



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:38 PM UTC

PDB ID : 3RSZ / pdb_00003rsz
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

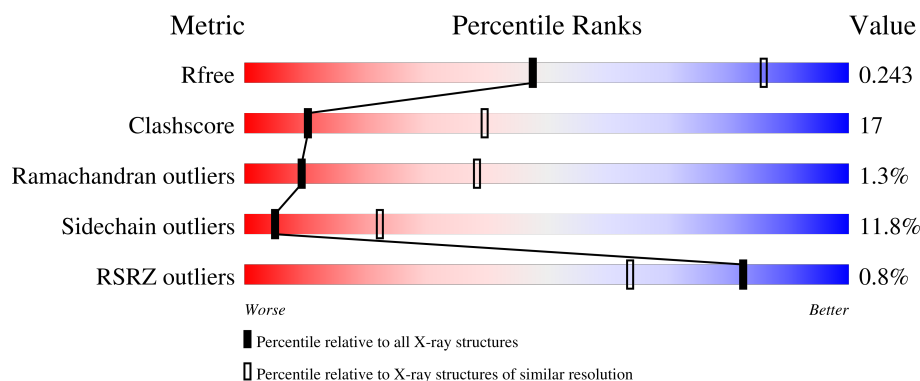
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.



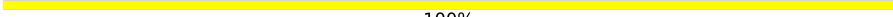
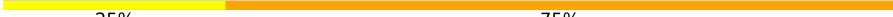
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	% 52% 27% 5% 16%
1	B	725	% 52% 27% 5% 16%
1	C	725	% 51% 27% 5% 15%
1	D	725	% 52% 27% 5% 15%
2	E	5	 40% 60%

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Mol	Chain	Length	Quality of chain
2	F	5	 100%
3	G	4	 75% 25%
3	H	4	 75% 25%
3	I	4	 100%
3	J	4	 25% 75%

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.

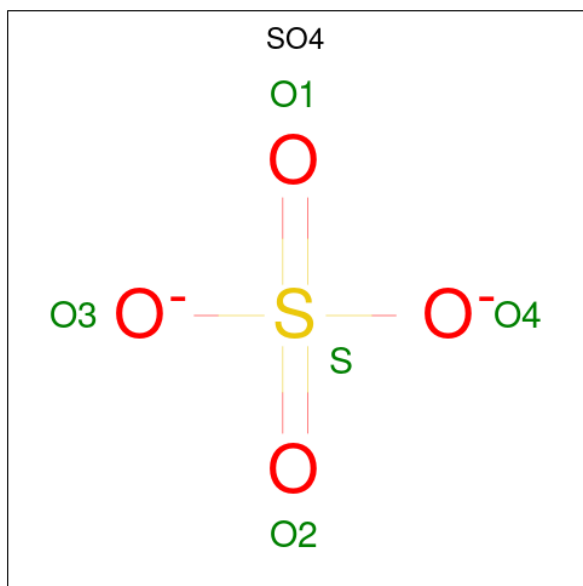
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	1	0	0
			10	6	2	2			
2	F	5	Total	C	N	O	1	0	0
			25	15	5	5			

- 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 (CCD ID: 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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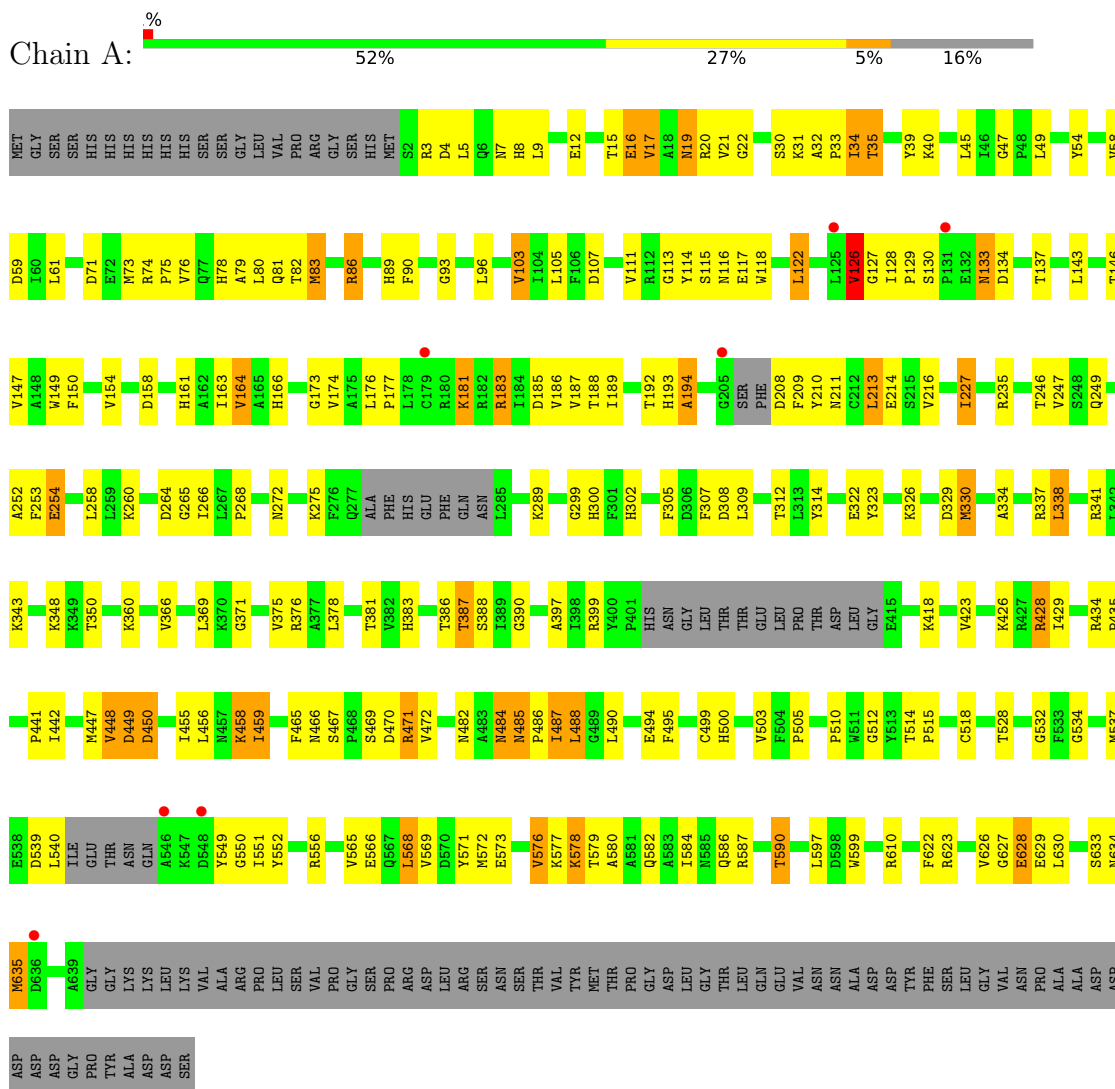
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			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		

3 Residue-property plots

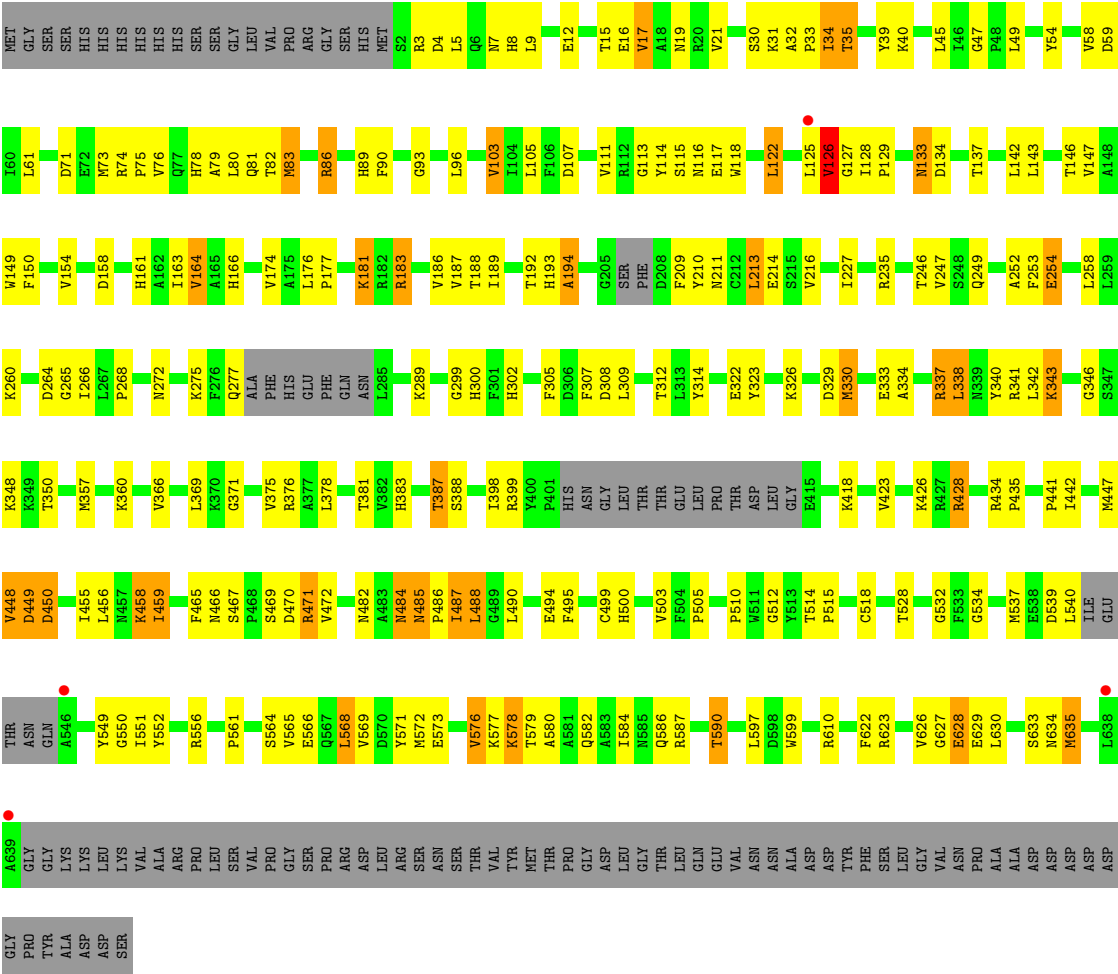
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycogen [starch] synthase isoform 2

