



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:01 PM UTC

PDB ID : 7ZA1 / pdb_00007za1
Title : GPC3-Unc5D octamer structure and role in cell migration
Authors : Akkermans, O.; Delloye-Bourgeois, C.; Peregrina, C.; Carrasquero, M.; Kokolaki, M.; Berbeira-Santana, M.; Chavent, M.; Reynaud, F.; Ritu, R.; Agirre, J.; Aksu, M.; White, E.; Lowe, E.; Ben Amar, D.; Zaballa, S.; Huo, J.; Pakos, I.; McCubbin, P.; Comoletti, D.; Owens, R.; Robinson, C.; Castellani, V.; del Toro, D.; Seiradake, E.
Deposited on : 2022-03-21
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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:

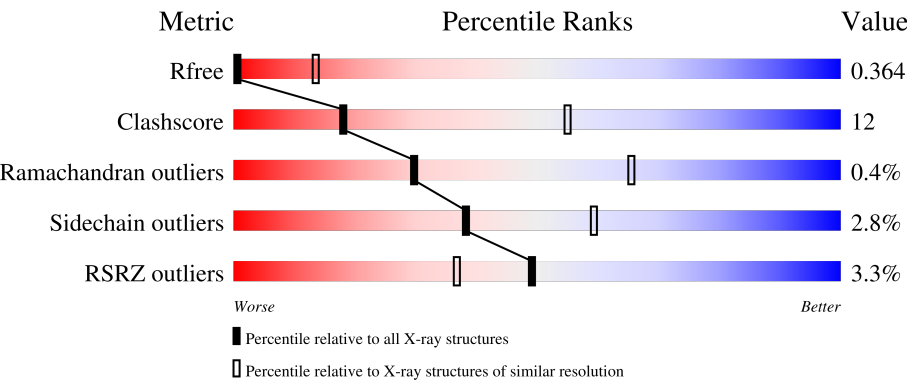
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	E	268	2% 64% 28% 6%
1	F	268	3% 66% 26% 6%
1	G	268	4% 65% 26% 6%
1	H	268	4% 67% 25% 6%

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Mol	Chain	Length	Quality of chain
2	A	464	
2	B	464	
2	C	464	
2	D	464	
3	I	2	
4	J	4	
4	K	4	
4	M	4	
4	N	4	

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	K	1	-	-	X	-
5	NAG	D	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39050 atoms, of which 19404 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 Netrin receptor UNC5D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	251	Total	C	H	N	O	S	49	0	0
			3903	1237	1912	363	376	15			
1	F	251	Total	C	H	N	O	S	49	0	0
			3903	1237	1912	363	376	15			
1	G	251	Total	C	H	N	O	S	50	0	0
			3906	1237	1915	363	376	15			
1	H	251	Total	C	H	N	O	S	49	0	0
			3903	1237	1912	363	376	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	308	HIS	-	expression tag	UNP F1LW30
E	309	HIS	-	expression tag	UNP F1LW30
E	310	HIS	-	expression tag	UNP F1LW30
E	311	HIS	-	expression tag	UNP F1LW30
E	312	HIS	-	expression tag	UNP F1LW30
E	313	HIS	-	expression tag	UNP F1LW30
F	308	HIS	-	expression tag	UNP F1LW30
F	309	HIS	-	expression tag	UNP F1LW30
F	310	HIS	-	expression tag	UNP F1LW30
F	311	HIS	-	expression tag	UNP F1LW30
F	312	HIS	-	expression tag	UNP F1LW30
F	313	HIS	-	expression tag	UNP F1LW30
G	308	HIS	-	expression tag	UNP F1LW30
G	309	HIS	-	expression tag	UNP F1LW30
G	310	HIS	-	expression tag	UNP F1LW30
G	311	HIS	-	expression tag	UNP F1LW30
G	312	HIS	-	expression tag	UNP F1LW30
G	313	HIS	-	expression tag	UNP F1LW30
H	308	HIS	-	expression tag	UNP F1LW30
H	309	HIS	-	expression tag	UNP F1LW30
H	310	HIS	-	expression tag	UNP F1LW30

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Chain	Residue	Modelled	Actual	Comment	Reference
H	311	HIS	-	expression tag	UNP F1LW30
H	312	HIS	-	expression tag	UNP F1LW30
H	313	HIS	-	expression tag	UNP F1LW30

