



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 PM UTC

PDB ID : 3LPO / pdb_00003lpo
Title : Crystal structure of the N-terminal domain of sucrase-isomaltase
Authors : Sim, L.; Rose, D.R.
Deposited on : 2010-02-05
Resolution : 3.20 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

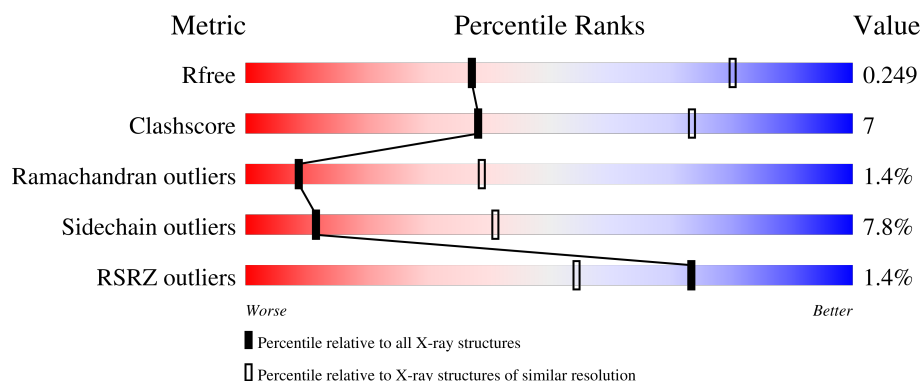
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



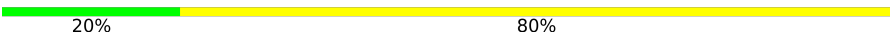
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	898	2% 79% 15% ...
1	B	898	2% 78% 16% ..
1	C	898	% 79% 15% ..
1	D	898	% 79% 14% ..
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	2	 50% 50%
3	F	5	 20% 80%
3	H	5	 80% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	2001	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27668 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 Sucrase-isomaltase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	870	Total	C	N	O	S	0	0	0
			6853	4402	1146	1276	29			
1	B	870	Total	C	N	O	S	0	0	0
			6784	4353	1138	1264	29			
1	C	870	Total	C	N	O	S	0	0	0
			6904	4429	1157	1290	28			
1	D	870	Total	C	N	O	S	0	0	0
			6879	4414	1153	1283	29			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	UNP P14410
A	2	SER	-	expression tag	UNP P14410
A	3	SER	-	expression tag	UNP P14410
A	4	HIS	-	expression tag	UNP P14410
A	5	HIS	-	expression tag	UNP P14410
A	6	HIS	-	expression tag	UNP P14410
A	7	HIS	-	expression tag	UNP P14410
A	8	HIS	-	expression tag	UNP P14410
A	9	HIS	-	expression tag	UNP P14410
A	10	GLY	-	expression tag	UNP P14410
A	11	GLU	-	expression tag	UNP P14410
A	12	PHE	-	expression tag	UNP P14410
A	13	ASP	-	expression tag	UNP P14410
A	14	ILE	-	expression tag	UNP P14410
A	15	PRO	-	expression tag	UNP P14410
A	16	THR	-	expression tag	UNP P14410
A	17	THR	-	expression tag	UNP P14410
A	18	GLU	-	expression tag	UNP P14410
A	19	ASN	-	expression tag	UNP P14410
A	20	LEU	-	expression tag	UNP P14410
A	21	TYR	-	expression tag	UNP P14410

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	PHE	-	expression tag	UNP P14410
A	23	GLN	-	expression tag	UNP P14410
A	24	SER	-	expression tag	UNP P14410
A	25	GLY	-	expression tag	UNP P14410
A	26	ILE	-	expression tag	UNP P14410
A	27	ARG	-	expression tag	UNP P14410
A	28	ARG	-	expression tag	UNP P14410
B	1	ARG	-	expression tag	UNP P14410
B	2	SER	-	expression tag	UNP P14410
B	3	SER	-	expression tag	UNP P14410
B	4	HIS	-	expression tag	UNP P14410
B	5	HIS	-	expression tag	UNP P14410
B	6	HIS	-	expression tag	UNP P14410
B	7	HIS	-	expression tag	UNP P14410
B	8	HIS	-	expression tag	UNP P14410
B	9	HIS	-	expression tag	UNP P14410
B	10	GLY	-	expression tag	UNP P14410
B	11	GLU	-	expression tag	UNP P14410
B	12	PHE	-	expression tag	UNP P14410
B	13	ASP	-	expression tag	UNP P14410
B	14	ILE	-	expression tag	UNP P14410
B	15	PRO	-	expression tag	UNP P14410
B	16	THR	-	expression tag	UNP P14410
B	17	THR	-	expression tag	UNP P14410
B	18	GLU	-	expression tag	UNP P14410
B	19	ASN	-	expression tag	UNP P14410
B	20	LEU	-	expression tag	UNP P14410
B	21	TYR	-	expression tag	UNP P14410
B	22	PHE	-	expression tag	UNP P14410
B	23	GLN	-	expression tag	UNP P14410
B	24	SER	-	expression tag	UNP P14410
B	25	GLY	-	expression tag	UNP P14410
B	26	ILE	-	expression tag	UNP P14410
B	27	ARG	-	expression tag	UNP P14410
B	28	ARG	-	expression tag	UNP P14410
C	1	ARG	-	expression tag	UNP P14410
C	2	SER	-	expression tag	UNP P14410
C	3	SER	-	expression tag	UNP P14410
C	4	HIS	-	expression tag	UNP P14410
C	5	HIS	-	expression tag	UNP P14410
C	6	HIS	-	expression tag	UNP P14410
C	7	HIS	-	expression tag	UNP P14410

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	HIS	-	expression tag	UNP P14410
C	9	HIS	-	expression tag	UNP P14410
C	10	GLY	-	expression tag	UNP P14410
C	11	GLU	-	expression tag	UNP P14410
C	12	PHE	-	expression tag	UNP P14410
C	13	ASP	-	expression tag	UNP P14410
C	14	ILE	-	expression tag	UNP P14410
C	15	PRO	-	expression tag	UNP P14410
C	16	THR	-	expression tag	UNP P14410
C	17	THR	-	expression tag	UNP P14410
C	18	GLU	-	expression tag	UNP P14410
C	19	ASN	-	expression tag	UNP P14410
C	20	LEU	-	expression tag	UNP P14410
C	21	TYR	-	expression tag	UNP P14410
C	22	PHE	-	expression tag	UNP P14410
C	23	GLN	-	expression tag	UNP P14410
C	24	SER	-	expression tag	UNP P14410
C	25	GLY	-	expression tag	UNP P14410
C	26	ILE	-	expression tag	UNP P14410
C	27	ARG	-	expression tag	UNP P14410
C	28	ARG	-	expression tag	UNP P14410
D	1	ARG	-	expression tag	UNP P14410
D	2	SER	-	expression tag	UNP P14410
D	3	SER	-	expression tag	UNP P14410
D	4	HIS	-	expression tag	UNP P14410
D	5	HIS	-	expression tag	UNP P14410
D	6	HIS	-	expression tag	UNP P14410
D	7	HIS	-	expression tag	UNP P14410
D	8	HIS	-	expression tag	UNP P14410
D	9	HIS	-	expression tag	UNP P14410
D	10	GLY	-	expression tag	UNP P14410
D	11	GLU	-	expression tag	UNP P14410
D	12	PHE	-	expression tag	UNP P14410
D	13	ASP	-	expression tag	UNP P14410
D	14	ILE	-	expression tag	UNP P14410
D	15	PRO	-	expression tag	UNP P14410
D	16	THR	-	expression tag	UNP P14410
D	17	THR	-	expression tag	UNP P14410
D	18	GLU	-	expression tag	UNP P14410
D	19	ASN	-	expression tag	UNP P14410
D	20	LEU	-	expression tag	UNP P14410
D	21	TYR	-	expression tag	UNP P14410

Continued on next page...

Continued from previous page...

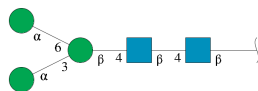
Chain	Residue	Modelled	Actual	Comment	Reference
D	22	PHE	-	expression tag	UNP P14410
D	23	GLN	-	expression tag	UNP P14410
D	24	SER	-	expression tag	UNP P14410
D	25	GLY	-	expression tag	UNP P14410
D	26	ILE	-	expression tag	UNP P14410
D	27	ARG	-	expression tag	UNP P14410
D	28	ARG	-	expression tag	UNP P14410

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



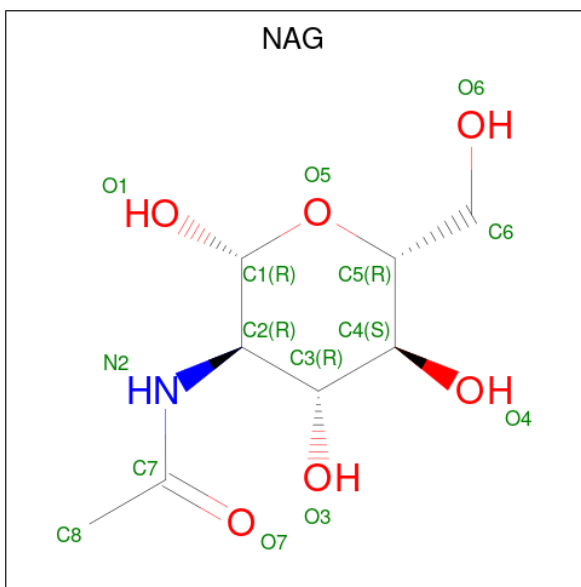
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

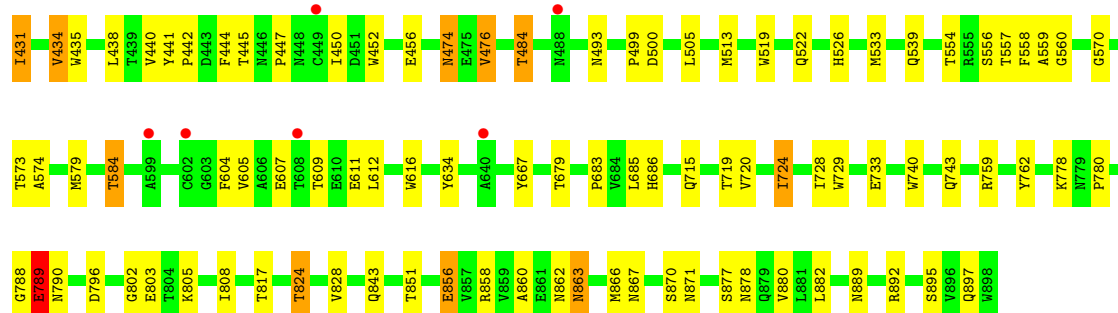
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