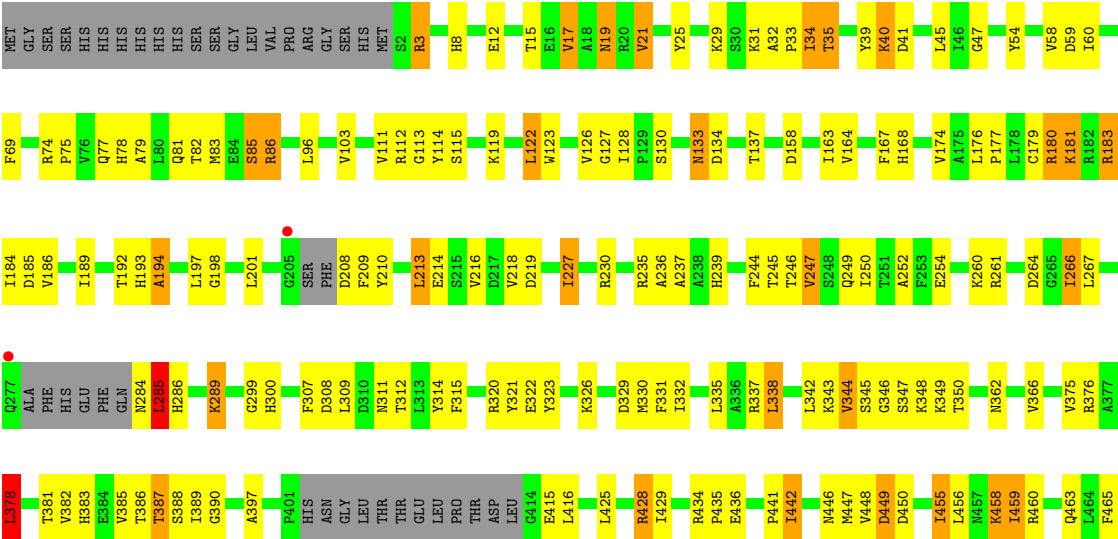


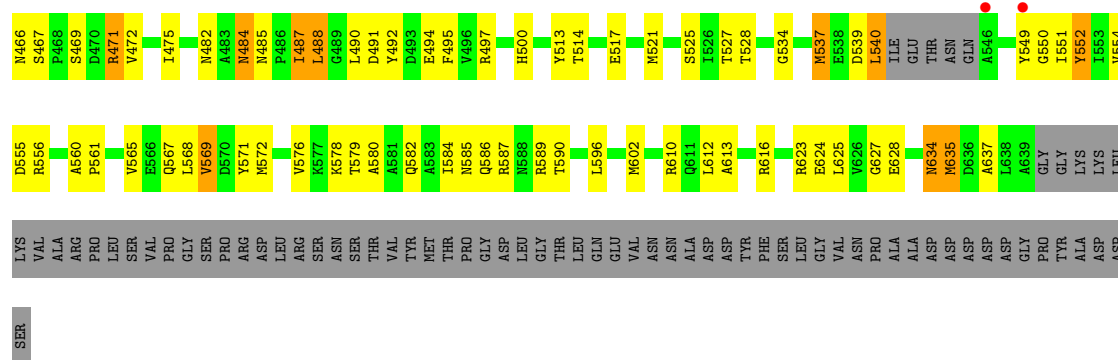
• Molecule 1: Glycogen [starch] synthase isoform 2



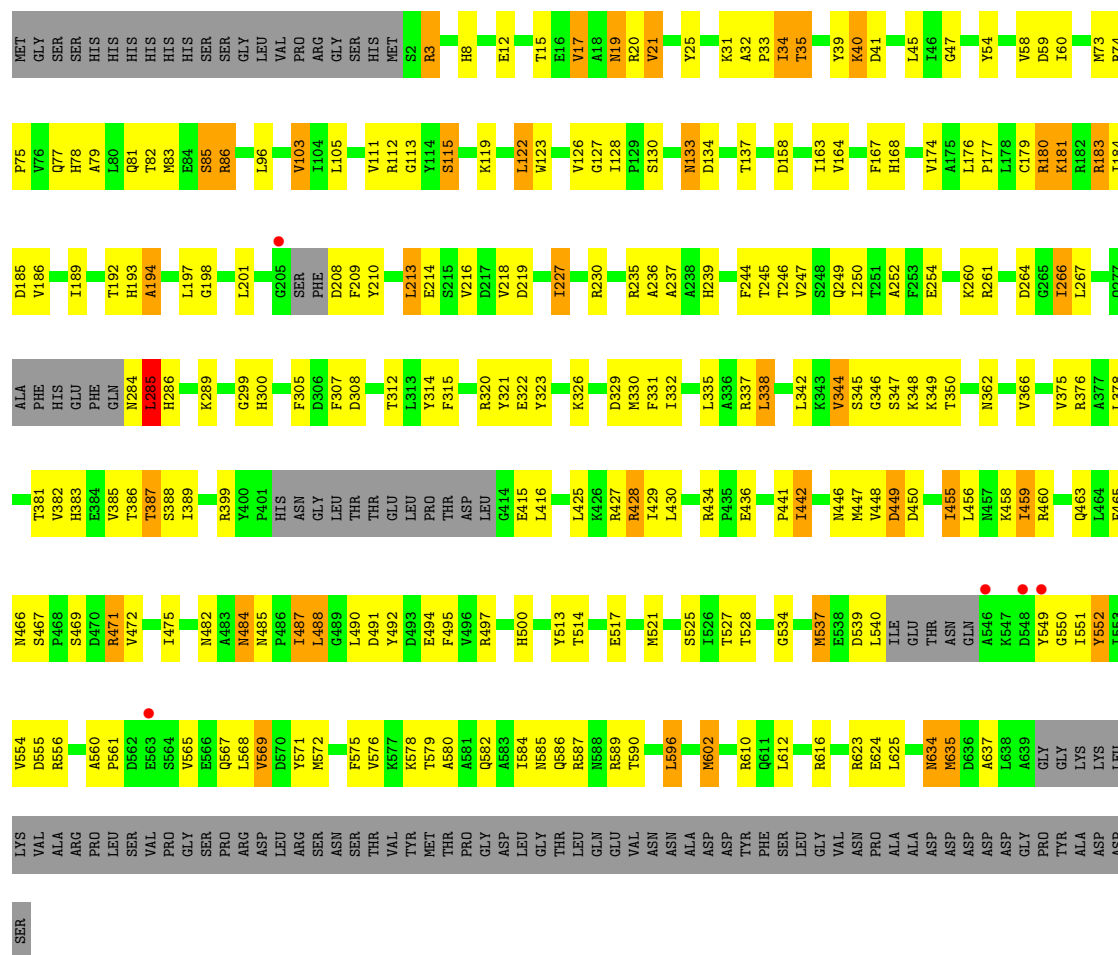


● Molecule 1: Glycogen [starch] synthase isoform 2

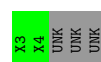




• Molecule 1: Glycogen [starch] synthase isoform 2



• Molecule 2: Glycogen [starch] synthase isoform 2

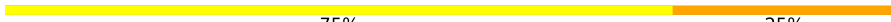


- Molecule 2: Glycogen [starch] synthase isoform 2

Chain F:  100%

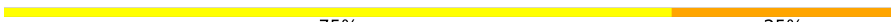
There are no outlier residues recorded for this chain.