- Molecule 2 is a protein called Glypican-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	351	Total	C	H	N	O	S	68	0	0
			5634	1793	2827	469	517	28			
2	C	351	Total	C	H	N	O	S	67	0	0
			5635	1793	2828	469	517	28			
2	D	351	Total	C	H	N	O	S	70	0	0
			5621	1789	2822	468	514	28			
2	B	351	Total	C	H	N	O	S	68	0	0
			5634	1793	2827	469	517	28			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLU	-	expression tag	UNP P51654
A	30	THR	-	expression tag	UNP P51654
A	31	GLY	-	expression tag	UNP P51654
A	359	PHE	SER	variant	UNP P51654
A	484	GLY	-	expression tag	UNP P51654
A	485	THR	-	expression tag	UNP P51654
A	486	LYS	-	expression tag	UNP P51654
A	487	HIS	-	expression tag	UNP P51654
A	488	HIS	-	expression tag	UNP P51654
A	489	HIS	-	expression tag	UNP P51654
A	490	HIS	-	expression tag	UNP P51654
A	491	HIS	-	expression tag	UNP P51654
A	492	HIS	-	expression tag	UNP P51654
C	29	GLU	-	expression tag	UNP P51654
C	30	THR	-	expression tag	UNP P51654
C	31	GLY	-	expression tag	UNP P51654
C	359	PHE	SER	variant	UNP P51654
C	484	GLY	-	expression tag	UNP P51654
C	485	THR	-	expression tag	UNP P51654
C	486	LYS	-	expression tag	UNP P51654
C	487	HIS	-	expression tag	UNP P51654
C	488	HIS	-	expression tag	UNP P51654
C	489	HIS	-	expression tag	UNP P51654

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Chain	Residue	Modelled	Actual	Comment	Reference
C	490	HIS	-	expression tag	UNP P51654
C	491	HIS	-	expression tag	UNP P51654
C	492	HIS	-	expression tag	UNP P51654
D	29	GLU	-	expression tag	UNP P51654
D	30	THR	-	expression tag	UNP P51654
D	31	GLY	-	expression tag	UNP P51654
D	359	PHE	SER	variant	UNP P51654
D	484	GLY	-	expression tag	UNP P51654
D	485	THR	-	expression tag	UNP P51654
D	486	LYS	-	expression tag	UNP P51654
D	487	HIS	-	expression tag	UNP P51654
D	488	HIS	-	expression tag	UNP P51654
D	489	HIS	-	expression tag	UNP P51654
D	490	HIS	-	expression tag	UNP P51654
D	491	HIS	-	expression tag	UNP P51654
D	492	HIS	-	expression tag	UNP P51654
B	29	GLU	-	expression tag	UNP P51654
B	30	THR	-	expression tag	UNP P51654
B	31	GLY	-	expression tag	UNP P51654
B	359	PHE	SER	variant	UNP P51654
B	484	GLY	-	expression tag	UNP P51654
B	485	THR	-	expression tag	UNP P51654
B	486	LYS	-	expression tag	UNP P51654
B	487	HIS	-	expression tag	UNP P51654
B	488	HIS	-	expression tag	UNP P51654
B	489	HIS	-	expression tag	UNP P51654
B	490	HIS	-	expression tag	UNP P51654
B	491	HIS	-	expression tag	UNP P51654
B	492	HIS	-	expression tag	UNP P51654

- Molecule 3 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
3	I	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

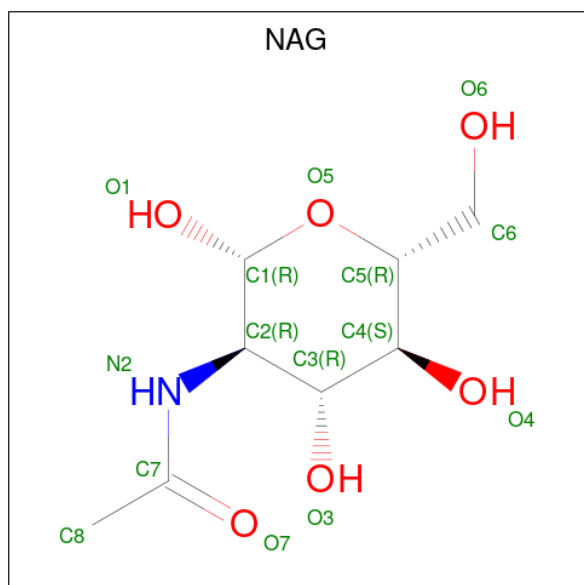
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose

e-(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
4	J	4	Total 97	C 28	H 47	N 2	O 20	11	0	0
4	K	4	Total 97	C 28	H 47	N 2	O 20	11	0	0
4	M	4	Total 97	C 28	H 47	N 2	O 20	11	0	0
4	N	4	Total 97	C 28	H 47	N 2	O 20	11	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



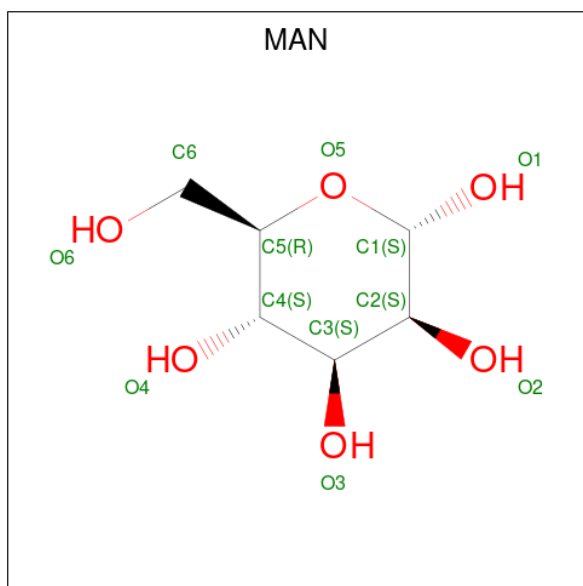
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total 28	C 8	H 14	N 1	O 5	3	0
5	E	1	Total 28	C 8	H 14	N 1	O 5	3	0
5	F	1	Total 28	C 8	H 14	N 1	O 5	3	0
5	F	1	Total 28	C 8	H 14	N 1	O 5	3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	H	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	C	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	D	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 6 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	H	O	4	0
			22	6	11	5		
6	E	1	Total	C	H	O	4	0
			22	6	11	5		
6	F	1	Total	C	H	O	4	0
			22	6	11	5		