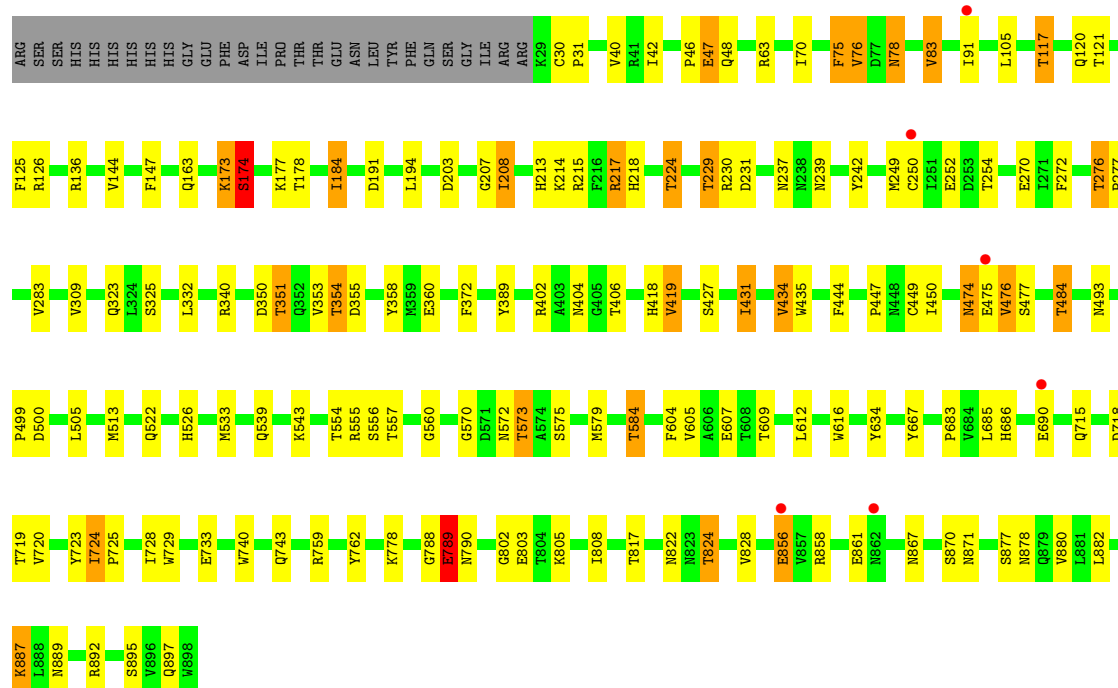
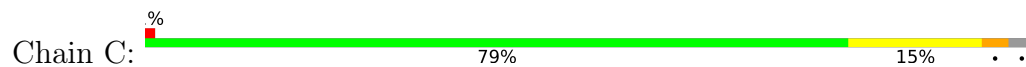
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 1: Sucrase-isomaltase

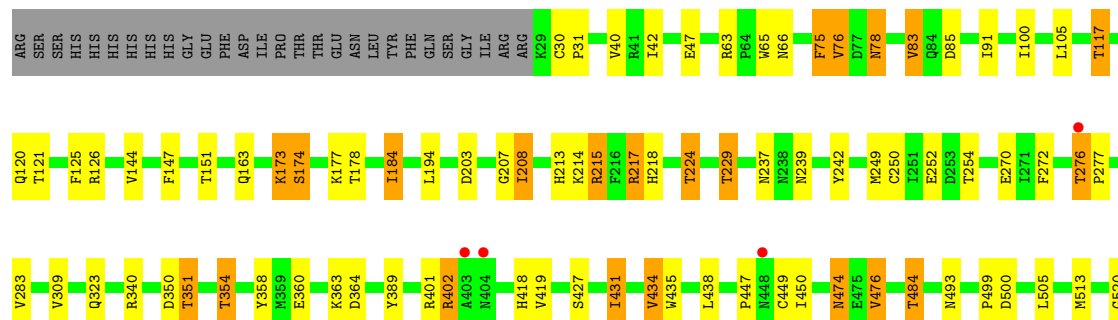
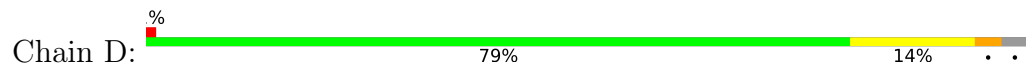


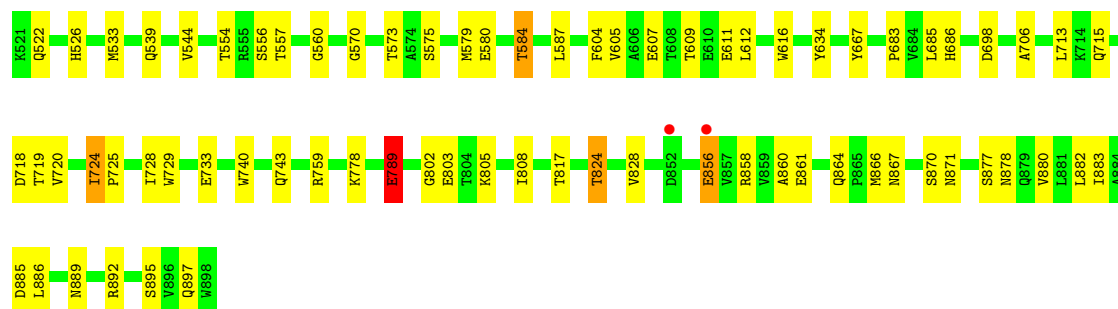


• Molecule 1: Sucrase-isomaltase



• Molecule 1: Sucrase-isomaltase





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

Chain E: 100%

NAG1
NAG2

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

Chain G: 50% 50%

NAG1
NAG2

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

Chain F: 20% 80%

NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain H: 80% 20%

NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.34Å 172.59Å 343.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.83 – 3.20 45.83 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.83-3.20) 99.6 (45.83-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.251 0.224 , 0.249	Depositor DCC
R_{free} test set	3802 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.2	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	0.89	EDS
Total number of atoms	27668	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: MAN, BMA, NAG

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	0.66	0/7054	0.89	5/9644 (0.1%)
1	B	0.68	0/6980	0.88	1/9545 (0.0%)
1	C	0.63	0/7105	0.87	4/9707 (0.0%)
1	D	0.63	0/7080	0.88	7/9675 (0.1%)
All	All	0.65	0/28219	0.88	17/38571 (0.0%)

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

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

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	474	ASN	N-CA-C	6.72	118.60	111.28
1	D	474	ASN	N-CA-C	6.29	118.94	111.71
1	C	718	ASP	N-CA-C	-5.97	106.61	114.31
1	C	474	ASN	N-CA-C	5.96	118.56	111.71
1	A	276	THR	N-CA-CB	5.93	120.92	110.37
1	A	474	ASN	N-CA-C	5.91	118.48	111.33
1	D	718	ASP	N-CA-C	-5.70	106.67	113.97
1	A	159	VAL	N-CA-C	5.58	114.77	106.85
1	D	520	GLY	N-CA-C	5.48	118.16	110.38
1	D	100	ILE	N-CA-C	-5.46	103.00	108.96
1	C	723	TYR	CA-C-N	-5.43	117.37	123.02
1	C	723	TYR	C-N-CA	-5.43	117.37	123.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	TYR	N-CA-C	-5.36	106.69	113.18
1	D	65	TRP	N-CA-C	5.21	117.10	109.24
1	D	544	VAL	N-CA-C	5.13	115.35	110.53
1	A	565	ALA	N-CA-C	5.11	116.57	108.96
1	D	706	ALA	N-CA-C	5.00	119.51	113.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	475	GLU	Peptide

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	6853	0	6381	93	0
1	B	6784	0	6276	95	0
1	C	6904	0	6474	93	0
1	D	6879	0	6424	89	0
2	E	28	0	25	0	0
2	G	28	0	25	1	0
3	F	61	0	52	0	0
3	H	61	0	52	4	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	28	0	26	1	0
All	All	27668	0	25774	368	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 7.