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

Chain G:  75% 25%

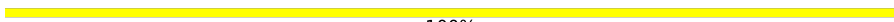
GLC1
GLC2
GLC3
GLC4

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

Chain H:  75% 25%

GLC1
GLC2
GLC3
GLC4

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

Chain I:  100%

GLC1
GLC2
GLC3
GLC4

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

Chain J:  25% 75%

GLC1
GLC2
GLC3
GLC4

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) 98.8 (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 0.203 , 0.243	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 , 41.6	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.48	0/5038	0.85	6/6819 (0.1%)
1	B	0.46	0/5038	0.85	8/6819 (0.1%)
1	C	0.48	0/5050	0.86	11/6835 (0.2%)
1	D	0.51	0/5050	0.86	11/6835 (0.2%)
All	All	0.48	0/20176	0.86	36/27308 (0.1%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	VAL	N-CA-C	-6.78	106.62	113.47
1	D	17	VAL	CA-C-N	-6.28	112.04	123.34
1	D	17	VAL	C-N-CA	-6.28	112.04	123.34
1	A	21	VAL	N-CA-C	-6.26	107.15	113.47
1	A	58	VAL	N-CA-C	6.22	116.82	108.11
1	C	17	VAL	CA-C-N	-6.11	112.34	123.34
1	C	17	VAL	C-N-CA	-6.11	112.34	123.34
1	C	285	LEU	N-CA-C	6.04	123.66	110.80
1	D	285	LEU	N-CA-C	5.98	123.55	110.80
1	C	434	ARG	CA-C-N	5.98	127.32	119.84
1	C	434	ARG	C-N-CA	5.98	127.32	119.84
1	B	434	ARG	CA-C-N	5.94	127.26	119.84
1	B	434	ARG	C-N-CA	5.94	127.26	119.84
1	D	58	VAL	N-CA-C	5.81	116.49	108.12
1	D	485	ASN	CA-C-N	5.79	125.65	119.28
1	D	485	ASN	C-N-CA	5.79	125.65	119.28
1	C	485	ASN	CA-C-N	5.77	125.62	119.28
1	C	485	ASN	C-N-CA	5.77	125.62	119.28
1	B	485	ASN	CA-C-N	5.71	125.56	119.28
1	B	485	ASN	C-N-CA	5.71	125.56	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	434	ARG	CA-C-N	5.69	126.95	119.84
1	D	434	ARG	C-N-CA	5.69	126.95	119.84
1	A	485	ASN	CA-C-N	5.67	125.52	119.28
1	A	485	ASN	C-N-CA	5.67	125.52	119.28
1	B	58	VAL	N-CA-C	5.54	115.87	108.11
1	C	58	VAL	N-CA-C	5.43	115.94	108.12
1	D	115	SER	N-CA-C	5.34	116.78	111.07
1	A	434	ARG	CA-C-N	5.33	126.50	119.84
1	A	434	ARG	C-N-CA	5.33	126.50	119.84
1	D	467	SER	CA-C-N	5.23	125.53	119.47
1	D	467	SER	C-N-CA	5.23	125.53	119.47
1	C	378	LEU	N-CA-C	-5.15	105.56	111.07
1	C	467	SER	CA-C-N	5.13	125.42	119.47
1	C	467	SER	C-N-CA	5.13	125.42	119.47
1	B	357	MET	CA-C-N	5.09	124.85	119.76
1	B	357	MET	C-N-CA	5.09	124.85	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4923	0	4850	171	0
1	B	4923	0	4850	162	0
1	C	4935	0	4859	175	0
1	D	4935	0	4859	174	0
2	E	10	0	4	0	0
2	F	25	0	7	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	20	0	0	1	0
All	All	20011	0	19585	668	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (668) 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
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:HD22	1:C:484:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:D:484:ASN:ND2	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:H	1:C:484:ASN:ND2	1.88	0.69
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:A:213:LEU:HD12	1:A:213:LEU:C	2.18	0.69
1:C:210:TYR:HE1	1:C:250:ILE:HD11	1.56	0.69
1:C:86:ARG:HB3	1:C:86:ARG:HH11	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:TYR:H	1:B:500:HIS:HD2	1.39	0.68
1:D:86:ARG:HH11	1:D:86:ARG:HB3	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:213:LEU:C	1:B:213:LEU:HD12	2.18	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: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:A:113:GLY:C	1:A:115:SER:H	2.04	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
1:B:580:ALA:O	1:B:584:ILE:HG13	1.98	0.64
1:C:448:VAL:O	1:C:448:VAL:HG12	1.96	0.64
1:B:113:GLY:C	1:B:115:SER:H	2.04	0.64
1:C:634:ASN:ND2	1:C:637:ALA:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LYS:HD3	1:B:181:LYS:C	2.23	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:B:484:ASN:ND2	1:B:484:ASN:H	1.94	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:A:181:LYS:HD3	1:A:181:LYS:C	2.23	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:D:213:LEU:HD12	1:D:213:LEU:C	2.24	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:A:577:LYS:O	1:A:578:LYS:C	2.44	0.61
1:B:577:LYS:O	1:B:578:LYS:C	2.42	0.61
1:C:181:LYS:C	1:C:181:LYS:HD3	2.26	0.61
1:D:134:ASP:CG	1:D:137:THR:HG23	2.26	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:C:134:ASP:CG	1:C:137:THR:HG23	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:314:TYR:H	1:B:500:HIS:CD2	2.20	0.59
1:B:484:ASN:H	1:B:484:ASN:HD22	1.48	0.59
1:D:245:THR:OG1	1:D:267:LEU:HD12	2.02	0.59
1:D:181:LYS:HD3	1:D:181:LYS:C	2.27	0.59
1:D:344:VAL:C	1:D:346:GLY:H	2.10	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: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:C:19:ASN:N	1:C:19:ASN:HD22	2.01	0.59
1:C:213:LEU:C	1:C:213:LEU:HD12	2.27	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:A:305:PHE:HZ	1:A:309:LEU:HG	1.69	0.58
1:D:79:ALA:O	1:D:83:MET:HG2	2.04	0.58
1:D:218:VAL:HG23	1:D:219:ASP:H	1.68	0.58
1:D:338:LEU:HD22	1:D:338:LEU:O	2.04	0.58
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:484:ASN:H	1:A:484:ASN:HD22	1.52	0.57
1:A:86:ARG:HH11	1:A:86:ARG:HB3	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:344:VAL:C	1:C:346:GLY:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:113:GLY:O	1:A:115:SER:N	2.38	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: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: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:193:HIS:O	1:B:194:ALA:HB2	2.06	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:484:ASN:HD22	1:D:484:ASN:N	2.03	0.55
1:A:20:ARG:NH1	4:A:801:SO4:O1	2.40	0.55
1:A:143:LEU:O	1:A:147:VAL:HG23	2.06	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: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
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.88	0.54
1:A:338:LEU:HD22	1:A:338:LEU:O	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:H	1:A:133:ASN:ND2	2.06	0.54
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HG	1:B:93:GLY:HA2	1.90	0.53
1:B:338:LEU:O	1:B:338:LEU:HD22	2.08	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:H	1:B:133:ASN:ND2	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:113:GLY:C	1:C:115:SER:H	2.17	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:86:ARG:HB3	1:C:86:ARG:NH1	2.22	0.52
1:C:350:THR:OG1	1:C:471:ARG:NH1	2.43	0.52
1:D:21:VAL:HG12	1:D:21:VAL:O	2.09	0.52
1:B:113:GLY:C	1:B:115:SER:N	2.68	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:12:GLU:HG3	1:A:166:HIS:HB3	1.91	0.52
1:A:163:ILE:CG2	1:A:186:VAL:HG12	2.40	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:285:LEU:HD13	1:C:497:ARG:HD3	1.91	0.51
1:C:484:ASN:ND2	1:C:484:ASN:N	2.58	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:81:GLN:O	1:A:82:THR:C	2.53	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:321:TYR:CD1	1:C:321:TYR:C	2.89	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:HA	1:B:428:ARG:NH1	2.25	0.51
1:C:82:THR:O	1:C:85:SER:HB2	2.10	0.51
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.92	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:D:113:GLY:C	1:D:115:SER:H	2.20	0.50
1:A:386:THR:CG2	1:C:390:GLY:HA2	2.37	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:81:GLN:O	1:B:82:THR:C	2.53	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
1:D:112:ARG:O	1:D:115:SER:HB2	2.12	0.49
1:D:54:TYR:CE1	1:D:60:ILE:HD11	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ASP:O	1:D:312:THR:HG23	2.12	0.49
1:A:586:GLN:O	1:A:590:THR:HG23	2.12	0.49
1:B:30:SER:O	1:B:599:TRP:CD1	2.65	0.49
1:B:448:VAL:O	1:B:449:ASP:CB	2.55	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:D:321:TYR:CD1	1:D:321:TYR:C	2.91	0.49
1:B:447:MET:HB2	1:B:450:ASP:OD2	2.12	0.49
1:B:116:ASN:C	1:B:118:TRP:N	2.69	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:HA	1:D:471:ARG:NE	2.28	0.48
1:A:34:ILE:HD12	1:A:34:ILE:HA	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:8:HIS:CE1	1:D:39:TYR:OH	2.64	0.48