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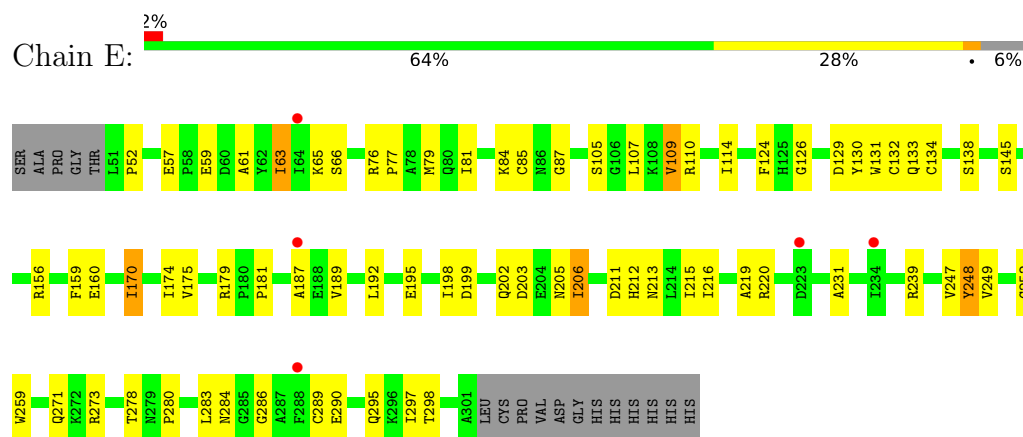
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	H	O	4	0
			22	6	11	5		
6	H	1	Total	C	H	O	4	0
			22	6	11	5		
6	H	1	Total	C	H	O	4	0
			22	6	11	5		

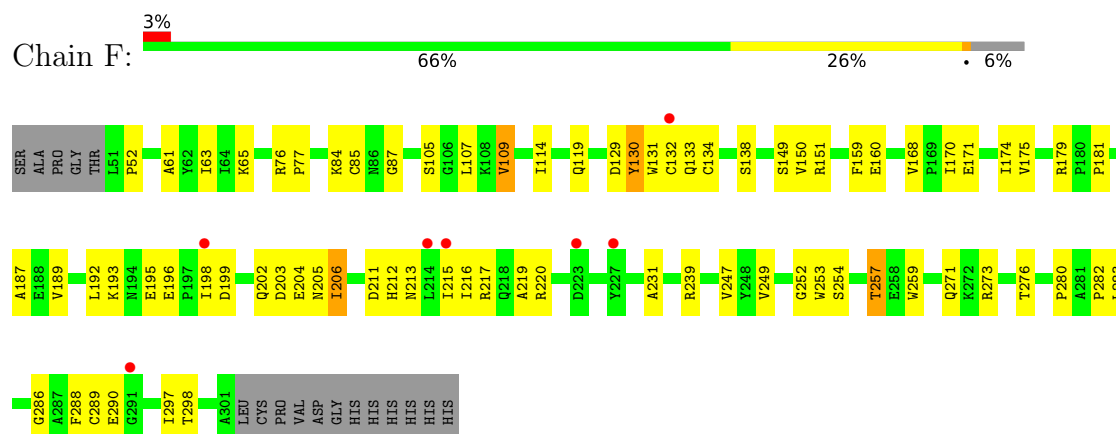
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