All (368) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PRO:O	1:B:276:THR:HG22	1.29	1.32
1:B:860:ALA:HB2	1:B:866:MET:HG3	1.40	1.03
1:A:522:GLN:HE21	1:A:526:HIS:HD2	1.16	0.93
1:C:822:ASN:HD21	3:H:1:NAG:H2	1.33	0.92
1:B:474:ASN:HB3	1:B:556:SER:HB3	1.50	0.92
1:A:402:ARG:HH11	1:A:402:ARG:CG	1.82	0.91
1:D:323:GLN:HG2	1:D:351:THR:HG23	1.53	0.91
1:C:522:GLN:HE21	1:C:526:HIS:HD2	1.18	0.90
1:A:402:ARG:HH11	1:A:402:ARG:HG2	1.34	0.89
1:D:522:GLN:HE21	1:D:526:HIS:HD2	1.16	0.88
1:C:474:ASN:HB3	1:C:556:SER:HB3	1.57	0.87
1:B:522:GLN:HE21	1:B:526:HIS:HD2	1.21	0.86
1:B:275:PRO:O	1:B:276:THR:CG2	2.21	0.85
1:A:474:ASN:HB3	1:A:556:SER:HB3	1.58	0.85
1:C:323:GLN:HG2	1:C:351:THR:HG23	1.57	0.85
1:A:323:GLN:HG2	1:A:351:THR:HG23	1.56	0.85
1:D:474:ASN:HB3	1:D:556:SER:HB3	1.58	0.85
1:B:48:GLN:HG3	1:C:48:GLN:HG3	1.58	0.83
1:B:323:GLN:HG2	1:B:351:THR:HG23	1.60	0.82
1:A:522:GLN:NE2	1:A:526:HIS:HD2	1.80	0.80
1:D:860:ALA:HB2	1:D:866:MET:CG	2.13	0.79
1:C:522:GLN:HE21	1:C:526:HIS:CD2	2.02	0.78
1:C:522:GLN:NE2	1:C:526:HIS:HD2	1.82	0.78
1:A:522:GLN:HE21	1:A:526:HIS:CD2	2.02	0.77
1:B:276:THR:HG21	1:B:278:ILE:HD12	1.67	0.77
1:B:522:GLN:HE21	1:B:526:HIS:CD2	2.03	0.76
1:B:237:ASN:HD22	1:B:239:ASN:H	1.31	0.76
1:D:224:THR:HG23	1:D:272:PHE:HD1	1.51	0.75
1:D:522:GLN:HE21	1:D:526:HIS:CD2	2.02	0.75
1:B:224:THR:HG23	1:B:272:PHE:HD1	1.50	0.75
1:C:237:ASN:HD22	1:C:239:ASN:H	1.35	0.75
1:B:117:THR:HG23	1:B:125:PHE:HE1	1.51	0.75
1:D:522:GLN:NE2	1:D:526:HIS:HD2	1.83	0.74
1:A:237:ASN:HD22	1:A:239:ASN:H	1.36	0.73
1:D:117:THR:HG23	1:D:125:PHE:HE1	1.53	0.73
1:D:237:ASN:HD22	1:D:239:ASN:H	1.36	0.73
1:C:117:THR:HG23	1:C:125:PHE:HE1	1.53	0.72
1:A:117:THR:HG23	1:A:125:PHE:HE1	1.52	0.72
1:A:224:THR:HG23	1:A:272:PHE:HD1	1.54	0.71
1:B:522:GLN:NE2	1:B:526:HIS:HD2	1.87	0.71
1:D:860:ALA:HB2	1:D:866:MET:HG3	1.72	0.71
1:C:224:THR:HG23	1:C:272:PHE:HD1	1.54	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:THR:HG21	1:B:389:TYR:OH	1.92	0.70
1:A:402:ARG:HG2	1:A:402:ARG:NH1	1.98	0.69
1:C:229:THR:HG22	1:C:526:HIS:CE1	2.28	0.68
1:B:824:THR:HB	1:B:897:GLN:HG2	1.75	0.68
1:A:474:ASN:C	1:A:476:VAL:H	2.00	0.67
1:C:887:LYS:HB2	1:C:887:LYS:NZ	2.09	0.67
1:C:824:THR:HB	1:C:897:GLN:HG2	1.77	0.66
1:A:474:ASN:ND2	1:A:554:THR:OG1	2.28	0.66
1:A:856:GLU:HG2	1:A:858:ARG:NH1	2.10	0.66
1:C:475:GLU:CD	1:C:475:GLU:H	2.04	0.66
1:C:889:ASN:HB2	1:C:892:ARG:HH21	1.60	0.66
1:C:822:ASN:ND2	3:H:1:NAG:H2	2.10	0.66
1:A:354:THR:HG21	1:A:389:TYR:OH	1.95	0.65
1:D:434:VAL:HG12	1:D:435:TRP:H	1.62	0.65
1:B:474:ASN:ND2	1:B:554:THR:OG1	2.29	0.65
1:A:824:THR:HB	1:A:897:GLN:HG2	1.76	0.65
1:B:275:PRO:C	1:B:276:THR:HG22	2.18	0.65
1:A:459:ILE:HG12	1:B:111:ASN:ND2	2.12	0.65
1:D:76:VAL:H	1:D:78:ASN:ND2	1.95	0.65
1:C:474:ASN:C	1:C:476:VAL:H	2.04	0.64
1:C:207:GLY:O	1:C:218:HIS:HE1	1.80	0.64
1:B:889:ASN:HB2	1:B:892:ARG:HH21	1.63	0.64
1:A:889:ASN:HB2	1:A:892:ARG:HH21	1.62	0.64
1:B:229:THR:HG22	1:B:526:HIS:CE1	2.32	0.64
1:C:856:GLU:HG2	1:C:858:ARG:NH1	2.13	0.64
1:B:860:ALA:CB	1:B:866:MET:HG3	2.23	0.63
1:C:177:LYS:HE3	1:C:252:GLU:HB3	1.79	0.63
1:A:207:GLY:O	1:A:218:HIS:HE1	1.82	0.63
1:D:824:THR:HB	1:D:897:GLN:HG2	1.81	0.63
1:D:860:ALA:HB2	1:D:866:MET:HG2	1.79	0.63
1:B:177:LYS:HE3	1:B:252:GLU:HB3	1.80	0.63
1:D:856:GLU:HG2	1:D:858:ARG:NH1	2.14	0.63
1:C:354:THR:HG21	1:C:389:TYR:OH	2.00	0.62
1:D:740:TRP:HA	1:D:743:GLN:NE2	2.13	0.62
1:D:354:THR:HG21	1:D:389:TYR:OH	1.99	0.62
1:D:474:ASN:C	1:D:476:VAL:H	2.07	0.62
1:C:740:TRP:HA	1:C:743:GLN:NE2	2.14	0.61
1:C:203:ASP:O	1:C:217:ARG:NH1	2.33	0.61
1:B:856:GLU:HG2	1:B:858:ARG:NH1	2.15	0.61
1:C:493:ASN:HD21	1:C:513:MET:H	1.47	0.60
1:A:860:ALA:HB2	1:A:866:MET:HG2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:889:ASN:HB2	1:D:892:ARG:HH21	1.65	0.60
1:B:474:ASN:C	1:B:476:VAL:H	2.10	0.60
1:D:203:ASP:O	1:D:217:ARG:NH1	2.34	0.60
1:A:740:TRP:HA	1:A:743:GLN:NE2	2.17	0.60
1:B:434:VAL:HG12	1:B:435:TRP:H	1.67	0.60
1:B:740:TRP:HA	1:B:743:GLN:NE2	2.17	0.59
1:D:207:GLY:O	1:D:218:HIS:HE1	1.84	0.59
1:C:360:GLU:OE1	1:C:402:ARG:NH2	2.31	0.59
1:A:142:GLN:HA	1:A:142:GLN:NE2	2.18	0.59
1:A:493:ASN:HD21	1:A:513:MET:H	1.51	0.58
1:C:214:LYS:O	1:C:584:THR:HG21	2.03	0.58
1:B:207:GLY:O	1:B:218:HIS:HE1	1.86	0.58
1:D:208:ILE:O	1:D:213:HIS:HE1	1.87	0.58
1:A:208:ILE:O	1:A:213:HIS:HE1	1.86	0.58
1:D:177:LYS:HE3	1:D:252:GLU:HB3	1.86	0.58
1:A:177:LYS:HE3	1:A:252:GLU:HB3	1.85	0.58
1:A:203:ASP:O	1:A:217:ARG:NH1	2.36	0.58
1:D:419:VAL:HG13	1:D:449:CYS:HA	1.84	0.58
1:B:208:ILE:O	1:B:213:HIS:HE1	1.86	0.57
1:D:214:LYS:O	1:D:584:THR:HG21	2.04	0.56
1:D:724:ILE:HG12	1:D:740:TRP:HB3	1.86	0.56
1:A:579:MET:HE3	1:A:612:LEU:HD12	1.86	0.56
1:C:117:THR:HG23	1:C:125:PHE:CE1	2.40	0.56
1:D:474:ASN:ND2	1:D:554:THR:OG1	2.39	0.56
1:D:229:THR:HG22	1:D:526:HIS:CE1	2.41	0.56
1:A:434:VAL:HG12	1:A:435:TRP:H	1.71	0.56
1:A:672:LYS:HE3	1:A:796:ASP:OD1	2.05	0.56
1:B:724:ILE:HG12	1:B:740:TRP:HB3	1.88	0.56
1:C:729:TRP:CZ3	1:C:759:ARG:HB2	2.41	0.56
1:C:822:ASN:HD21	3:H:1:NAG:C2	2.10	0.56
1:B:203:ASP:O	1:B:217:ARG:NH1	2.40	0.55
1:D:434:VAL:HG12	1:D:435:TRP:N	2.21	0.55
1:C:208:ILE:O	1:C:213:HIS:HE1	1.89	0.55
1:D:493:ASN:HD21	1:D:513:MET:H	1.53	0.55
1:C:431:ILE:HB	1:C:484:THR:HB	1.89	0.55
1:D:419:VAL:HG12	1:D:449:CYS:SG	2.47	0.55
1:A:724:ILE:HG12	1:A:740:TRP:HB3	1.88	0.55
1:B:683:PRO:HG2	1:B:686:HIS:CD2	2.42	0.55
1:B:276:THR:HG21	1:B:278:ILE:CD1	2.37	0.54
1:C:360:GLU:CD	1:C:402:ARG:HH21	2.16	0.54
1:A:91:ILE:HG23	1:A:147:PHE:HE2	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:PRO:HG2	1:C:686:HIS:CD2	2.43	0.54
1:D:83:VAL:HG13	1:D:163:GLN:HA	1.90	0.54
1:D:418:HIS:CD2	4:D:3001:NAG:H62	2.43	0.53
1:A:214:LYS:O	1:A:584:THR:HG21	2.08	0.53
1:A:229:THR:HG22	1:A:526:HIS:CE1	2.43	0.53
1:C:419:VAL:HG13	1:C:449:CYS:SG	2.49	0.53
1:A:30:CYS:HB3	1:A:63:ARG:NH2	2.24	0.53
1:C:474:ASN:ND2	1:C:554:THR:OG1	2.41	0.53
1:B:860:ALA:HB2	1:B:866:MET:CG	2.28	0.52
1:B:83:VAL:HG13	1:B:163:GLN:HA	1.92	0.52
1:B:493:ASN:HD21	1:B:513:MET:H	1.57	0.52
1:A:474:ASN:C	1:A:476:VAL:N	2.68	0.52
1:C:579:MET:HE2	1:C:616:TRP:HB2	1.91	0.52
1:C:724:ILE:HG12	1:C:740:TRP:HB3	1.91	0.52
1:D:866:MET:HE1	1:D:897:GLN:OE1	2.08	0.52
1:B:76:VAL:H	1:B:78:ASN:ND2	2.06	0.52
1:D:360:GLU:OE2	1:D:402:ARG:HG3	2.10	0.52
1:C:522:GLN:NE2	1:C:526:HIS:CD2	2.68	0.52
1:D:30:CYS:HB3	1:D:63:ARG:NH2	2.25	0.52
1:C:42:ILE:HG22	1:C:75:PHE:CE2	2.44	0.52
1:A:683:PRO:HG2	1:A:686:HIS:CD2	2.44	0.52
1:B:91:ILE:HG23	1:B:147:PHE:HE2	1.75	0.52
1:B:434:VAL:HG12	1:B:435:TRP:N	2.25	0.52
1:D:579:MET:HE3	1:D:612:LEU:HD12	1.91	0.52
1:B:579:MET:HE3	1:B:612:LEU:HD12	1.92	0.51
1:C:83:VAL:HG13	1:C:163:GLN:HA	1.92	0.51
1:C:309:VAL:HG12	1:C:560:GLY:HA3	1.91	0.51
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.73	0.51
1:A:83:VAL:HG13	1:A:163:GLN:HA	1.92	0.51
1:B:431:ILE:HB	1:B:484:THR:HB	1.93	0.51
1:B:354:THR:HG23	1:B:358:TYR:CD2	2.46	0.51
1:C:607:GLU:HG2	1:C:634:TYR:HB3	1.91	0.51
1:D:173:LYS:O	1:D:174:SER:C	2.54	0.51
1:D:354:THR:HG23	1:D:358:TYR:CD2	2.46	0.51
1:B:214:LYS:O	1:B:584:THR:HG21	2.11	0.51
1:B:579:MET:HE2	1:B:616:TRP:HB2	1.93	0.51
1:C:76:VAL:H	1:C:78:ASN:ND2	2.08	0.51
1:D:117:THR:HG23	1:D:125:PHE:CE1	2.41	0.51
1:D:323:GLN:HG2	1:D:351:THR:CG2	2.35	0.51
1:D:402:ARG:HH11	1:D:402:ARG:CG	2.24	0.51
1:A:354:THR:HG23	1:A:358:TYR:CD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:VAL:HG12	1:B:560:GLY:HA3	1.93	0.51
1:C:573:THR:HG23	1:C:605:VAL:HB	1.92	0.50
1:C:354:THR:HG23	1:C:358:TYR:CD2	2.47	0.50
1:A:431:ILE:HB	1:A:484:THR:HB	1.92	0.50
1:A:522:GLN:NE2	1:A:526:HIS:CD2	2.68	0.50
1:B:309:VAL:CG1	1:B:560:GLY:HA3	2.41	0.50
1:D:431:ILE:HB	1:D:484:THR:HB	1.92	0.50
1:D:522:GLN:NE2	1:D:526:HIS:CD2	2.71	0.50
1:A:434:VAL:HG12	1:A:435:TRP:N	2.27	0.50
1:B:173:LYS:O	1:B:174:SER:C	2.54	0.50
1:C:120:GLN:NE2	1:C:126:ARG:HD2	2.27	0.50
1:D:42:ILE:HG22	1:D:75:PHE:CE2	2.47	0.50
1:A:609:THR:HG22	1:A:611:GLU:H	1.77	0.49
1:B:30:CYS:HA	1:B:76:VAL:HG21	1.93	0.49
1:C:270:GLU:HG3	1:C:499:PRO:CB	2.43	0.49
1:C:609:THR:HB	1:C:612:LEU:H	1.77	0.49
1:D:729:TRP:CZ3	1:D:759:ARG:HB2	2.47	0.49
1:A:76:VAL:H	1:A:78:ASN:ND2	2.11	0.49
1:A:309:VAL:CG1	1:A:560:GLY:HA3	2.42	0.49
1:B:729:TRP:CZ3	1:B:759:ARG:HB2	2.48	0.49
1:A:117:THR:HG23	1:A:125:PHE:CE1	2.41	0.49
1:D:363:LYS:NZ	1:D:401:ARG:O	2.45	0.49
1:C:325:SER:HB2	1:C:353:VAL:HB	1.95	0.49
1:D:91:ILE:HG23	1:D:147:PHE:HE2	1.78	0.49
1:D:587:LEU:HD13	1:D:683:PRO:HB3	1.95	0.49
1:A:249:MET:HG2	1:A:250:CYS:N	2.27	0.49
1:D:309:VAL:CG1	1:D:560:GLY:HA3	2.43	0.49
1:C:249:MET:HG2	1:C:250:CYS:N	2.28	0.48
1:B:30:CYS:HB3	1:B:63:ARG:NH2	2.28	0.48
1:C:355:ASP:O	1:C:358:TYR:HD2	1.96	0.48
1:A:728:ILE:HD12	1:A:789:GLU:H	1.78	0.48
1:B:224:THR:HG23	1:B:272:PHE:CD1	2.39	0.48
1:C:242:TYR:CE2	1:C:570:GLY:HA3	2.48	0.48
1:C:91:ILE:HG23	1:C:147:PHE:HE2	1.79	0.48
1:D:309:VAL:HG12	1:D:560:GLY:HA3	1.96	0.48
1:D:474:ASN:C	1:D:476:VAL:N	2.71	0.48
1:C:579:MET:HE3	1:C:612:LEU:HD12	1.96	0.48
1:D:276:THR:N	1:D:277:PRO:HA	2.28	0.48
1:D:683:PRO:HG2	1:D:686:HIS:CD2	2.48	0.48
1:A:276:THR:N	1:A:277:PRO:HA	2.28	0.48
1:B:117:THR:HG23	1:B:125:PHE:CE1	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:ILE:HD12	1:C:789:GLU:H	1.78	0.48
1:A:401:ARG:NH1	1:A:405:GLY:O	2.33	0.48
1:C:579:MET:HG3	1:C:616:TRP:CD2	2.49	0.48
1:A:364:ASP:OD2	1:A:394:ASP:O	2.32	0.47
1:C:309:VAL:CG1	1:C:560:GLY:HA3	2.44	0.47
1:C:759:ARG:HD3	1:C:762:TYR:CE2	2.49	0.47
1:B:30:CYS:HB3	1:B:31:PRO:HD2	1.95	0.47
1:B:452:TRP:O	1:B:456:GLU:HG2	2.15	0.47
1:C:173:LYS:O	1:C:174:SER:C	2.57	0.47
1:D:609:THR:HG22	1:D:611:GLU:H	1.79	0.47
1:A:42:ILE:HG22	1:A:75:PHE:CE2	2.50	0.47
1:B:52:GLU:HG3	1:B:62:TRP:CD1	2.49	0.47
1:D:76:VAL:H	1:D:78:ASN:HD21	1.63	0.47
1:D:419:VAL:CG1	1:D:449:CYS:SG	3.03	0.47
1:A:667:TYR:OH	1:A:802:GLY:HA2	2.15	0.47
1:A:740:TRP:HA	1:A:743:GLN:HE22	1.79	0.47
1:D:30:CYS:HA	1:D:76:VAL:HG21	1.96	0.47
1:A:275:PRO:O	1:A:276:THR:HG23	2.14	0.47
1:B:293:LEU:N	1:B:293:LEU:HD12	2.30	0.47
1:C:887:LYS:HB2	1:C:887:LYS:HZ1	1.80	0.47
1:D:579:MET:HG3	1:D:616:TRP:CD2	2.49	0.47
1:D:609:THR:HB	1:D:612:LEU:H	1.80	0.47
1:C:224:THR:HG23	1:C:272:PHE:CD1	2.43	0.47
1:A:607:GLU:HG2	1:A:634:TYR:HB3	1.97	0.47
1:A:609:THR:HB	1:A:612:LEU:H	1.79	0.47
1:D:224:THR:HG23	1:D:272:PHE:CD1	2.39	0.47
1:A:270:GLU:HG3	1:A:499:PRO:CB	2.45	0.47
1:A:579:MET:HG3	1:A:616:TRP:CD2	2.50	0.46
1:C:230:ARG:HG3	1:C:231:ASP:N	2.31	0.46
1:D:728:ILE:HD12	1:D:789:GLU:H	1.80	0.46
1:B:447:PRO:O	1:B:450:ILE:HG12	2.15	0.46
1:B:522:GLN:NE2	1:B:526:HIS:CD2	2.73	0.46
1:C:822:ASN:ND2	3:H:1:NAG:C2	2.76	0.46
1:B:120:GLN:NE2	1:B:126:ARG:HD2	2.31	0.46
1:C:276:THR:N	1:C:277:PRO:HA	2.30	0.46
1:D:580:GLU:HG3	1:D:713:LEU:HD13	1.96	0.46
1:A:444:PHE:CE2	1:A:533:MET:HG3	2.51	0.46
1:B:728:ILE:HD12	1:B:789:GLU:H	1.81	0.46
1:B:474:ASN:CB	1:B:556:SER:HB3	2.35	0.46
1:D:270:GLU:HG3	1:D:499:PRO:CB	2.46	0.46
1:A:579:MET:HE2	1:A:616:TRP:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:HG22	1:B:75:PHE:CE2	2.51	0.46
1:B:573:THR:HG23	1:B:605:VAL:HB	1.97	0.46
1:B:609:THR:HB	1:B:612:LEU:H	1.80	0.46
1:B:740:TRP:HA	1:B:743:GLN:HE22	1.80	0.45
1:C:447:PRO:O	1:C:450:ILE:HG12	2.16	0.45
1:A:861:GLU:OE2	1:A:892:ARG:HD2	2.16	0.45
1:D:573:THR:HG23	1:D:605:VAL:HB	1.98	0.45
1:B:579:MET:HG3	1:B:616:TRP:CD2	2.51	0.45
1:A:579:MET:HE3	1:A:612:LEU:CD1	2.46	0.45
1:A:30:CYS:HB3	1:A:31:PRO:HD2	1.98	0.45
1:A:120:GLN:NE2	1:A:126:ARG:HD2	2.31	0.45
1:D:242:TYR:CE2	1:D:570:GLY:HA3	2.52	0.45
1:D:883:ILE:HG22	1:D:886:LEU:HD11	1.99	0.45
1:A:66:ASN:OD1	1:A:66:ASN:N	2.50	0.45
1:B:276:THR:N	1:B:277:PRO:HA	2.32	0.45
1:C:30:CYS:HB3	1:C:63:ARG:NH2	2.32	0.45
1:D:120:GLN:NE2	1:D:126:ARG:HD2	2.32	0.45
1:A:724:ILE:HG13	1:A:724:ILE:O	2.17	0.44
1:B:579:MET:HE3	1:B:612:LEU:CD1	2.47	0.44
1:C:418:HIS:HB2	2:G:2:NAG:H61	1.98	0.44
1:A:475:GLU:O	1:A:476:VAL:HG23	2.17	0.44
1:A:759:ARG:HD3	1:A:762:TYR:CE2	2.52	0.44
1:A:862:ASN:HB3	1:A:863:ASN:H	1.58	0.44
1:D:724:ILE:HA	1:D:725:PRO:HD3	1.75	0.44
1:B:299:GLU:OE2	1:B:679:THR:OG1	2.27	0.44
1:C:30:CYS:HB3	1:C:31:PRO:HD2	1.98	0.44
1:A:49:PHE:HA	1:A:50:PRO:HD3	1.85	0.44
1:C:878:ASN:HB3	1:C:880:VAL:HG23	2.00	0.44
1:A:309:VAL:HG12	1:A:560:GLY:HA3	2.00	0.44
1:B:270:GLU:HG3	1:B:499:PRO:CB	2.48	0.44
1:C:207:GLY:O	1:C:218:HIS:CE1	2.67	0.44
1:A:173:LYS:O	1:A:174:SER:C	2.60	0.44
1:B:607:GLU:HG2	1:B:634:TYR:HB3	2.00	0.44
1:B:152:VAL:HG12	1:B:155:THR:HG22	2.00	0.43
1:B:242:TYR:CE2	1:B:570:GLY:HA3	2.52	0.43
1:D:740:TRP:HA	1:D:743:GLN:HE22	1.82	0.43
1:A:355:ASP:O	1:A:358:TYR:HD2	2.01	0.43
1:B:609:THR:HG22	1:B:611:GLU:H	1.83	0.43
1:B:355:ASP:O	1:B:358:TYR:HD2	2.01	0.43
1:D:607:GLU:HG2	1:D:634:TYR:HB3	2.00	0.43
1:D:878:ASN:HB3	1:D:880:VAL:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:TRP:CZ3	1:A:759:ARG:HB2	2.53	0.43
1:B:444:PHE:CE2	1:B:533:MET:HG3	2.53	0.43
1:C:740:TRP:HA	1:C:743:GLN:HE22	1.84	0.43
1:C:475:GLU:CD	1:C:555:ARG:HH21	2.26	0.43
1:D:402:ARG:CG	1:D:402:ARG:NH1	2.82	0.43
1:A:724:ILE:HA	1:A:725:PRO:HD3	1.72	0.43
1:B:249:MET:HG2	1:B:250:CYS:N	2.34	0.43
1:C:213:HIS:O	1:C:214:LYS:HB2	2.18	0.43
1:B:136:ARG:HH12	1:B:191:ASP:HA	1.83	0.43
1:C:40:VAL:O	1:C:40:VAL:CG1	2.67	0.43
1:C:42:ILE:HG22	1:C:75:PHE:CD2	2.54	0.43
1:C:889:ASN:HB2	1:C:892:ARG:NH2	2.32	0.43
1:D:237:ASN:ND2	1:D:239:ASN:CG	2.76	0.43
1:B:270:GLU:HG3	1:B:499:PRO:HB2	2.00	0.43
1:D:184:ILE:HD12	1:D:184:ILE:HA	1.83	0.43
1:D:447:PRO:O	1:D:450:ILE:HG12	2.17	0.43
1:A:224:THR:HG23	1:A:272:PHE:CD1	2.43	0.43
1:D:215:ARG:NH1	1:D:698:ASP:OD2	2.51	0.43
1:D:249:MET:HG2	1:D:250:CYS:N	2.34	0.43
1:D:474:ASN:OD1	1:D:533:MET:SD	2.78	0.42
1:B:788:GLY:O	1:B:790:ASN:N	2.53	0.42
1:C:444:PHE:CE2	1:C:533:MET:HG3	2.54	0.42
1:B:474:ASN:C	1:B:476:VAL:N	2.73	0.42
1:B:866:MET:HE3	1:B:866:MET:HB2	1.97	0.42
1:C:434:VAL:HG12	1:C:435:TRP:H	1.82	0.42
1:C:690:GLU:CD	1:C:690:GLU:H	2.27	0.42
1:D:667:TYR:OH	1:D:802:GLY:HA2	2.19	0.42
1:A:242:TYR:CE2	1:A:570:GLY:HA3	2.54	0.42
1:A:40:VAL:O	1:A:40:VAL:HG12	2.19	0.42
1:A:788:GLY:O	1:A:790:ASN:N	2.53	0.42
1:C:667:TYR:OH	1:C:802:GLY:HA2	2.19	0.42
1:D:579:MET:HE2	1:D:616:TRP:HB2	2.01	0.42
1:A:203:ASP:HB3	1:A:220:LEU:HD11	2.02	0.42
1:C:724:ILE:HA	1:C:725:PRO:HD3	1.74	0.42
1:C:788:GLY:O	1:C:790:ASN:N	2.53	0.42
1:D:30:CYS:HB3	1:D:31:PRO:HD2	2.01	0.42
1:A:763:ILE:HG12	1:A:785:VAL:HG22	2.02	0.42
1:B:759:ARG:HD3	1:B:762:TYR:CE2	2.55	0.42
1:C:474:ASN:OD1	1:C:533:MET:SD	2.78	0.42
1:A:234:PRO:HD2	1:A:571:ASP:O	2.20	0.41
1:B:276:THR:HG23	1:B:277:PRO:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:HH12	1:C:191:ASP:HA	1.85	0.41
1:C:332:LEU:HB2	1:C:372:PHE:HA	2.02	0.41
1:A:40:VAL:O	1:A:40:VAL:CG1	2.67	0.41
1:A:323:GLN:HG2	1:A:351:THR:CG2	2.40	0.41
1:B:332:LEU:HB2	1:B:372:PHE:HA	2.02	0.41
1:B:667:TYR:OH	1:B:802:GLY:HA2	2.20	0.41
1:D:40:VAL:O	1:D:40:VAL:CG1	2.68	0.41
1:D:861:GLU:OE2	1:D:892:ARG:HD2	2.21	0.41
1:A:136:ARG:HH12	1:A:191:ASP:HA	1.86	0.41
1:D:579:MET:HE3	1:D:612:LEU:CD1	2.51	0.41
1:A:84:GLN:O	1:A:85:ASP:HB3	2.21	0.41
1:A:92:GLY:HA3	1:A:117:THR:HG22	2.02	0.41
1:B:445:THR:HB	1:B:519:TRP:CE2	2.56	0.41
1:C:474:ASN:C	1:C:476:VAL:N	2.71	0.41
1:C:572:ASN:O	1:C:604:PHE:HB3	2.21	0.41
1:B:181:ASP:HB3	1:B:199:ARG:HB3	2.03	0.41
1:B:441:TYR:HA	1:B:442:PRO:HD3	1.90	0.41
1:D:40:VAL:O	1:D:40:VAL:HG12	2.21	0.41
1:D:42:ILE:HG22	1:D:75:PHE:CD2	2.56	0.41
1:B:49:PHE:HA	1:B:50:PRO:HD3	1.87	0.41
1:B:76:VAL:H	1:B:78:ASN:HD21	1.69	0.41
1:B:780:PRO:HB3	1:B:843:GLN:CD	2.46	0.41
1:B:878:ASN:HB3	1:B:880:VAL:HG23	2.03	0.41
1:C:40:VAL:O	1:C:40:VAL:HG12	2.21	0.41
1:C:323:GLN:HG2	1:C:351:THR:CG2	2.41	0.41
1:C:861:GLU:OE2	1:C:892:ARG:HD2	2.21	0.41
1:D:91:ILE:CG2	1:D:147:PHE:HE2	2.34	0.41
1:B:558:PHE:CG	1:B:559:ALA:N	2.89	0.40
1:A:91:ILE:CG2	1:A:147:PHE:HE2	2.33	0.40
1:C:46:PRO:HD2	1:C:47:GLU:HG3	2.02	0.40
1:A:447:PRO:O	1:A:450:ILE:HG12	2.21	0.40
1:A:474:ASN:O	1:A:476:VAL:N	2.54	0.40
1:A:889:ASN:HB2	1:A:892:ARG:NH2	2.34	0.40
1:D:885:ASP:O	1:D:885:ASP:CG	2.65	0.40
1:A:83:VAL:CG1	1:A:163:GLN:HA	2.52	0.40
1:B:275:PRO:C	1:B:276:THR:CG2	2.87	0.40
1:B:862:ASN:HB3	1:B:863:ASN:H	1.65	0.40
1:C:42:ILE:HG22	1:C:75:PHE:HE2	1.87	0.40
1:C:184:ILE:HA	1:C:184:ILE:HD12	1.87	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	868/898 (97%)	802 (92%)	55 (6%)	11 (1%)	9	40
1	B	868/898 (97%)	802 (92%)	51 (6%)	15 (2%)	7	35
1	C	868/898 (97%)	804 (93%)	53 (6%)	11 (1%)	9	40
1	D	868/898 (97%)	805 (93%)	50 (6%)	13 (2%)	8	37
All	All	3472/3592 (97%)	3213 (92%)	209 (6%)	50 (1%)	9	39