1:D:198:GLY:HA3	1:D:254:GLU:OE1	2.13	0.48
1:D:227:ILE:HD12	1:D:230:ARG:HD2	1.94	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:A:465:PHE:CE1	3:H:3:GLC:H2	2.49	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:113:GLY:C	1:A:115:SER:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLY:O	1:A:266:ILE:HD13	2.14	0.47
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: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:A:512:GLY:O	1:A:515:PRO:HD2	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:D:3:ARG:NH1	1:D:185:ASP:OD2	2.41	0.47
1:D:168:HIS:HD2	1:D:193:HIS:NE2	2.13	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:76:VAL:O	1:A:79:ALA:HB3	2.15	0.46
1:B:134:ASP:CG	1:B:137:THR:HG23	2.40	0.46
1:D:133:ASN:H	1:D:133:ASN:ND2	2.13	0.46
1:D:362:ASN:HB2	1:D:446:ASN:HB2	1.98	0.46
1:B:213:LEU:HD21	1:B:253:PHE:CE1	2.50	0.46
1:B:623:ARG:HG3	1:B:628:GLU:C	2.40	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:40:LYS:HB3	1:C:41:ASP:H	1.57	0.46
1:C:197:LEU:HD23	1:C:197:LEU:HA	1.77	0.46
1:C:465:PHE:O	1:C:466:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:C	1:B:118:TRP:H	2.24	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: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:344:VAL:C	1:D:346:GLY:N	2.73	0.46
1:A:623:ARG:HG3	1:A:628:GLU:C	2.40	0.45
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:HD12	1:B:398:ILE:HA	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: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:25:TYR:C	1:C:25:TYR:CD2	2.94	0.45
1:A:116:ASN:C	1:A:118:TRP:N	2.73	0.45
1:A:73:MET:C	1:A:75:PRO:HD2	2.41	0.45
1:A:134:ASP:CG	1:A:137:THR:HG23	2.41	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:25:TYR:C	1:D:25:TYR:CD2	2.94	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:321:TYR:C	1:C:321:TYR:HD1	2.25	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:80:LEU:O	1:A:83:MET:HB2	2.17	0.44
1:B:512:GLY:C	1:B:515:PRO:HD2	2.42	0.44
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:D:180:ARG:CG	2.31	0.44
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: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:A:512:GLY:C	1:A:515:PRO:HD2	2.43	0.44
1:B:146:THR:O	1:B:149:TRP:HB3	2.18	0.44
1:B:330:MET:HE2	1:B:505:PRO:HB3	2.00	0.44
1:B:485:ASN:HA	1:B:486:PRO:HD3	1.87	0.44
1:A:4:ASP:OD2	1:A:7:ASN:HB3	2.18	0.44
1:A:307:PHE:HD1	1:A:312:THR:HG21	1.83	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:491:ASP:O	1:D:492:TYR:C	2.61	0.44
1:B:73:MET:C	1:B:75:PRO:HD2	2.42	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:74:ARG:HG3	1:D:78:HIS:CE1	2.53	0.43
1:D:490:LEU:HD22	1:D:494:GLU:HB3	2.00	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:A:537:MET:HE2	1:A:597:LEU:HD21	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:PHE:O	1:A:466:ASN:HB2	2.18	0.43
1:B:80:LEU:O	1:B:83:MET:HB2	2.19	0.43
1:B:465:PHE:O	1:B:466:ASN:HB2	2.19	0.43
1:C:29:LYS:HE2	4:C:801:SO4:O3	2.18	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: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:HD3	1:C:458:LYS:O	2.18	0.43
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:74:ARG:N	1:D:75:PRO:CD	2.82	0.43
1:D:575:PHE:O	1:D:578:LYS:HB2	2.19	0.43
1:A:96:LEU:CD1	1:D:430:LEU:HD12	2.49	0.43
1:C:183:ARG:HE	1:C:183:ARG:HB2	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: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:O	1:B:227:ILE:CG2	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:HE	1:C:623:ARG:HB2	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:HD12	1:B:34:ILE:HA	1.73	0.42
1:B:471:ARG:HA	1:B:471:ARG:NE	2.34	0.42
1:C:549:TYR:C	1:C:590:THR:HG22	2.42	0.42
1:C:560:ALA:HB1	1:C:561:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:503:VAL:C	1:B:505:PRO:HD3	2.43	0.42
1:B:537:MET:HE2	1:B:597:LEU:HD21	2.00	0.42
1:C:180:ARG:HH11	1:C:180:ARG:CG	2.31	0.42
1:C:197:LEU:O	1:C:198:GLY:C	2.62	0.42
1:C:321:TYR:CD1	1:C:321:TYR:O	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:A:330:MET:HE3	1:A:568:LEU:HD12	2.02	0.42
1:B:116:ASN:O	1:B:117:GLU:C	2.62	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
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:73:MET:C	1:D:75:PRO:HD2	2.45	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:A:116:ASN:O	1:A:117:GLU:C	2.62	0.42
1:C:201:LEU:HD23	1:C:201:LEU:HA	1.88	0.42
1:C:527:THR:HG21	1:C:534:GLY:HA2	2.01	0.42
1:D:321:TYR:C	1:D:321:TYR:HD1	2.28	0.42
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.94	0.42
1:D:552:TYR:HD1	1:D:571:TYR:CD2	2.38	0.42
1:A:330:MET:HE2	1:A:505:PRO:HB3	2.01	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:81:GLN:HE21	1:A:81:GLN:C	2.26	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:A:465:PHE:CZ	3:H:3:GLC:H2	2.54	0.42
1:B:565:VAL:O	1:B:569:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:PRO:CB	1:D:158:ASP:HB2	2.50	0.42
1:D:428:ARG:NH1	1:D:428:ARG:HA	2.34	0.42
1:A:89:HIS:O	1:A:107:ASP:CB	2.68	0.42
1:D:602:MET:HE3	1:D:602:MET:HB3	1.91	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.88	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:C:491:ASP:O	1:C:492:TYR:C	2.62	0.41
1:D:183:ARG:HE	1:D:183:ARG:HB2	1.53	0.41
1:D:197:LEU:O	1:D:198:GLY:C	2.62	0.41
1:A:17:VAL:HG22	1:A:47:GLY:HA3	2.01	0.41
1:C:344:VAL:C	1:C:346:GLY:N	2.73	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
1:A:31:LYS:HZ3	1:A:35:THR:HG21	1.85	0.41
1:A:300:HIS:HE1	1:A:441:PRO:O	2.03	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: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:83:MET:HE2	1:A:83:MET:HB3	1.59	0.41
1:A:227:ILE:O	1:A:227:ILE:CG2	2.68	0.41
1:B:266:ILE:HD13	1:B:266:ILE:HA	1.81	0.41
1:B:299:GLY:HA2	1:B:375:VAL:HG21	2.02	0.41
1:B:334:ALA:CB	1:B:568:LEU:HD13	2.50	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:77:GLN:O	1:D:81:GLN:HG3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:76:VAL:O	1:B:79:ALA:HB3	2.21	0.41
1:B:337:ARG:O	1:B:341:ARG:HG3	2.20	0.41
1:B:340:TYR:O	1:B:341:ARG:C	2.63	0.41
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.86	0.41
1:C:77:GLN:O	1:C:81:GLN:HG3	2.21	0.41
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.55	0.41
1:D:180:ARG:NH1	1:D:180:ARG:HG3	2.36	0.41
1:A:369:LEU:HD23	1:A:487:ILE:HD13	2.03	0.41
1:A:369:LEU:HD23	1:A:487:ILE:CD1	2.50	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
1:B:125:LEU:C	1:B:126:VAL:CG2	2.93	0.41
1:B:369:LEU:HD23	1:B:487:ILE:CD1	2.50	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:416:LEU:HD23	1:D:416:LEU:HA	1.90	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:17:VAL:HG12	1:A:45:LEU:HB3	2.02	0.41
1:A:126:VAL:O	1:A:128:ILE:HG13	2.21	0.41
1:A:369:LEU:HD23	1:A:369:LEU:HA	1.82	0.41
1:B:626:VAL:HG11	1:B:630:LEU:HD12	2.02	0.41
1:C:309:LEU:C	1:C:311:ASN:H	2.28	0.41
1:A:626:VAL:HG11	1:A:630:LEU:HD12	2.01	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:B:209:PHE:O	1:B:211:ASN:N	2.53	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:HA	1:D:487:ILE:HD12	1.83	0.40
1:A:397:ALA:HB3	1:C:378:LEU:HD11	2.02	0.40
1:B:17:VAL:HG12	1:B:45:LEU:HB3	2.03	0.40
1:B:142:LEU:HA	1:B:142:LEU:HD23	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:213:LEU:C	1:A:213:LEU:CD1	2.89	0.40
1:A:399:ARG:NH2	1:C:308:ASP:HA	2.36	0.40
1:B:71:ASP:O	1:B:74:ARG:HB2	2.21	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:C:113:GLY:C	1:C:115:SER:N	2.80	0.40
1:C:193:HIS:O	1:C:194:ALA:HB2	2.21	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:B:17:VAL:CG1	1:B:45:LEU:HB3	2.52	0.40
1:C:69:PHE:CD2	1:C:77:GLN:HB2	2.57	0.40
1:D:201:LEU:HD23	1:D:201:LEU:HA	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 [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	601/725 (83%)	535 (89%)	56 (9%)	10 (2%)	7	32
1	B	601/725 (83%)	542 (90%)	49 (8%)	10 (2%)	7	32
1	C	603/725 (83%)	550 (91%)	46 (8%)	7 (1%)	10	40
1	D	603/725 (83%)	548 (91%)	50 (8%)	5 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2408/2900 (83%)	2175 (90%)	201 (8%)	32 (1%)	9	38