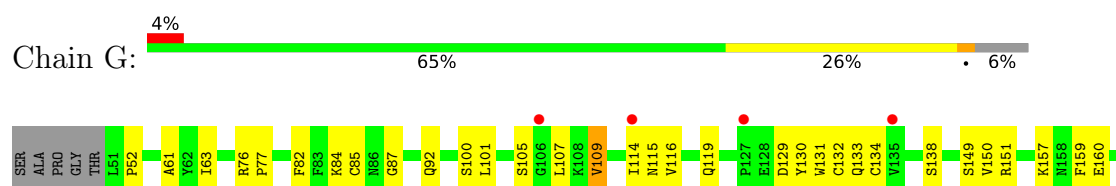
• Molecule 1: Netrin receptor UNC5D

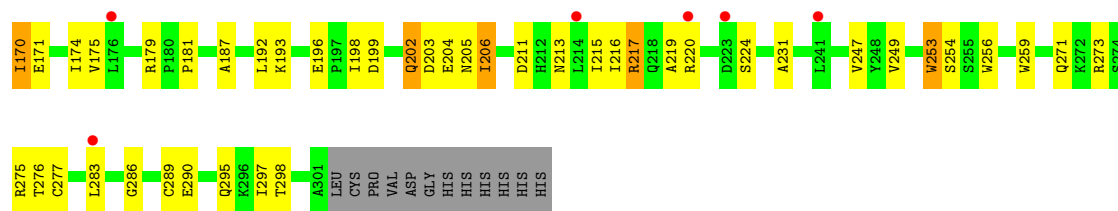


• Molecule 1: Netrin receptor UNC5D

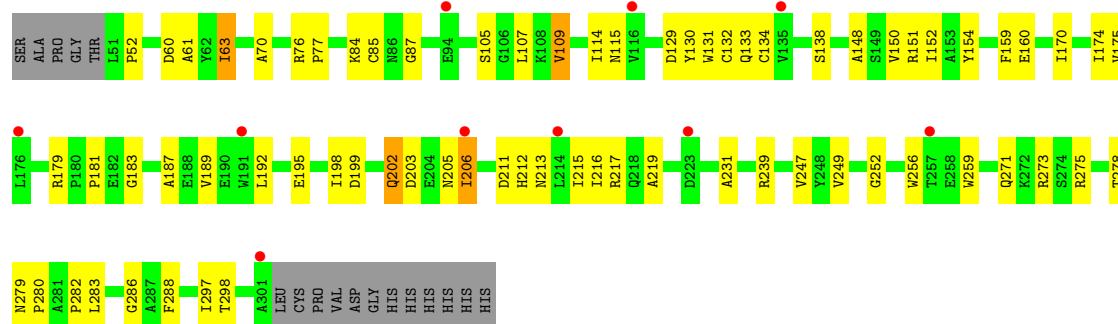


• Molecule 1: Netrin receptor UNC5D

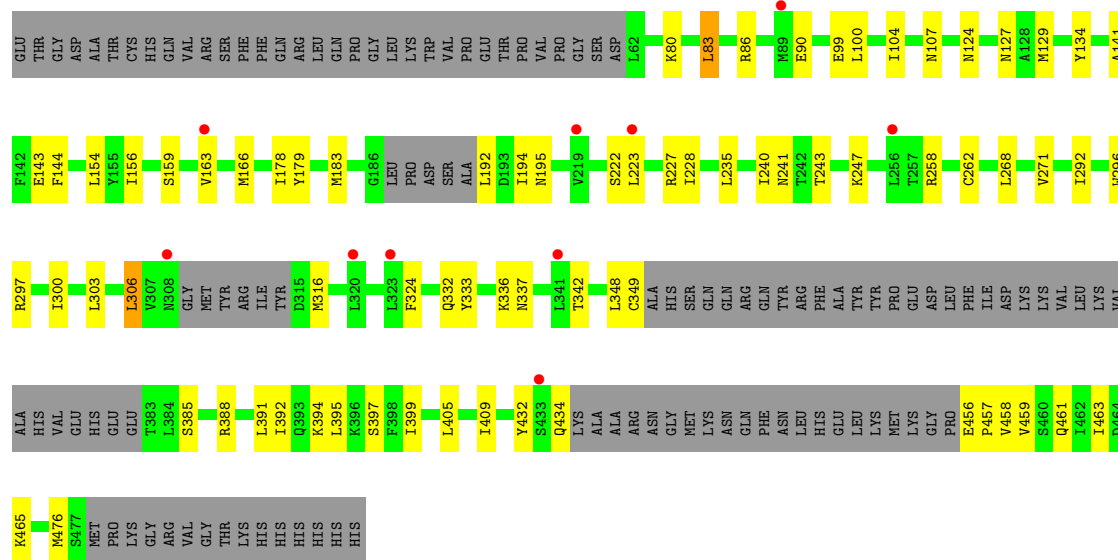




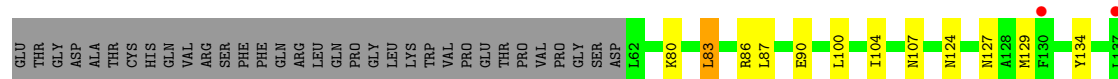
● Molecule 1: Netrin receptor UNC5D

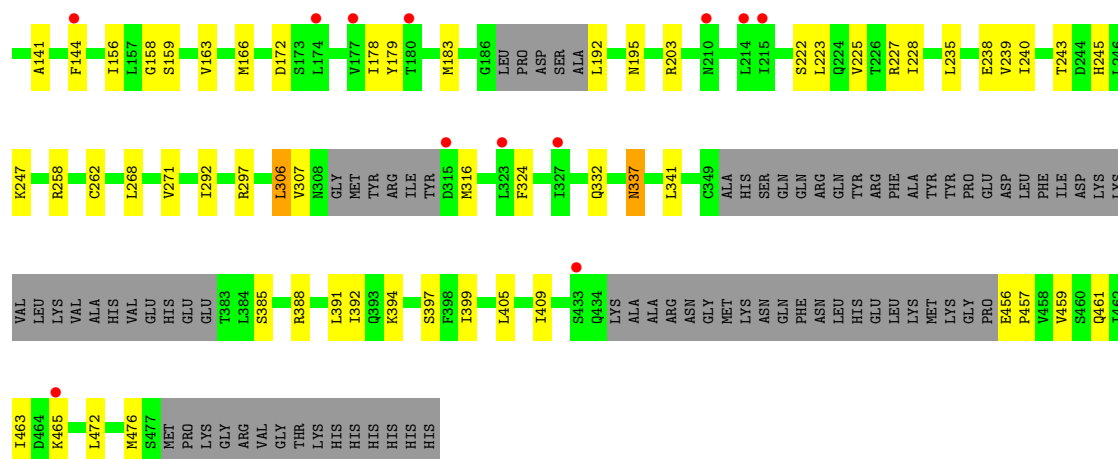


● Molecule 2: Glypican-3

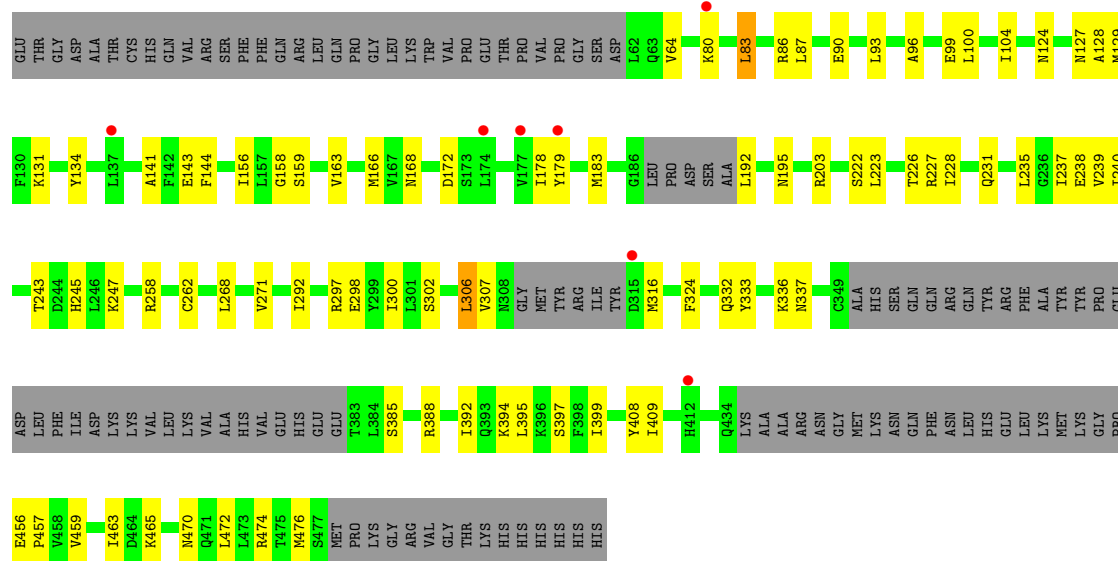


● Molecule 2: Glypican-3

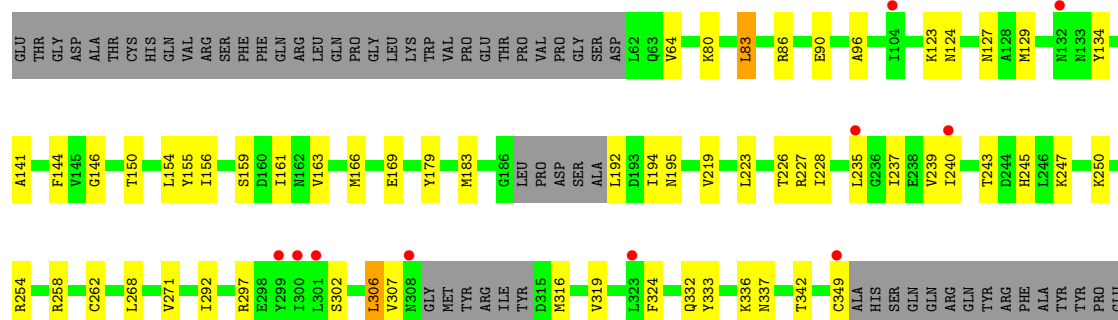


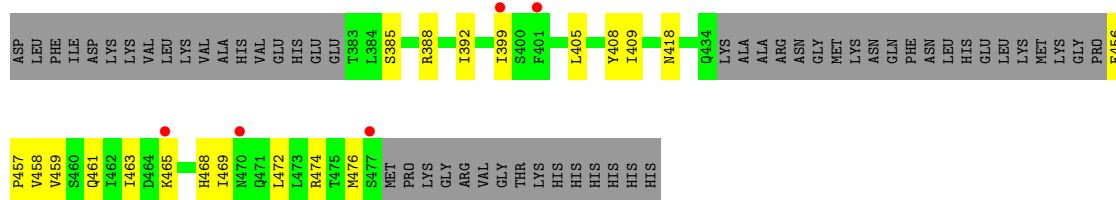


• Molecule 2: Glypican-3



• Molecule 2: Glypican-3





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



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

Chain J: 50%



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

Chain K: 50%



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

Chain M: 50%



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

Chain N: 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.64Å 157.58Å 126.60Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	97.34 – 4.10 97.34 – 4.10	Depositor EDS
% Data completeness (in resolution range)	59.5 (97.34-4.10) 59.5 (97.34-4.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 4.15Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.324 , 0.365 0.323 , 0.364	Depositor DCC
R_{free} test set	899 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	158.7	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 158.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	39050	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	E	0.80	0/2038	0.72	2/2764 (0.1%)
1	F	0.82	1/2038 (0.0%)	0.76	0/2764
1	G	0.81	0/2038	0.75	1/2764 (0.0%)
1	H	0.81	0/2038	0.70	0/2764
2	A	0.80	0/2855	0.69	0/3849