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	A	789	GLU
1	B	276	THR
1	B	789	GLU
1	C	276	THR
1	C	789	GLU
1	D	276	THR
1	D	789	GLU
1	A	76	VAL
1	A	208	ILE
1	B	76	VAL
1	B	208	ILE
1	C	76	VAL
1	C	208	ILE
1	D	208	ILE
1	A	174	SER
1	A	404	ASN
1	B	174	SER
1	B	404	ASN
1	C	174	SER
1	A	604	PHE
1	B	803	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	66	ASN
1	D	76	VAL
1	D	174	SER
1	D	604	PHE
1	A	475	GLU
1	B	85	ASP
1	B	403	ALA
1	B	500	ASP
1	B	574	ALA
1	C	500	ASP
1	C	803	GLU
1	D	803	GLU
1	A	476	VAL
1	B	604	PHE
1	C	404	ASN
1	D	85	ASP
1	D	500	ASP
1	A	434	VAL
1	B	434	VAL
1	C	434	VAL
1	C	476	VAL
1	D	144	VAL
1	D	434	VAL
1	D	476	VAL
1	A	144	VAL
1	B	144	VAL
1	B	476	VAL
1	C	144	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	720/797 (90%)	662 (92%)	58 (8%)	11	39
1	B	703/797 (88%)	646 (92%)	57 (8%)	11	39
1	C	734/797 (92%)	677 (92%)	57 (8%)	11	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	728/797 (91%)	674 (93%)	54 (7%)	13	43
All	All	2885/3188 (90%)	2659 (92%)	226 (8%)	11	41

