 114, 153	0
1	B	611/725 (84%)	-0.20	7 (1%)	80 56	57, 80, 114, 154	0
1	C	613/725 (84%)	-0.31	3 (0%)	91 75	50, 78, 106, 133	0
1	D	613/725 (84%)	-0.27	2 (0%)	94 84	50, 77, 106, 133	0
2	E	0/5	-	-	-	-	-
2	F	0/5	-	-	-	-	-
All	All	2448/2910 (84%)	-0.24	19 (0%)	86 65	50, 78, 111, 154	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	631	ASN	4.3
1	A	549	TYR	4.1
1	B	630	LEU	3.5
1	A	548	ASP	3.4
1	B	549	TYR	3.0
1	C	548	ASP	2.7
1	A	547	LYS	2.6
1	A	625	LEU	2.6
1	B	548	ASP	2.5
1	B	626	VAL	2.5
1	A	546	ALA	2.3
1	D	548	ASP	2.3
1	C	549	TYR	2.2
1	C	592	ARG	2.1
1	B	415	GLU	2.1
1	B	436	GLU	2.1
1	A	550	GLY	2.1
1	A	416	LEU	2.1
1	D	414	GLY	2.0

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 ⓘ

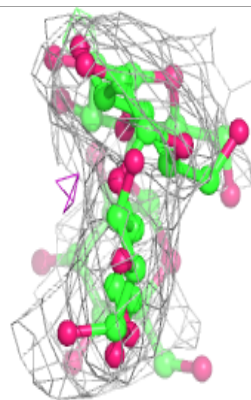
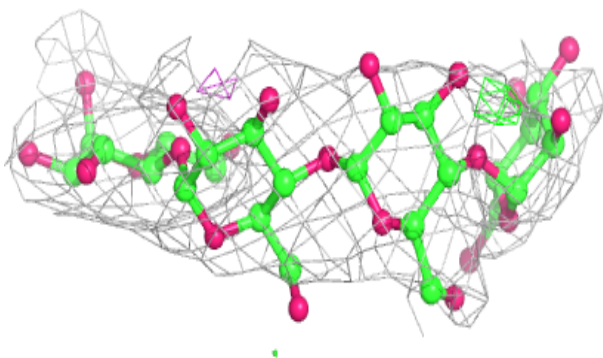
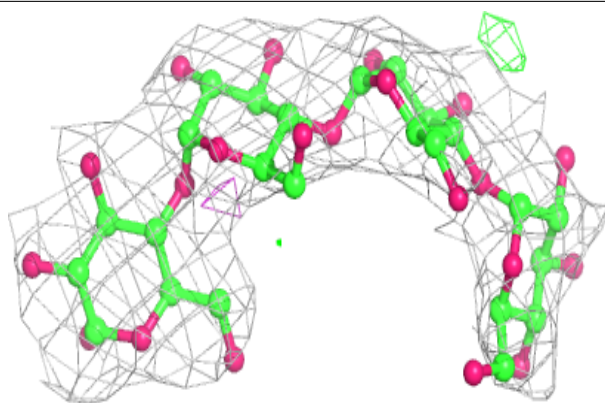
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	J	4	11/12	0.69	0.45	123,130,136,140	0
3	GLC	G	4	11/12	0.76	0.33	127,138,144,144	0
3	GLC	J	1	12/12	0.79	0.52	91,108,114,118	0
3	GLC	H	1	12/12	0.82	0.25	82,95,103,106	0
3	GLC	J	3	11/12	0.85	0.27	99,114,129,131	0
3	GLC	H	4	11/12	0.86	0.24	98,110,116,123	0
3	GLC	I	4	11/12	0.87	0.27	119,124,127,131	0
3	GLC	J	2	11/12	0.87	0.36	90,93,105,112	0
3	GLC	G	1	12/12	0.89	0.16	89,95,100,100	0
3	GLC	I	1	12/12	0.89	0.20	92,95,100,110	0
3	GLC	G	3	11/12	0.91	0.15	105,117,130,131	0
3	GLC	G	2	11/12	0.92	0.19	95,100,108,112	0
3	GLC	H	3	11/12	0.92	0.19	84,89,108,112	0
3	GLC	I	2	11/12	0.93	0.21	89,96,104,112	0
3	GLC	I	3	11/12	0.94	0.14	96,106,116,117	0
3	GLC	H	2	11/12	0.95	0.27	80,86,92,92	0

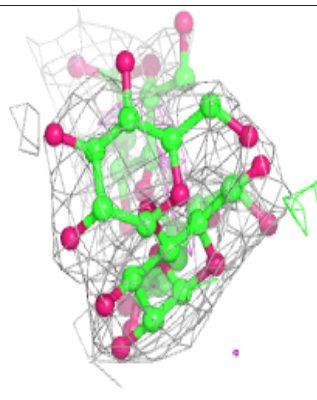
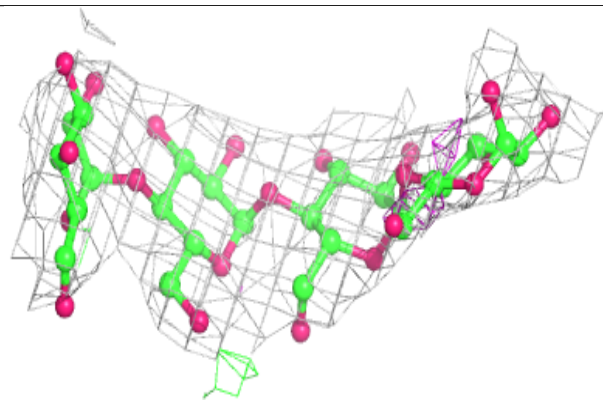
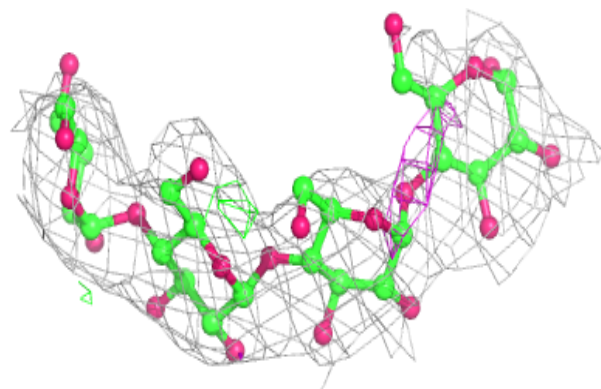
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