2	B	0.81	0/2855	0.70	0/3849
2	C	0.81	0/2855	0.70	0/3849
2	D	0.81	0/2847	0.70	0/3839
All	All	0.81	1/19564 (0.0%)	0.71	3/26442 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	257	THR	N-CA	5.87	1.53	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	217	ARG	CG-CD-NE	-6.39	97.94	112.00
1	E	248	TYR	CA-CB-CG	5.56	123.91	113.90
1	E	248	TYR	CB-CA-C	5.05	118.48	109.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1991	1912	1905	79	0
1	F	1991	1912	1906	87	0
1	G	1991	1915	1907	83	0
1	H	1991	1912	1905	44	0
2	A	2807	2827	2816	57	0
2	B	2807	2827	2817	66	0
2	C	2807	2828	2818	56	0
2	D	2799	2822	2808	72	0
3	I	28	27	25	0	0
4	J	50	47	43	2	0
4	K	50	47	43	9	0
4	M	50	47	43	3	0
4	N	50	47	43	4	0
5	A	28	28	26	0	0
5	B	28	28	26	3	0
5	C	14	14	13	0	0
5	D	14	14	12	22	0
5	E	28	28	26	0	0
5	F	28	28	26	0	0
5	H	28	28	26	1	0
6	E	22	22	20	1	0
6	F	22	22	20	2	0
6	H	22	22	20	0	0
All	All	19646	19404	19294	475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (475) 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:F:253:TRP:CZ3	1:F:289:CYS:HB3	1.13	1.64
2:D:131:LYS:NZ	5:D:501:NAG:H82	1.35	1.41
1:F:253:TRP:CZ3	1:F:289:CYS:CB	2.02	1.41
1:F:119:GLN:OE1	5:D:501:NAG:C6	1.67	1.40
1:F:253:TRP:CH2	1:F:289:CYS:HB3	1.64	1.30
2:C:245:HIS:CG	4:K:1:NAG:O6	1.95	1.20
2:B:245:HIS:CD2	4:N:1:NAG:H62	1.81	1.12
2:D:131:LYS:CE	5:D:501:NAG:H82	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:GLN:CD	5:D:501:NAG:C6	2.32	1.01
1:G:253:TRP:CE2	1:G:289:CYS:HB3	1.97	1.00
1:G:253:TRP:CZ2	1:G:289:CYS:HB3	1.95	1.00
1:E:256:TRP:CE3	1:E:273:ARG:HG2	1.96	0.99
2:D:131:LYS:NZ	5:D:501:NAG:C8	2.26	0.97
1:E:256:TRP:HE3	1:E:273:ARG:HG2	1.28	0.96
1:F:119:GLN:OE1	5:D:501:NAG:H61	1.61	0.96
2:D:131:LYS:HZ1	5:D:501:NAG:H82	1.12	0.94
1:E:220:ARG:CZ	2:B:461:GLN:HG2	1.97	0.93