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	66	ASN
1	A	75	PHE
1	A	78	ASN
1	A	83	VAL
1	A	85	ASP
1	A	105	LEU
1	A	117	THR
1	A	121	THR
1	A	151	THR
1	A	173	LYS
1	A	174	SER
1	A	178	THR
1	A	194	LEU
1	A	215	ARG
1	A	217	ARG
1	A	224	THR
1	A	229	THR
1	A	254	THR
1	A	283	VAL
1	A	340	ARG
1	A	350	ASP
1	A	351	THR
1	A	354	THR
1	A	401	ARG
1	A	402	ARG
1	A	406	THR
1	A	419	VAL
1	A	427	SER
1	A	431	ILE
1	A	438	LEU
1	A	476	VAL
1	A	484	THR
1	A	505	LEU
1	A	539	GLN
1	A	557	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	584	THR
1	A	685	LEU
1	A	715	GLN
1	A	719	THR
1	A	720	VAL
1	A	724	ILE
1	A	733	GLU
1	A	778	LYS
1	A	789	GLU
1	A	796	ASP
1	A	805	LYS
1	A	808	ILE
1	A	817	THR
1	A	824	THR
1	A	828	VAL
1	A	856	GLU
1	A	867	ASN
1	A	870	SER
1	A	871	ASN
1	A	877	SER
1	A	882	LEU
1	A	895	SER
1	B	47	GLU
1	B	75	PHE
1	B	76	VAL
1	B	78	ASN
1	B	83	VAL
1	B	105	LEU
1	B	112	SER
1	B	117	THR
1	B	121	THR
1	B	173	LYS
1	B	174	SER
1	B	178	THR
1	B	194	LEU
1	B	215	ARG
1	B	217	ARG
1	B	223	LYS
1	B	224	THR
1	B	229	THR
1	B	254	THR
1	B	276	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	283	VAL
1	B	340	ARG
1	B	350	ASP
1	B	351	THR
1	B	354	THR
1	B	427	SER
1	B	431	ILE
1	B	438	LEU
1	B	440	VAL
1	B	484	THR
1	B	505	LEU
1	B	539	GLN
1	B	557	THR
1	B	584	THR
1	B	685	LEU
1	B	715	GLN
1	B	719	THR
1	B	720	VAL
1	B	724	ILE
1	B	733	GLU
1	B	778	LYS
1	B	789	GLU
1	B	796	ASP
1	B	805	LYS
1	B	808	ILE
1	B	817	THR
1	B	824	THR
1	B	828	VAL
1	B	851	THR
1	B	856	GLU
1	B	863	ASN
1	B	867	ASN
1	B	870	SER
1	B	871	ASN
1	B	877	SER
1	B	882	LEU
1	B	895	SER
1	C	47	GLU
1	C	70	ILE
1	C	75	PHE
1	C	78	ASN
1	C	83	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	105	LEU
1	C	117	THR
1	C	121	THR
1	C	173	LYS
1	C	174	SER
1	C	178	THR
1	C	184	ILE
1	C	194	LEU
1	C	215	ARG
1	C	217	ARG
1	C	224	THR
1	C	229	THR
1	C	254	THR
1	C	283	VAL
1	C	340	ARG
1	C	350	ASP
1	C	351	THR
1	C	354	THR
1	C	406	THR
1	C	419	VAL
1	C	427	SER
1	C	431	ILE
1	C	477	SER
1	C	484	THR
1	C	505	LEU
1	C	539	GLN
1	C	543	LYS
1	C	557	THR
1	C	573	THR
1	C	575	SER
1	C	584	THR
1	C	685	LEU
1	C	715	GLN
1	C	719	THR
1	C	720	VAL
1	C	724	ILE
1	C	733	GLU
1	C	778	LYS
1	C	789	GLU
1	C	805	LYS
1	C	808	ILE
1	C	817	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	824	THR
1	C	828	VAL
1	C	856	GLU
1	C	867	ASN
1	C	870	SER
1	C	871	ASN
1	C	877	SER
1	C	882	LEU
1	C	887	LYS
1	C	895	SER
1	D	47	GLU
1	D	75	PHE
1	D	78	ASN
1	D	83	VAL
1	D	105	LEU
1	D	117	THR
1	D	121	THR
1	D	151	THR
1	D	173	LYS
1	D	178	THR
1	D	184	ILE
1	D	194	LEU
1	D	215	ARG
1	D	217	ARG
1	D	224	THR
1	D	229	THR
1	D	254	THR
1	D	283	VAL
1	D	340	ARG
1	D	350	ASP
1	D	351	THR
1	D	354	THR
1	D	364	ASP
1	D	402	ARG
1	D	427	SER
1	D	431	ILE
1	D	438	LEU
1	D	484	THR
1	D	505	LEU
1	D	539	GLN
1	D	557	THR
1	D	575	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	584	THR
1	D	685	LEU
1	D	715	GLN
1	D	719	THR
1	D	720	VAL
1	D	724	ILE
1	D	733	GLU
1	D	778	LYS
1	D	789	GLU
1	D	805	LYS
1	D	808	ILE
1	D	817	THR
1	D	824	THR
1	D	828	VAL
1	D	856	GLU
1	D	864	GLN
1	D	867	ASN
1	D	870	SER
1	D	871	ASN
1	D	877	SER
1	D	882	LEU
1	D	895	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	78	ASN
1	A	79	HIS
1	A	123	ASN
1	A	142	GLN
1	A	169	GLN
1	A	192	GLN
1	A	195	GLN
1	A	213	HIS
1	A	218	HIS
1	A	232	GLN
1	A	237	ASN
1	A	239	ASN
1	A	373	ASN
1	A	448	ASN
1	A	462	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	474	ASN
1	A	493	ASN
1	A	517	GLN
1	A	522	GLN
1	A	526	HIS
1	A	567	HIS
1	A	686	HIS
1	A	743	GLN
1	A	812	ASN
1	A	897	GLN
1	B	48	GLN
1	B	78	ASN
1	B	79	HIS
1	B	111	ASN
1	B	134	ASN
1	B	142	GLN
1	B	163	GLN
1	B	169	GLN
1	B	192	GLN
1	B	213	HIS
1	B	218	HIS
1	B	232	GLN
1	B	237	ASN
1	B	239	ASN
1	B	319	ASN
1	B	462	GLN
1	B	474	ASN
1	B	493	ASN
1	B	526	HIS
1	B	564	HIS
1	B	743	GLN
1	B	863	ASN
1	C	39	ASN
1	C	48	GLN
1	C	78	ASN
1	C	79	HIS
1	C	134	ASN
1	C	142	GLN
1	C	169	GLN
1	C	192	GLN
1	C	195	GLN
1	C	213	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	218	HIS
1	C	232	GLN
1	C	237	ASN
1	C	239	ASN
1	C	448	ASN
1	C	462	GLN
1	C	474	ASN
1	C	493	ASN
1	C	517	GLN
1	C	518	ASN
1	C	522	GLN
1	C	526	HIS
1	C	564	HIS
1	C	567	HIS
1	C	743	GLN
1	C	812	ASN
1	C	822	ASN
1	C	897	GLN
1	D	78	ASN
1	D	79	HIS
1	D	123	ASN
1	D	142	GLN
1	D	169	GLN
1	D	192	GLN
1	D	213	HIS
1	D	218	HIS
1	D	232	GLN
1	D	237	ASN
1	D	239	ASN
1	D	373	ASN
1	D	418	HIS
1	D	448	ASN
1	D	461	HIS
1	D	462	GLN
1	D	474	ASN
1	D	493	ASN
1	D	517	GLN
1	D	518	ASN
1	D	522	GLN
1	D	526	HIS
1	D	564	HIS
1	D	567	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	743	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	E	1	1,2	14,14,15	0.65	0	17,19,21	1.07	1 (5%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	2.03	3 (17%)
3	NAG	F	1	3,1	14,14,15	0.68	0	17,19,21	2.40	7 (41%)
3	NAG	F	2	3	14,14,15	0.62	0	17,19,21	1.10	1 (5%)
3	BMA	F	3	3	11,11,12	0.56	0	15,15,17	1.52	2 (13%)
3	MAN	F	4	3	11,11,12	0.76	0	15,15,17	1.65	4 (26%)
3	MAN	F	5	3	11,11,12	0.57	0	15,15,17	0.71	0
2	NAG	G	1	1,2	14,14,15	0.68	0	17,19,21	1.13	0
2	NAG	G	2	2	14,14,15	0.44	0	17,19,21	2.01	2 (11%)
3	NAG	H	1	3	14,14,15	0.64	0	17,19,21	1.86	3 (17%)
3	NAG	H	2	3	14,14,15	0.60	0	17,19,21	1.30	1 (5%)
3	BMA	H	3	3	11,11,12	0.54	0	15,15,17	2.12	6 (40%)
3	MAN	H	4	3	11,11,12	0.66	0	15,15,17	1.07	1 (6%)
3	MAN	H	5	3	11,11,12	0.74	0	15,15,17	2.33	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	7.31	121.98	112.19
3	F	1	NAG	C1-O5-C5	7.08	121.68	112.19
2	E	2	NAG	C1-O5-C5	5.69	119.81	112.19
3	H	1	NAG	C3-C4-C5	4.63	118.63	110.23
3	H	3	BMA	C1-O5-C5	4.63	118.39	112.19
3	H	5	MAN	C1-C2-C3	4.47	116.16	109.64
3	H	5	MAN	C1-O5-C5	4.37	118.05	112.19
3	H	1	NAG	C1-O5-C5	4.35	118.02	112.19
3	H	2	NAG	C4-C3-C2	4.29	117.31	111.02
3	H	5	MAN	C2-C3-C4	4.14	118.14	110.86
2	E	2	NAG	C4-C3-C2	3.84	116.65	111.02
3	H	5	MAN	C3-C4-C5	3.84	117.19	110.23
3	F	3	BMA	C1-C2-C3	3.59	114.87	109.64
3	F	4	MAN	C1-C2-C3	3.18	114.27	109.64
3	F	4	MAN	C3-C4-C5	3.08	115.81	110.23
3	H	3	BMA	C1-C2-C3	2.75	113.65	109.64
2	E	1	NAG	C3-C4-C5	-2.71	105.32	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C3-C4-C5	2.70	115.12	110.23
3	H	3	BMA	C2-C3-C4	2.69	115.58	110.86
2	E	2	NAG	O3-C3-C4	-2.68	104.07	110.38
3	F	1	NAG	C1-C2-N2	2.65	114.60	110.43
3	F	1	NAG	O5-C1-C2	-2.63	107.22	111.29
3	F	1	NAG	C3-C4-C5	2.63	115.00	110.23
3	H	3	BMA	O5-C5-C6	-2.59	102.63	107.66
3	F	1	NAG	C4-C3-C2	2.56	114.78	111.02
3	F	4	MAN	O3-C3-C2	-2.54	104.87	110.05
3	F	3	BMA	O6-C6-C5	-2.44	103.03	111.33
3	F	4	MAN	O2-C2-C3	-2.42	105.14	110.15
2	G	2	NAG	O5-C5-C6	2.36	112.26	107.66
3	H	1	NAG	O5-C5-C4	2.33	116.49	110.83
3	F	2	NAG	C4-C3-C2	2.23	114.29	111.02
3	H	5	MAN	O5-C5-C6	2.19	111.93	107.66
3	H	4	MAN	C1-O5-C5	2.13	115.04	112.19
3	F	1	NAG	O4-C4-C3	-2.10	105.42	110.38
3	H	3	BMA	O3-C3-C4	-2.08	105.47	110.38
3	F	1	NAG	O5-C5-C4	2.07	115.86	110.83