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
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%)	466 (89%)	60 (11%)	5	24
1	B	526/622 (85%)	467 (89%)	59 (11%)	6	24
1	C	527/622 (85%)	461 (88%)	66 (12%)	4	20
1	D	527/622 (85%)	463 (88%)	64 (12%)	5	21
All	All	2106/2488 (85%)	1857 (88%)	249 (12%)	5	22

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
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	83	MET
1	A	86	ARG
1	A	103	VAL
1	A	111	VAL
1	A	122	LEU
1	A	126	VAL
1	A	130	SER
1	A	133	ASN
1	A	164	VAL
1	A	181	LYS
1	A	183	ARG
1	A	213	LEU
1	A	214	GLU
1	A	216	VAL
1	A	227	ILE
1	A	247	VAL
1	A	249	GLN
1	A	254	GLU
1	A	289	LYS
1	A	330	MET

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Mol	Chain	Res	Type
1	A	337	ARG
1	A	338	LEU
1	A	343	LYS
1	A	348	LYS
1	A	366	VAL
1	A	376	ARG
1	A	378	LEU
1	A	381	THR
1	A	387	THR
1	A	388	SER
1	A	418	LYS
1	A	423	VAL
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	472	VAL
1	A	484	ASN
1	A	487	ILE
1	A	488	LEU
1	A	551	ILE
1	A	556	ARG
1	A	568	LEU
1	A	576	VAL
1	A	590	THR
1	A	633	SER
1	A	634	ASN
1	A	635	MET
1	B	9	LEU
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	83	MET
1	B	86	ARG

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Mol	Chain	Res	Type
1	B	103	VAL
1	B	111	VAL
1	B	122	LEU
1	B	126	VAL
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	330	MET
1	B	337	ARG
1	B	338	LEU
1	B	343	LYS
1	B	348	LYS
1	B	366	VAL
1	B	376	ARG
1	B	378	LEU
1	B	381	THR
1	B	387	THR
1	B	388	SER
1	B	418	LYS
1	B	423	VAL
1	B	426	LYS
1	B	428	ARG
1	B	450	ASP
1	B	455	ILE
1	B	458	LYS
1	B	459	ILE
1	B	469	SER
1	B	471	ARG
1	B	472	VAL
1	B	484	ASN
1	B	487	ILE
1	B	488	LEU
1	B	551	ILE

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Mol	Chain	Res	Type
1	B	556	ARG
1	B	568	LEU
1	B	576	VAL
1	B	590	THR
1	B	633	SER
1	B	634	ASN
1	B	635	MET
1	C	3	ARG
1	C	15	THR
1	C	19	ASN
1	C	34	ILE
1	C	35	THR
1	C	40	LYS
1	C	85	SER
1	C	86	ARG
1	C	103	VAL
1	C	111	VAL
1	C	119	LYS
1	C	122	LEU
1	C	126	VAL
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	285	LEU
1	C	289	LYS
1	C	337	ARG
1	C	338	LEU
1	C	343	LYS
1	C	344	VAL
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	381	THR
1	C	385	VAL
1	C	387	THR
1	C	388	SER
1	C	428	ARG
1	C	436	GLU
1	C	442	ILE
1	C	455	ILE
1	C	458	LYS
1	C	459	ILE
1	C	469	SER
1	C	471	ARG
1	C	472	VAL
1	C	484	ASN
1	C	487	ILE
1	C	488	LEU
1	C	513	TYR
1	C	514	THR
1	C	525	SER
1	C	537	MET
1	C	540	LEU
1	C	552	TYR
1	C	556	ARG
1	C	568	LEU
1	C	569	VAL
1	C	596	LEU
1	C	602	MET
1	C	624	GLU
1	C	625	LEU
1	C	634	ASN
1	C	635	MET
1	D	3	ARG
1	D	15	THR
1	D	19	ASN
1	D	34	ILE
1	D	35	THR
1	D	40	LYS
1	D	85	SER
1	D	86	ARG
1	D	103	VAL
1	D	111	VAL
1	D	119	LYS

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Mol	Chain	Res	Type
1	D	122	LEU
1	D	126	VAL
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
1	D	247	VAL
1	D	249	GLN
1	D	266	ILE
1	D	284	ASN
1	D	285	LEU
1	D	289	LYS
1	D	337	ARG
1	D	338	LEU
1	D	344	VAL
1	D	348	LYS
1	D	366	VAL
1	D	376	ARG
1	D	378	LEU
1	D	381	THR
1	D	385	VAL
1	D	387	THR
1	D	388	SER
1	D	428	ARG
1	D	436	GLU
1	D	442	ILE
1	D	455	ILE
1	D	458	LYS
1	D	459	ILE
1	D	469	SER
1	D	471	ARG
1	D	472	VAL
1	D	484	ASN
1	D	487	ILE
1	D	488	LEU
1	D	513	TYR
1	D	514	THR
1	D	525	SER

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Mol	Chain	Res	Type
1	D	537	MET
1	D	552	TYR
1	D	556	ARG
1	D	568	LEU
1	D	569	VAL
1	D	596	LEU
1	D	602	MET
1	D	624	GLU
1	D	625	LEU
1	D	634	ASN
1	D	635	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	HIS
1	A	19	ASN
1	A	38	GLN
1	A	78	HIS
1	A	133	ASN
1	A	156	HIS
1	A	168	HIS
1	A	239	HIS
1	A	300	HIS
1	A	302	HIS
1	A	362	ASN
1	A	484	ASN
1	A	500	HIS
1	A	567	GLN
1	A	634	ASN
1	B	7	ASN
1	B	8	HIS
1	B	38	GLN
1	B	78	HIS
1	B	133	ASN
1	B	168	HIS
1	B	239	HIS
1	B	300	HIS
1	B	362	ASN
1	B	484	ASN
1	B	500	HIS

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Mol	Chain	Res	Type
1	B	567	GLN
1	B	634	ASN
1	C	6	GLN
1	C	7	ASN
1	C	8	HIS
1	C	42	HIS
1	C	78	HIS
1	C	133	ASN
1	C	168	HIS
1	C	239	HIS
1	C	257	HIS
1	C	300	HIS
1	C	484	ASN
1	C	500	HIS
1	C	567	GLN
1	C	621	GLN
1	C	631	ASN
1	C	634	ASN
1	D	6	GLN
1	D	7	ASN
1	D	8	HIS
1	D	42	HIS
1	D	78	HIS
1	D	133	ASN
1	D	168	HIS
1	D	239	HIS
1	D	257	HIS
1	D	300	HIS
1	D	383	HIS
1	D	484	ASN
1	D	500	HIS
1	D	621	GLN
1	D	631	ASN
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	1.05	0
3	GLC	G	2	3	11,11,12	0.84	0	15,15,17	1.62	4 (26%)
3	GLC	G	3	3	11,11,12	1.36	1 (9%)	15,15,17	2.43	5 (33%)
3	GLC	G	4	3	11,11,12	1.16	1 (9%)	15,15,17	1.93	4 (26%)
3	GLC	H	1	3	12,12,12	1.09	1 (8%)	17,17,17	1.64	3 (17%)
3	GLC	H	2	3	11,11,12	0.79	0	15,15,17	1.75	5 (33%)
3	GLC	H	3	3	11,11,12	0.91	0	15,15,17	1.66	3 (20%)
3	GLC	H	4	3	11,11,12	0.82	0	15,15,17	1.66	4 (26%)
3	GLC	I	1	3	12,12,12	0.78	0	17,17,17	1.16	1 (5%)
3	GLC	I	2	3	11,11,12	0.82	1 (9%)	15,15,17	1.39	2 (13%)
3	GLC	I	3	3	11,11,12	0.81	0	15,15,17	2.01	5 (33%)
3	GLC	I	4	3	11,11,12	0.90	0	15,15,17	1.66	3 (20%)
3	GLC	J	1	3	12,12,12	0.84	0	17,17,17	1.32	1 (5%)
3	GLC	J	2	3	11,11,12	0.90	0	15,15,17	1.46	2 (13%)
3	GLC	J	3	3	11,11,12	1.17	1 (9%)	15,15,17	1.95	5 (33%)
3	GLC	J	4	3	11,11,12	0.81	0	15,15,17	1.68	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	GLC	C4-C5	2.97	1.59	1.53
3	G	4	GLC	O5-C1	2.95	1.48	1.43
3	H	1	GLC	O4-C4	2.41	1.48	1.43
3	J	3	GLC	O5-C1	2.09	1.47	1.43
3	I	2	GLC	O5-C5	2.01	1.47	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	GLC	O4-C4-C5	6.25	124.71	109.32
3	I	3	GLC	O4-C4-C5	5.05	121.75	109.32
3	G	4	GLC	C6-C5-C4	-4.44	102.12	113.02
3	H	4	GLC	C1-O5-C5	-4.24	106.50	112.19
3	J	2	GLC	O4-C4-C5	3.91	118.95	109.32
3	G	3	GLC	O4-C4-C3	-3.75	101.54	110.38
3	H	3	GLC	O5-C5-C6	3.71	114.89	107.66
3	J	3	GLC	C1-C2-C3	3.64	114.94	109.64
3	H	2	GLC	O4-C4-C5	3.61	118.21	109.32
3	J	3	GLC	O4-C4-C5	3.51	117.96	109.32
3	J	3	GLC	C2-C3-C4	-3.45	104.80	110.86
3	I	2	GLC	C3-C4-C5	-3.29	104.27	110.23
3	G	4	GLC	C2-C3-C4	-3.29	105.08	110.86
3	I	4	GLC	C2-C3-C4	-3.27	105.11	110.86
3	H	1	GLC	O4-C4-C5	3.27	117.37	109.32
3	I	4	GLC	O5-C5-C6	-3.17	101.49	107.66
3	H	1	GLC	O5-C5-C6	3.08	114.07	106.44
3	J	3	GLC	O4-C4-C3	-3.07	103.14	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	GLC	O4-C4-C3	-3.03	103.23	110.38
3	J	4	GLC	C1-O5-C5	3.02	116.24	112.19
3	G	3	GLC	O3-C3-C4	-3.01	103.28	110.38
3	H	3	GLC	O4-C4-C3	-3.01	103.29	110.38
3	G	3	GLC	O5-C5-C6	2.90	113.31	107.66
3	I	2	GLC	O4-C4-C5	2.88	116.42	109.32
3	G	2	GLC	O5-C5-C6	2.88	113.27	107.66
3	G	2	GLC	O4-C4-C5	2.85	116.34	109.32
3	H	2	GLC	C1-C2-C3	2.73	113.62	109.64
3	G	3	GLC	O5-C1-C2	-2.68	104.39	110.79
3	I	3	GLC	C1-C2-C3	2.68	113.55	109.64
3	G	4	GLC	O2-C2-C1	-2.65	103.15	109.22
3	G	2	GLC	C6-C5-C4	-2.63	106.57	113.02
3	J	2	GLC	O4-C4-C3	-2.58	104.28	110.38
3	H	2	GLC	O5-C1-C2	-2.58	104.63	110.79
3	H	2	GLC	O4-C4-C3	-2.55	104.37	110.38
3	H	3	GLC	C2-C3-C4	-2.47	106.51	110.86
3	I	3	GLC	O5-C1-C2	-2.46	104.92	110.79
3	I	1	GLC	C6-C5-C4	-2.45	107.01	113.02
3	J	4	GLC	C1-C2-C3	2.39	113.13	109.64
3	I	3	GLC	O5-C5-C6	2.38	112.29	107.66
3	G	2	GLC	C3-C4-C5	-2.31	106.04	110.23
3	I	4	GLC	C6-C5-C4	-2.27	107.43	113.02
3	G	4	GLC	O5-C5-C6	-2.27	103.25	107.66
3	H	1	GLC	O1-C1-C2	2.26	115.55	108.98
3	H	4	GLC	C3-C4-C5	-2.22	106.21	110.23
3	H	4	GLC	C2-C3-C4	-2.15	107.07	110.86
3	H	4	GLC	O5-C5-C4	2.15	116.06	110.83
3	J	3	GLC	O5-C1-C2	-2.12	105.74	110.79
3	H	2	GLC	C2-C3-C4	-2.05	107.26	110.86
3	J	1	GLC	O5-C5-C6	2.02	111.44	106.44