1:H:279:ASN:ND2	4:M:2:NAG:O6	2.03	0.92
1:F:253:TRP:HZ3	1:F:289:CYS:HB3	1.18	0.92
6:F:403:MAN:H4	4:K:4:MAN:O5	1.69	0.91
2:C:245:HIS:CD2	4:K:1:NAG:O6	2.25	0.89
1:E:220:ARG:NH1	2:B:461:GLN:CG	2.36	0.89
1:F:217:ARG:HB3	1:G:217:ARG:NH2	1.88	0.89
1:E:256:TRP:CH2	1:E:295:GLN:HB2	2.08	0.89
1:E:59:GLU:OE1	2:D:87:LEU:HD13	1.73	0.88
1:E:220:ARG:HH12	2:B:461:GLN:NE2	1.69	0.88
2:D:131:LYS:HE3	5:D:501:NAG:C8	2.04	0.87
1:E:253:TRP:CH2	1:E:289:CYS:HB3	2.10	0.87
1:F:253:TRP:CE3	1:F:289:CYS:SG	2.69	0.86
2:D:131:LYS:NZ	5:D:501:NAG:O3	2.10	0.84
1:F:217:ARG:HB3	1:G:217:ARG:CZ	2.08	0.84
2:D:131:LYS:CE	5:D:501:NAG:C8	2.55	0.84
2:B:228:ILE:HD11	2:B:472:LEU:HB3	1.58	0.83
1:G:256:TRP:HE3	1:G:273:ARG:HG2	1.43	0.83
1:G:119:GLN:NE2	5:B:501:NAG:H83	1.94	0.82
2:D:128:ALA:HA	5:D:501:NAG:H81	1.61	0.82
2:D:131:LYS:HZ2	5:D:501:NAG:H82	1.43	0.82
1:F:217:ARG:HB3	1:G:217:ARG:NH1	1.97	0.80
2:C:228:ILE:HD11	2:C:472:LEU:HB3	1.64	0.80
1:E:220:ARG:HH12	2:B:461:GLN:HE21	1.26	0.80
1:F:253:TRP:CH2	1:F:290:GLU:N	2.50	0.79
2:C:245:HIS:CD2	4:K:1:NAG:C6	2.66	0.78
2:C:297:ARG:HG2	2:C:399:ILE:HG12	1.66	0.77
2:D:297:ARG:HG2	2:D:399:ILE:HG12	1.67	0.77
1:F:65:LYS:O	2:D:143:GLU:OE2	2.03	0.76
2:B:156:ILE:HD11	2:B:223:LEU:HD22	1.66	0.76
2:A:156:ILE:HD11	2:A:223:LEU:HD22	1.65	0.76
1:G:119:GLN:HE21	5:B:501:NAG:H83	1.52	0.75
2:C:245:HIS:CG	4:K:1:NAG:HO6	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:ALA:HA	5:D:501:NAG:C8	2.17	0.75
1:E:220:ARG:NH1	2:B:461:GLN:HG2	2.01	0.74
1:F:119:GLN:NE2	5:D:501:NAG:C6	2.49	0.74
2:B:297:ARG:HG2	2:B:399:ILE:HG12	1.67	0.74
2:D:245:HIS:CD2	4:M:1:NAG:HO6	2.05	0.73
1:E:220:ARG:CZ	2:B:461:GLN:CG	2.64	0.73
1:G:253:TRP:CH2	1:G:289:CYS:HB3	2.23	0.72
2:D:245:HIS:CD2	4:M:1:NAG:O6	2.42	0.72
1:G:253:TRP:HZ2	1:G:290:GLU:C	1.96	0.72
2:D:156:ILE:HD11	2:D:223:LEU:HD22	1.71	0.72