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	4	MAN	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	H	3	BMA	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
3	F	3	BMA	C4-C5-C6-O6
2	E	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

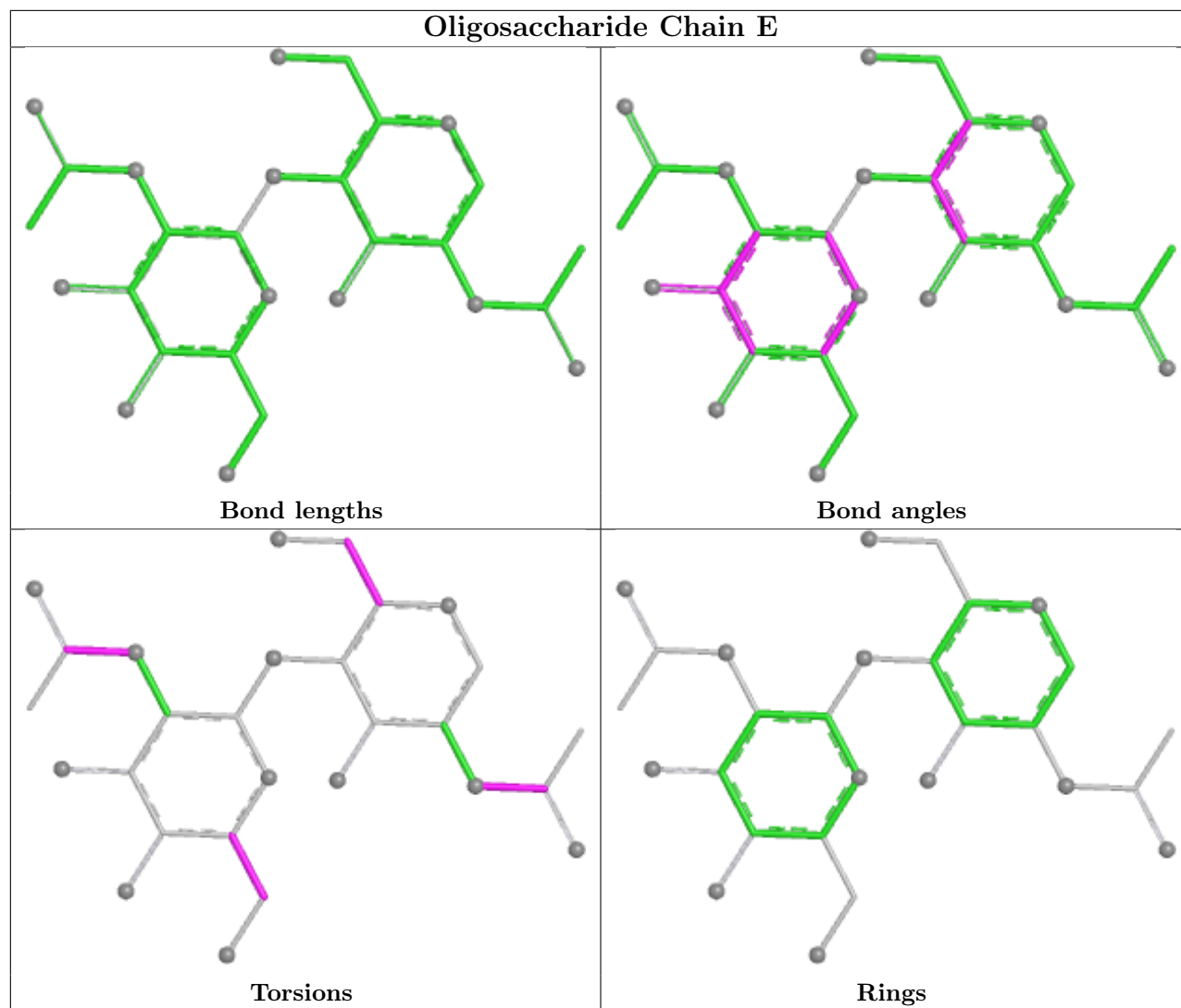
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	3	BMA	O5-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O7-C7-N2-C2
3	F	5	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7

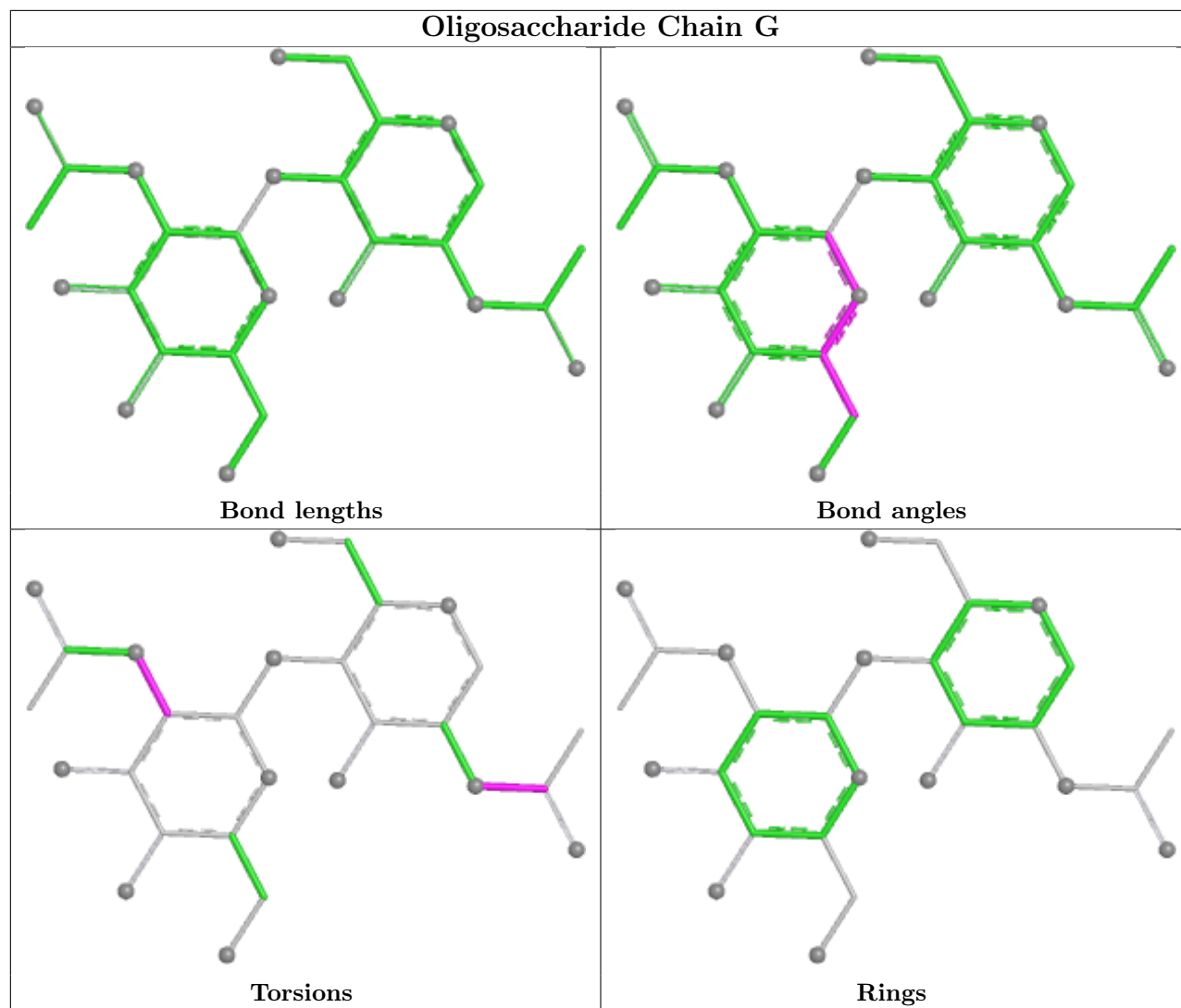
There are no ring outliers.