There are no chirality outliers.

All (3) torsion outliers are listed below:

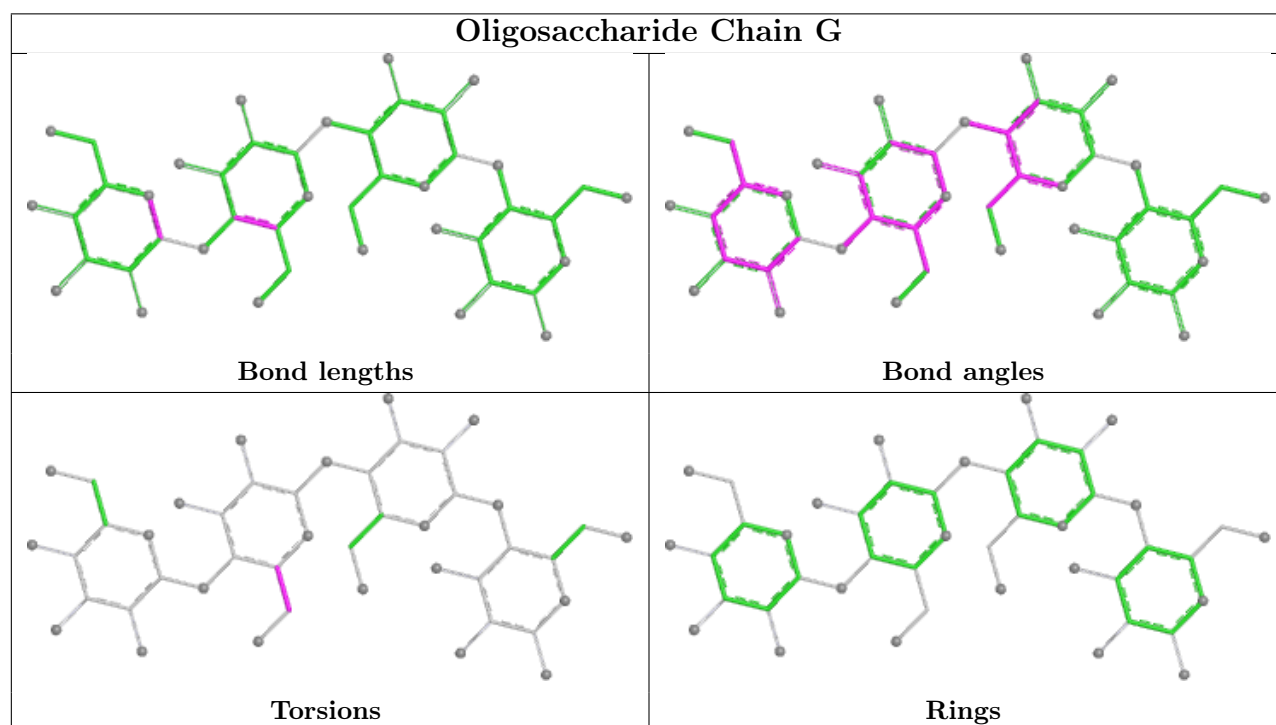
Mol	Chain	Res	Type	Atoms
3	H	4	GLC	O5-C5-C6-O6
3	G	3	GLC	O5-C5-C6-O6
3	H	4	GLC	C4-C5-C6-O6

There are no ring outliers.

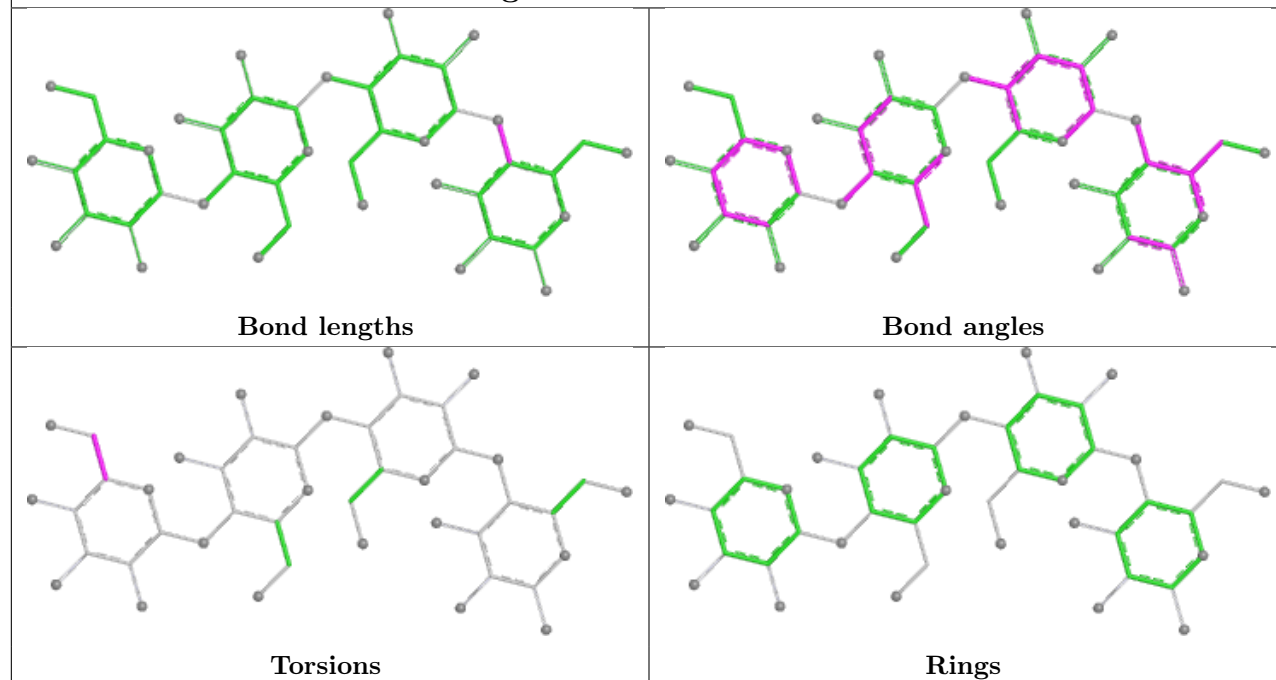
6 monomers are involved in 5 short contacts:

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

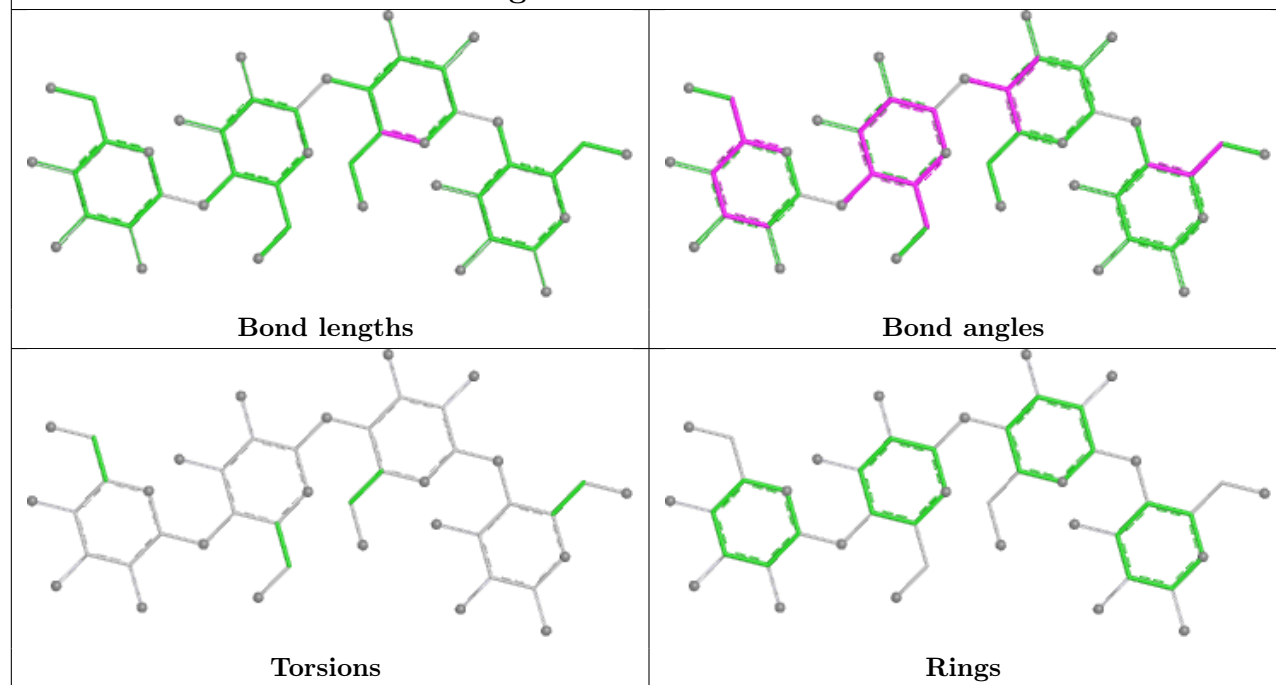
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

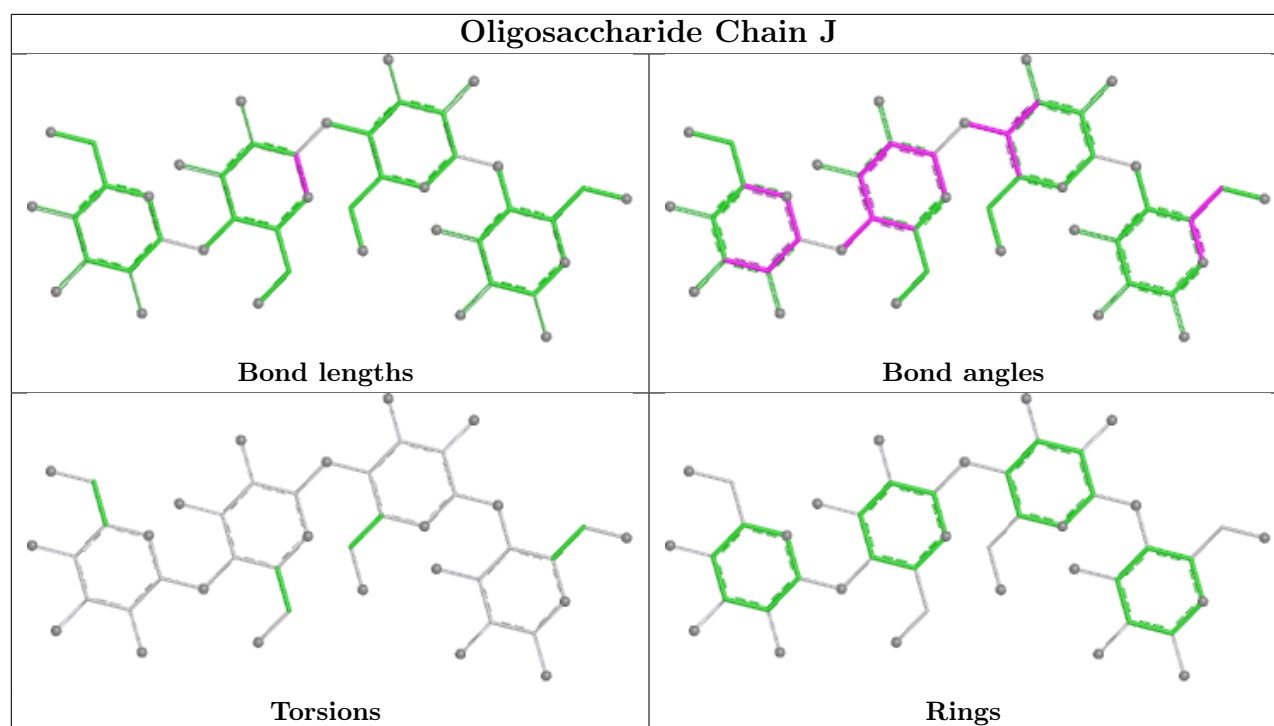


Oligosaccharide Chain H



Oligosaccharide Chain I





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	C	803	-	4,4,4	0.30	0	6,6,6	0.18	0
4	SO4	B	706	-	4,4,4	0.31	0	6,6,6	0.23	0
4	SO4	D	801	-	4,4,4	0.43	0	6,6,6	0.38	0
4	SO4	C	706	-	4,4,4	0.29	0	6,6,6	0.26	0
4	SO4	D	802	-	4,4,4	0.26	0	6,6,6	0.23	0
4	SO4	D	803	-	4,4,4	0.28	0	6,6,6	0.17	0
4	SO4	A	804	-	4,4,4	0.26	0	6,6,6	0.16	0
4	SO4	D	804	-	4,4,4	0.24	0	6,6,6	0.25	0
4	SO4	B	802	-	4,4,4	0.44	0	6,6,6	0.29	0
4	SO4	C	801	-	4,4,4	0.31	0	6,6,6	0.09	0
4	SO4	A	803	-	4,4,4	0.30	0	6,6,6	0.23	0
4	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	C	804	-	4,4,4	0.24	0	6,6,6	0.22	0
4	SO4	A	802	-	4,4,4	0.34	0	6,6,6	0.36	0
4	SO4	A	801	-	4,4,4	0.27	0	6,6,6	0.07	0
4	SO4	B	801	-	4,4,4	0.28	0	6,6,6	0.28	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	D	802	SO4	1	0
4	C	801	SO4	1	0
4	A	801	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.15	7 (1%)	78 57	56, 79, 114, 153	0
1	B	611/725 (84%)	-0.19	4 (0%)	84 66	57, 80, 114, 154	0
1	C	613/725 (84%)	-0.22	4 (0%)	84 66	50, 78, 106, 133	0
1	D	613/725 (84%)	-0.25	5 (0%)	82 64	50, 77, 106, 133	0
2	E	0/5	-	-	-	-	-
2	F	0/5	-	-	-	-	-
All	All	2448/2910 (84%)	-0.20	20 (0%)	82 64	50, 78, 111, 154	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	546	ALA	4.7
1	C	205	GLY	4.7
1	C	546	ALA	4.7
1	D	205	GLY	3.4
1	B	546	ALA	3.3
1	A	546	ALA	3.0
1	B	639	ALA	2.7
1	C	549	TYR	2.5
1	C	277	GLN	2.4
1	B	638	LEU	2.3
1	B	125	LEU	2.3
1	D	549	TYR	2.2
1	A	548	ASP	2.2
1	D	548	ASP	2.2
1	A	636	ASP	2.2
1	A	125	LEU	2.2
1	A	179	CYS	2.2
1	A	205	GLY	2.1
1	A	131	PRO	2.1
1	D	563	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