2:C:156:ILE:HD11	2:C:223:LEU:HD22	1.70	0.72
1:E:253:TRP:HZ2	1:E:290:GLU:O	1.73	0.71
1:G:254:SER:OG	1:G:276:THR:N	2.24	0.70
2:D:228:ILE:HD11	2:D:472:LEU:HB3	1.72	0.70
1:F:253:TRP:CH2	1:F:289:CYS:CB	2.52	0.70
1:F:253:TRP:CZ3	1:F:289:CYS:SG	2.83	0.70
2:B:90:GLU:OE2	2:B:247:LYS:NZ	2.25	0.70
1:F:217:ARG:HB3	1:G:217:ARG:HH22	1.57	0.69
1:E:129:ASP:HB3	1:E:151:ARG:HD3	1.73	0.69
2:A:159:SER:O	2:A:227:ARG:NH2	2.24	0.69
2:D:307:VAL:HG11	2:D:392:ILE:HG13	1.73	0.69
1:F:253:TRP:HH2	1:F:290:GLU:N	1.89	0.69
1:F:217:ARG:CB	1:G:217:ARG:NH2	2.56	0.69
1:E:220:ARG:NH1	2:B:461:GLN:NE2	2.40	0.69
2:D:240:ILE:O	2:D:243:THR:OG1	2.11	0.68
1:F:288:PHE:CE1	2:C:158:GLY:HA3	2.29	0.68
2:A:297:ARG:HG2	2:A:399:ILE:HG12	1.75	0.68
1:E:284:ASN:ND2	2:B:468:HIS:CE1	2.61	0.68
1:E:253:TRP:HZ2	1:E:290:GLU:C	2.02	0.67
1:F:204:GLU:HG2	1:G:204:GLU:CD	2.19	0.67
1:F:119:GLN:OE1	5:D:501:NAG:O6	2.12	0.67
1:F:252:GLY:HA3	1:F:280:PRO:HD2	1.76	0.67
2:A:235:LEU:HD11	2:A:465:LYS:HB3	1.76	0.67
1:G:256:TRP:CZ3	1:G:295:GLN:HB2	2.30	0.67
1:G:129:ASP:HB3	1:G:151:ARG:HD3	1.77	0.67
1:G:157:LYS:HE3	2:B:169:GLU:HG3	1.77	0.66
1:E:205:ASN:HD21	1:E:216:ILE:HG23	1.59	0.66
1:G:220:ARG:HH12	2:A:461:GLN:HE21	1.42	0.66
1:F:220:ARG:CZ	2:C:461:GLN:CD	2.68	0.66
2:A:129:MET:HG3	2:A:324:PHE:CD2	2.31	0.66
2:D:159:SER:O	2:D:227:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:ILE:O	2:A:243:THR:OG1	2.14	0.65
2:C:245:HIS:CD2	4:K:1:NAG:H62	2.30	0.65
1:F:204:GLU:HG2	1:G:204:GLU:HG2	1.78	0.65
2:D:134:TYR:OH	2:D:332:GLN:OE1	2.15	0.65
1:G:220:ARG:CZ	2:A:461:GLN:HG2	2.27	0.65
1:E:256:TRP:CE3	1:E:273:ARG:CG	2.79	0.64
1:G:256:TRP:CE3	1:G:273:ARG:NE	2.65	0.64
1:F:217:ARG:CB	1:G:217:ARG:HH22	2.10	0.64
1:E:253:TRP:CZ2	1:E:290:GLU:O	2.51	0.64
2:B:240:ILE:O	2:B:243:THR:OG1	2.16	0.64
1:F:220:ARG:NH2	2:C:461:GLN:CD	2.56	0.63