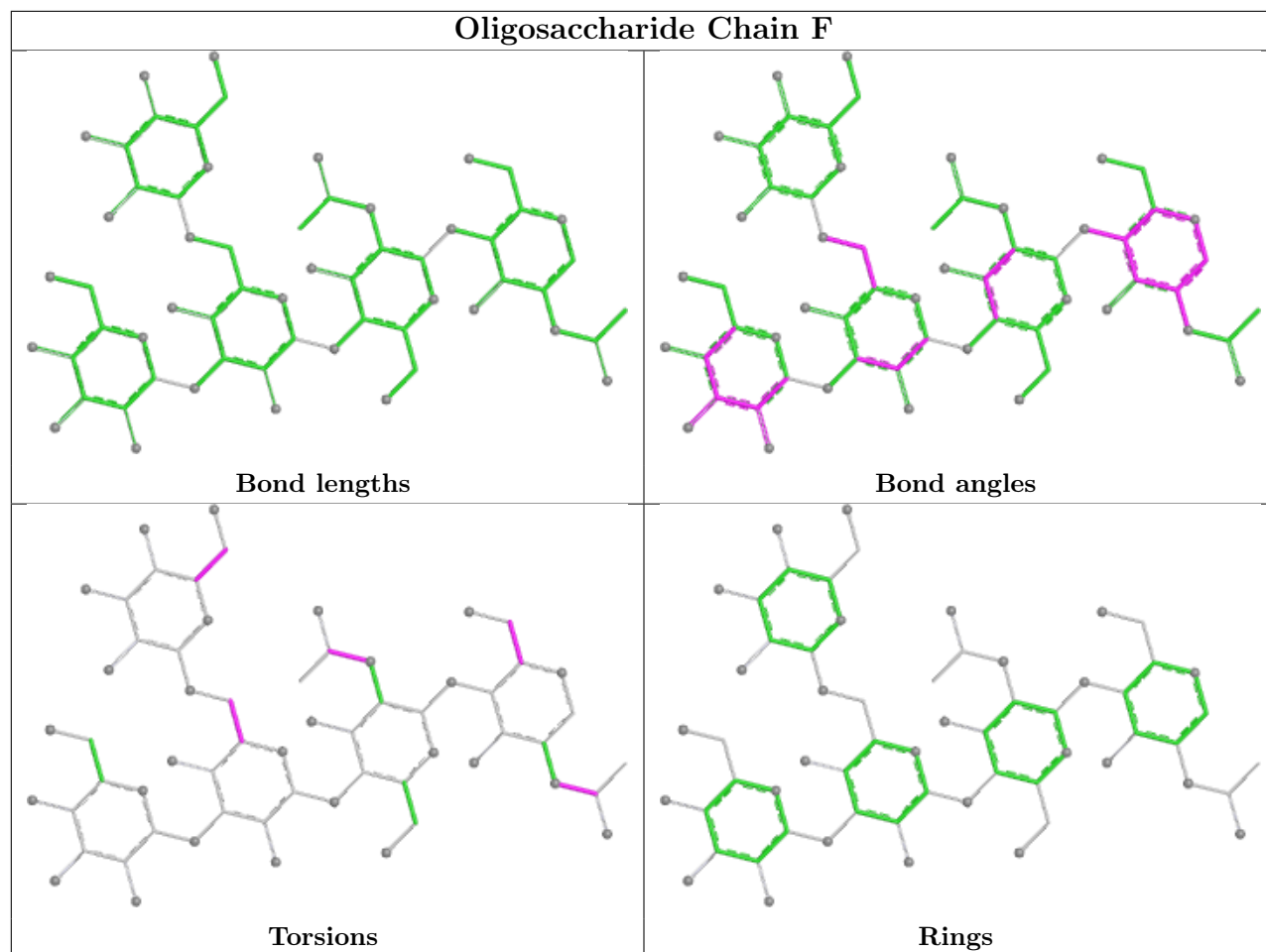
2 monomers are involved in 5 short contacts:

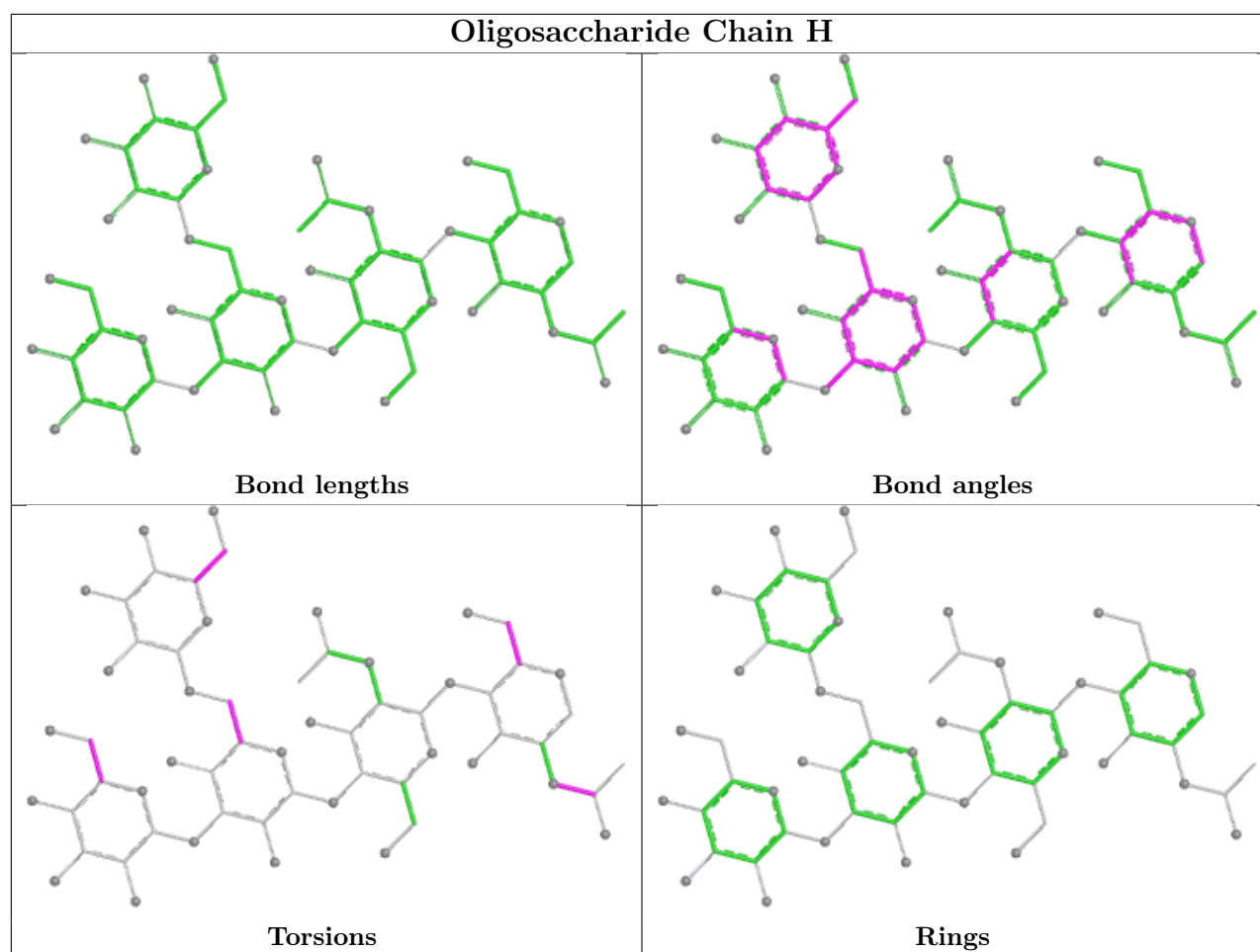
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
3	H	1	NAG	4	0

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](#)

5 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	NAG	B	2001	1	14,14,15	0.69	0	17,19,21	2.85	6 (35%)
4	NAG	D	3001	1	14,14,15	0.62	0	17,19,21	1.38	2 (11%)
4	NAG	D	2001	1	14,14,15	1.42	2 (14%)	17,19,21	3.69	6 (35%)
4	NAG	C	2001	1	14,14,15	0.72	0	17,19,21	1.50	2 (11%)
4	NAG	A	2001	1	14,14,15	0.53	0	17,19,21	1.45	3 (17%)

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
4	NAG	B	2001	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	D	3001	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2001	1	-	3/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	6/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2001	NAG	C1-C2	3.53	1.57	1.52
4	D	2001	NAG	C2-N2	2.42	1.50	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2001	NAG	C2-N2-C7	11.93	138.89	122.90
4	B	2001	NAG	C1-O5-C5	7.12	121.73	112.19
4	B	2001	NAG	C2-N2-C7	6.02	130.97	122.90
4	D	2001	NAG	C1-O5-C5	5.07	118.98	112.19
4	D	2001	NAG	C8-C7-N2	4.69	123.89	116.12
4	C	2001	NAG	C1-O5-C5	4.63	118.39	112.19
4	A	2001	NAG	C1-O5-C5	3.88	117.38	112.19
4	D	2001	NAG	O7-C7-C8	-3.70	115.46	122.05
4	B	2001	NAG	C3-C4-C5	3.26	116.14	110.23
4	D	2001	NAG	O3-C3-C2	3.06	115.76	109.40
4	B	2001	NAG	C4-C3-C2	3.04	115.48	111.02
4	C	2001	NAG	C2-N2-C7	2.77	126.62	122.90
4	B	2001	NAG	O7-C7-N2	2.67	126.70	121.98
4	B	2001	NAG	O7-C7-C8	-2.54	117.52	122.05
4	D	2001	NAG	O5-C5-C4	-2.47	104.81	110.83
4	D	3001	NAG	C4-C3-C2	2.37	114.49	111.02
4	D	3001	NAG	C3-C4-C5	-2.36	105.95	110.23
4	A	2001	NAG	O3-C3-C2	-2.25	104.73	109.40
4	A	2001	NAG	O7-C7-C8	-2.14	118.24	122.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2001	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2001	NAG	C8-C7-N2-C2
4	C	2001	NAG	O7-C7-N2-C2
4	D	2001	NAG	C3-C2-N2-C7
4	D	3001	NAG	C8-C7-N2-C2
4	D	3001	NAG	O7-C7-N2-C2
4	D	3001	NAG	O5-C5-C6-O6
4	C	2001	NAG	O5-C5-C6-O6
4	D	2001	NAG	C8-C7-N2-C2
4	D	2001	NAG	O7-C7-N2-C2
4	D	3001	NAG	C4-C5-C6-O6
4	B	2001	NAG	C8-C7-N2-C2
4	B	2001	NAG	O7-C7-N2-C2
4	C	2001	NAG	C4-C5-C6-O6
4	C	2001	NAG	C3-C2-N2-C7
4	A	2001	NAG	C4-C5-C6-O6
4	A	2001	NAG	O5-C5-C6-O6
4	C	2001	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3001	NAG	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	870/898 (96%)	0.36	17 (1%) 65 45	29, 49, 61, 69	0
1	B	870/898 (96%)	0.36	18 (2%) 63 43	29, 50, 61, 69	0
1	C	870/898 (96%)	0.15	6 (0%) 84 69	29, 49, 61, 69	0
1	D	870/898 (96%)	0.19	6 (0%) 84 69	29, 49, 61, 69	0
All	All	3480/3592 (96%)	0.27	47 (1%) 73 54	29, 49, 61, 69	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	602	CYS	4.0
1	A	36	ASP	3.5
1	A	231	ASP	3.3
1	D	403	ALA	3.2
1	A	30	CYS	3.0
1	B	111	ASN	3.0
1	A	32	ASN	2.9
1	B	449	CYS	2.9
1	D	852	ASP	2.5
1	A	826	ASP	2.5
1	A	865	PRO	2.5
1	B	84	GLN	2.5
1	A	29	LYS	2.5
1	B	409	ALA	2.4
1	C	690	GLU	2.4
1	A	154	ASP	2.4
1	A	852	ASP	2.4
1	D	276	THR	2.4
1	A	476	VAL	2.4
1	B	608	THR	2.4
1	B	364	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	407	THR	2.3
1	D	404	ASN	2.3
1	A	296	ASP	2.3
1	C	475	GLU	2.3
1	C	856	GLU	2.3
1	B	422	ASN	2.3
1	A	863	ASN	2.2
1	B	375	LEU	2.2
1	A	874	TYR	2.2
1	A	810	ASN	2.2
1	B	488	ASN	2.2
1	B	419	VAL	2.2
1	A	853	SER	2.2
1	A	433	GLU	2.2
1	A	823	ASN	2.2
1	B	373	ASN	2.1
1	B	361	ASP	2.1
1	B	640	ALA	2.1
1	C	862	ASN	2.1
1	D	856	GLU	2.1
1	D	448	ASN	2.1
1	B	420	TRP	2.1
1	B	599	ALA	2.1
1	C	250	CYS	2.0
1	B	404	ASN	2.0
1	C	91	ILE	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.