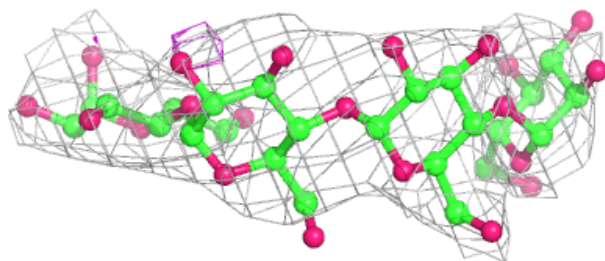
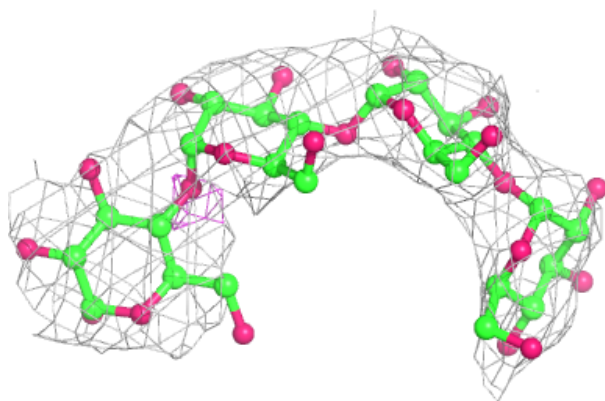
**Electron density around Chain H:**

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

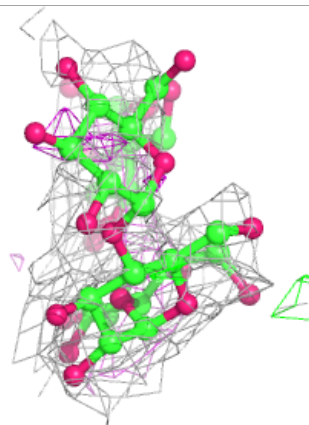
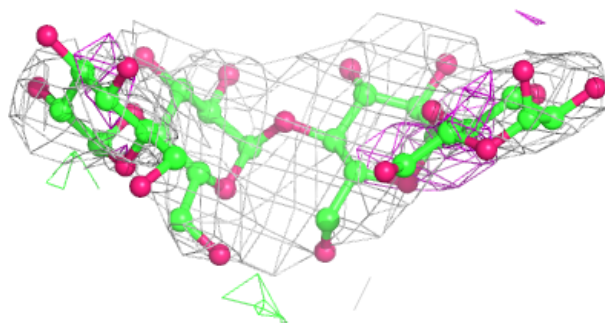
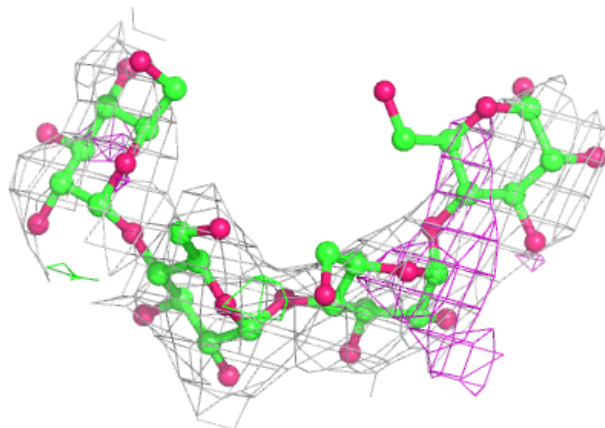


Electron density around Chain I:

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

**Electron density around Chain J:**

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



6.4 Ligands [i](#)

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, 95th 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
4	SO4	D	801	5/5	0.47	0.30	95,97,124,140	0
4	SO4	D	803	5/5	0.83	0.20	109,116,122,132	0
4	SO4	C	803	5/5	0.83	0.26	105,118,128,139	0
4	SO4	B	802	5/5	0.88	0.29	84,95,108,127	0
4	SO4	D	804	5/5	0.88	0.27	121,122,126,138	0
4	SO4	A	804	5/5	0.89	0.19	122,133,134,143	0
4	SO4	C	706	5/5	0.90	0.20	103,106,122,136	0
4	SO4	A	803	5/5	0.90	0.18	93,99,118,120	0
4	SO4	B	804	5/5	0.90	0.21	129,130,133,146	0
4	SO4	B	801	5/5	0.91	0.22	87,89,108,114	0
4	SO4	B	706	5/5	0.91	0.17	96,107,112,125	0
4	SO4	A	802	5/5	0.92	0.26	77,83,98,116	0
4	SO4	C	804	5/5	0.94	0.28	126,128,131,133	0
4	SO4	A	801	5/5	0.95	0.15	83,90,100,102	0
4	SO4	D	802	5/5	0.95	0.16	89,93,109,112	0
4	SO4	C	801	5/5	0.96	0.12	90,90,110,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.