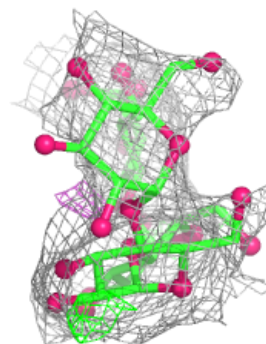
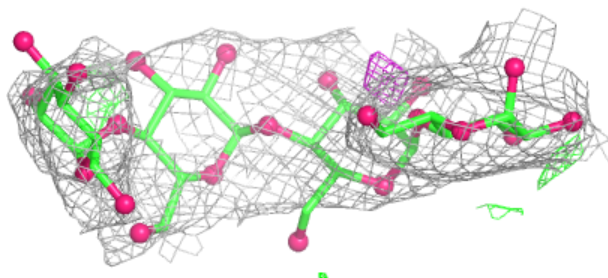
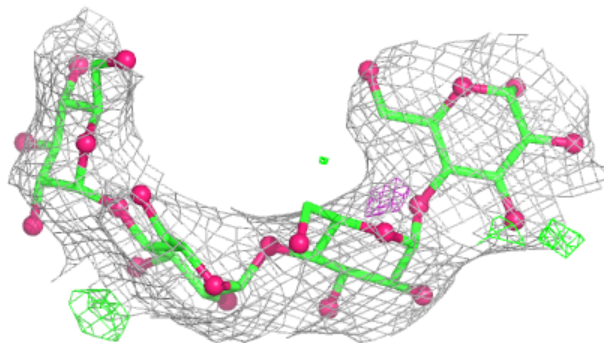
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	J	4	11/12	0.53	0.17	123,130,136,140	0
3	GLC	G	4	11/12	0.54	0.12	127,138,144,144	0
3	GLC	I	4	11/12	0.64	0.12	119,124,127,131	0
3	GLC	H	4	11/12	0.70	0.12	98,110,116,123	0
3	GLC	J	3	11/12	0.72	0.17	99,114,129,131	0
3	GLC	I	1	12/12	0.76	0.10	92,95,100,110	0
3	GLC	G	1	12/12	0.78	0.10	89,95,100,100	0
3	GLC	G	3	11/12	0.79	0.11	105,117,130,131	0
3	GLC	J	1	12/12	0.79	0.13	91,108,114,118	0
3	GLC	I	3	11/12	0.82	0.10	96,106,116,117	0
3	GLC	H	1	12/12	0.83	0.13	82,95,103,106	0
3	GLC	H	3	11/12	0.84	0.11	84,89,108,112	0
3	GLC	J	2	11/12	0.86	0.15	90,93,105,112	0
3	GLC	H	2	11/12	0.91	0.11	80,86,92,92	0
3	GLC	I	2	11/12	0.91	0.13	89,96,104,112	0
3	GLC	G	2	11/12	0.92	0.11	95,100,108,112	0

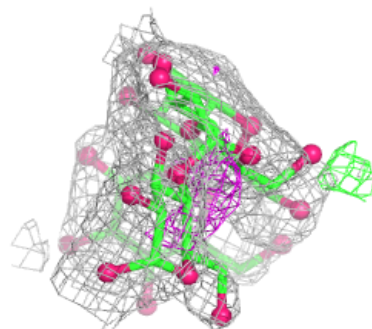
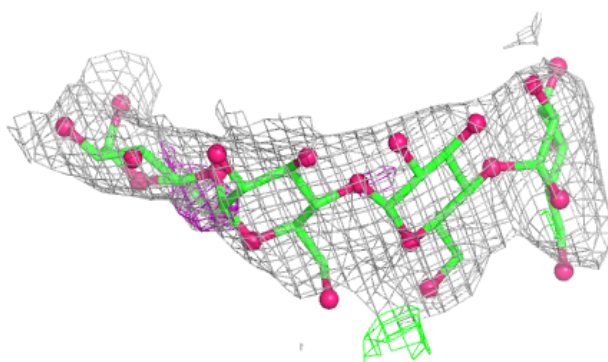
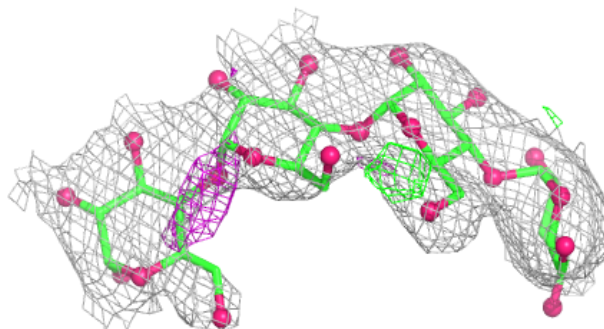
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

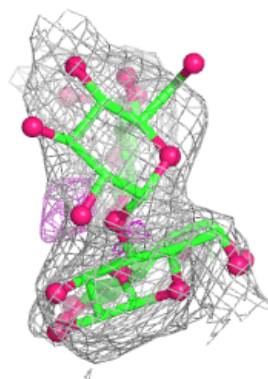
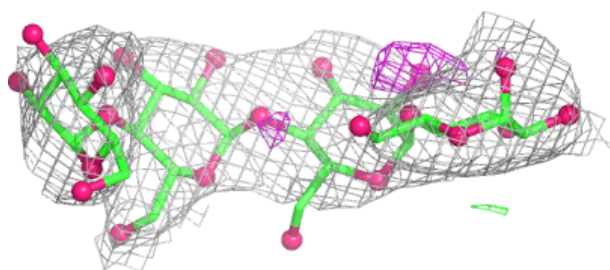
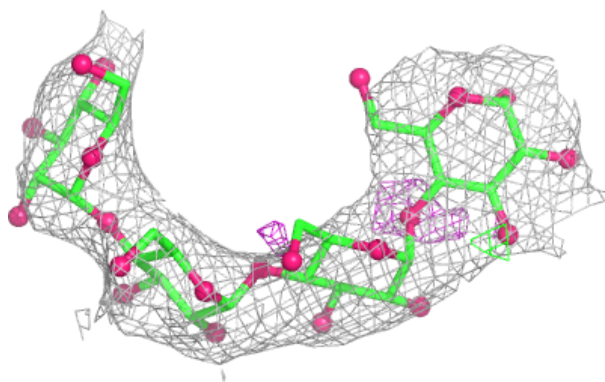
**Electron density around Chain H:**

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

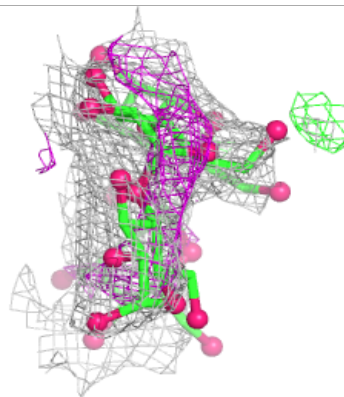
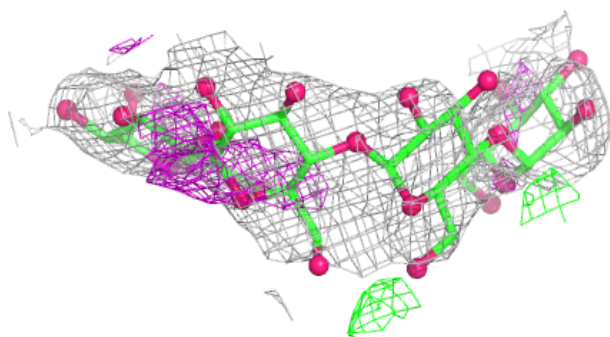
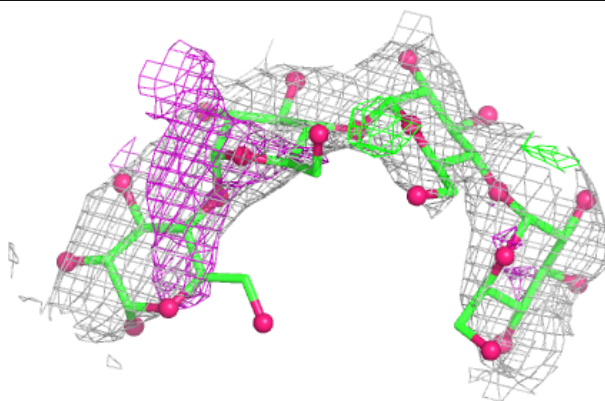


Electron density around Chain I:

$2mF_o-DF_c$ (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

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	0.62	0.15	95,97,124,140	0
4	SO4	C	804	5/5	0.66	0.19	126,128,131,133	0
4	SO4	A	804	5/5	0.72	0.14	122,133,134,143	0
4	SO4	D	804	5/5	0.72	0.16	121,122,126,138	0
4	SO4	D	803	5/5	0.73	0.22	109,116,122,132	0
4	SO4	B	802	5/5	0.75	0.15	84,95,108,127	0
4	SO4	C	803	5/5	0.75	0.20	105,118,128,139	0
4	SO4	C	706	5/5	0.76	0.14	103,106,122,136	0
4	SO4	B	804	5/5	0.78	0.07	129,130,133,146	0
4	SO4	A	802	5/5	0.84	0.12	77,83,98,116	0
4	SO4	A	803	5/5	0.85	0.17	93,99,118,120	0
4	SO4	B	706	5/5	0.86	0.15	96,107,112,125	0
4	SO4	D	802	5/5	0.87	0.21	89,93,109,112	0
4	SO4	C	801	5/5	0.88	0.18	90,90,110,114	0
4	SO4	A	801	5/5	0.89	0.16	83,90,100,102	0
4	SO4	B	801	5/5	0.92	0.13	87,89,108,114	0

6.5 Other polymers

There are no such residues in this entry.