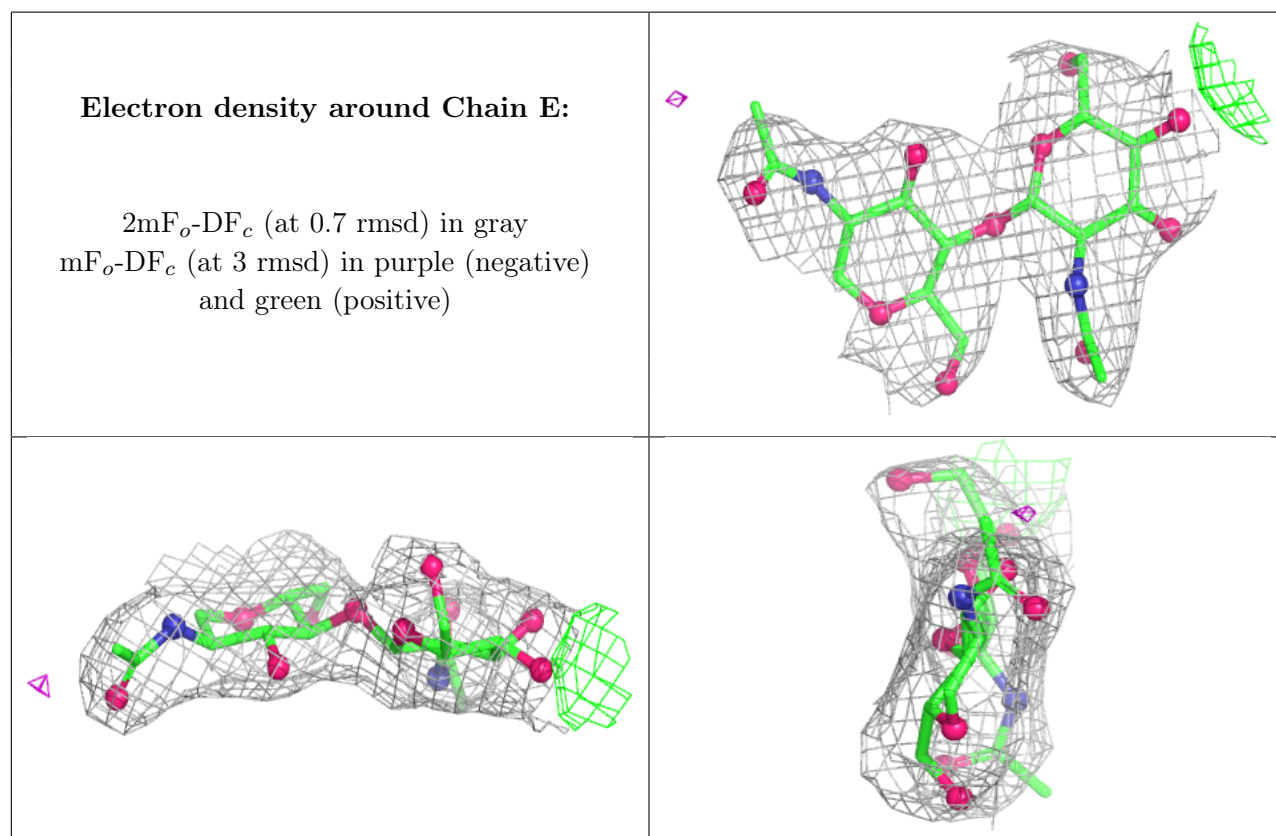
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	H	5	11/12	0.68	0.12	74,76,76,77	0
3	NAG	H	1	14/15	0.73	0.13	77,80,81,81	0

Continued on next page...

Continued from previous page...

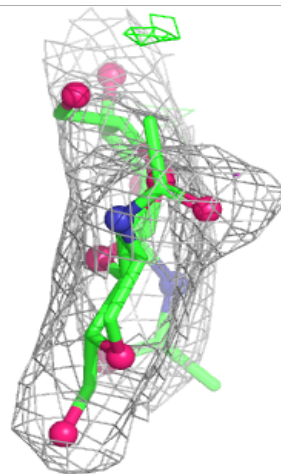
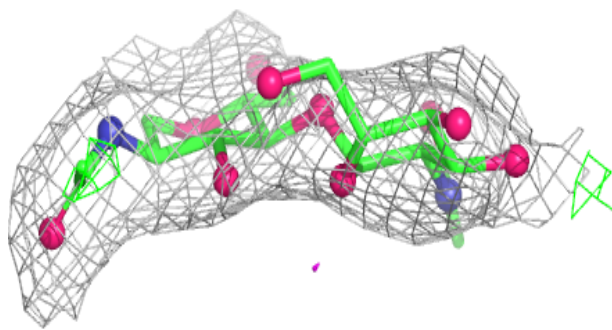
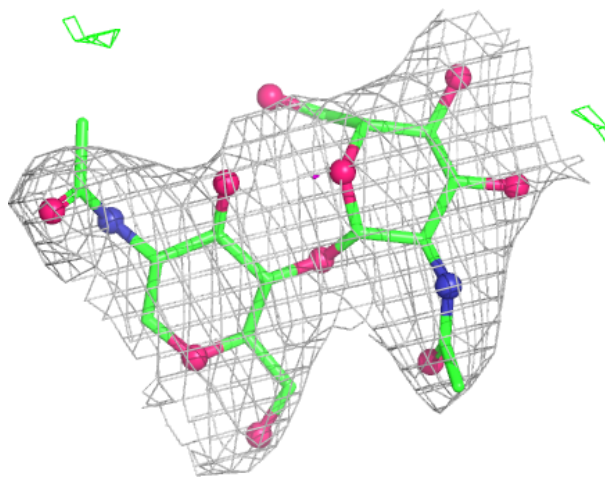
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	F	5	11/12	0.77	0.14	68,69,70,71	0
2	NAG	E	2	14/15	0.78	0.10	62,63,65,65	0
3	NAG	F	1	14/15	0.80	0.11	61,62,65,66	0
3	MAN	F	4	11/12	0.82	0.13	52,54,55,55	0
2	NAG	G	2	14/15	0.83	0.12	65,66,69,70	0
3	NAG	H	2	14/15	0.85	0.10	70,75,78,79	0
3	BMA	H	3	11/12	0.86	0.12	64,67,71,75	0
3	NAG	F	2	14/15	0.88	0.11	60,63,66,66	0
2	NAG	G	1	14/15	0.90	0.09	55,60,62,64	0
2	NAG	E	1	14/15	0.91	0.10	57,59,60,62	0
3	MAN	H	4	11/12	0.91	0.11	60,61,63,63	0
3	BMA	F	3	11/12	0.91	0.10	56,59,64,67	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.



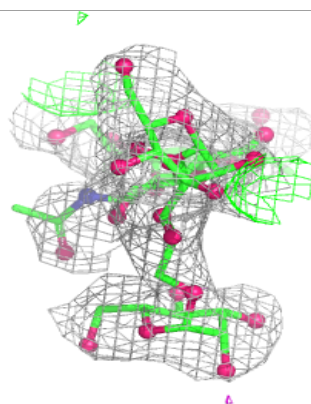
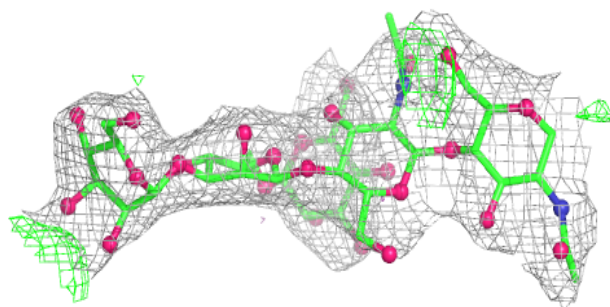
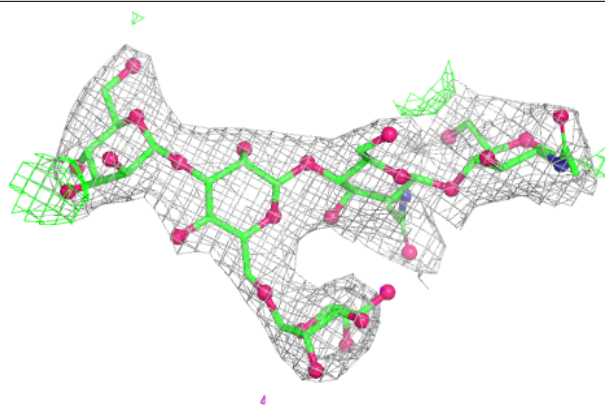
Electron density around Chain G:

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

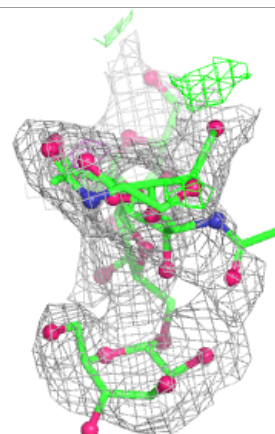
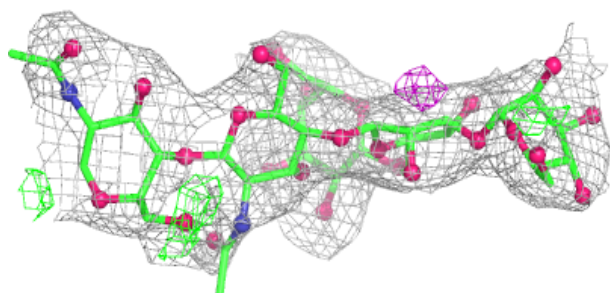
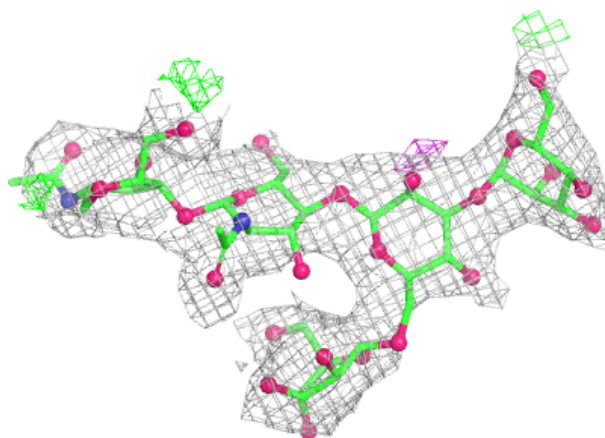


Electron density around Chain F:

$2mF_o-DF_c$ (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)



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($\text{\AA}^2$)	Q<0.9
4	NAG	D	2001	14/15	0.66	0.17	40,45,46,46	0
4	NAG	B	2001	14/15	0.72	0.14	48,51,53,53	0
4	NAG	C	2001	14/15	0.80	0.12	57,61,62,62	0
4	NAG	A	2001	14/15	0.82	0.11	48,50,53,55	0
4	NAG	D	3001	14/15	0.83	0.14	60,61,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.