1:F:119:GLN:HE22	5:D:501:NAG:C6	2.09	0.63
1:H:76:ARG:HD3	1:H:109:VAL:HG22	1.80	0.63
1:F:253:TRP:CH2	1:F:289:CYS:C	2.77	0.63
1:G:61:ALA:HB3	1:G:150:VAL:HG22	1.81	0.63
1:H:76:ARG:HD2	1:H:107:LEU:HB3	1.80	0.63
2:C:159:SER:O	2:C:227:ARG:NH2	2.31	0.63
1:F:76:ARG:HD2	1:F:107:LEU:HB3	1.81	0.63
2:B:124:ASN:HA	2:B:127:ASN:HB2	1.81	0.63
1:G:175:VAL:HG22	1:G:215:ILE:HG23	1.81	0.63
2:D:129:MET:HG3	2:D:324:PHE:CD2	2.33	0.63
1:H:252:GLY:HA3	1:H:280:PRO:HD2	1.81	0.63
1:E:52:PRO:HG3	1:E:138:SER:HB2	1.81	0.62
2:B:245:HIS:NE2	4:N:1:NAG:H62	2.13	0.62
1:E:220:ARG:NH1	2:B:461:GLN:CD	2.58	0.62
1:E:220:ARG:CZ	2:B:461:GLN:CD	2.73	0.62
1:H:288:PHE:CD1	2:D:158:GLY:HA3	2.34	0.62
1:F:220:ARG:CZ	2:C:461:GLN:CG	2.78	0.62
1:G:52:PRO:HG3	1:G:138:SER:HB2	1.81	0.62
2:C:307:VAL:HG11	2:C:392:ILE:HG13	1.82	0.61
1:G:76:ARG:HH12	1:G:105:SER:HB2	1.65	0.61
1:E:131:TRP:HA	1:E:149:SER:HA	1.81	0.61
2:B:159:SER:O	2:B:227:ARG:NH2	2.33	0.61
1:G:253:TRP:CD2	1:G:289:CYS:HB3	2.35	0.61
2:C:80:LYS:HA	2:C:83:LEU:HD23	1.83	0.61
1:F:76:ARG:HD3	1:F:109:VAL:HG22	1.82	0.61
1:F:205:ASN:OD1	1:F:217:ARG:HG3	2.01	0.61
1:E:253:TRP:CZ2	1:E:289:CYS:HB3	2.34	0.61
1:E:253:TRP:CZ3	1:E:289:CYS:HB3	2.35	0.61
1:G:220:ARG:CZ	2:A:461:GLN:CG	2.79	0.60
2:C:90:GLU:OE2	2:C:247:LYS:NZ	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:LEU:HD11	2:B:465:LYS:HB3	1.83	0.60
1:G:254:SER:OG	1:G:275:ARG:HA	2.00	0.60
1:G:256:TRP:HZ3	1:G:295:GLN:HB2	1.66	0.60
2:A:178:ILE:HG22	2:A:183:MET:HE2	1.82	0.60
2:B:306:LEU:HD11	2:B:476:MET:HB2	1.84	0.60
2:D:90:GLU:OE2	2:D:247:LYS:NZ	2.32	0.60
2:B:307:VAL:HG11	2:B:392:ILE:HG13	1.84	0.60
1:F:175:VAL:HG22	1:F:215:ILE:HG23	1.83	0.60
2:C:129:MET:HG3	2:C:324:PHE:CD2	2.36	0.60
1:F:249:VAL:O	1:F:286:GLY:HA3	2.02	0.60
1:F:52:PRO:HG3	1:F:138:SER:HB2	1.84	0.60
1:H:175:VAL:HG22	1:H:215:ILE:HG23	1.83	0.60
2:D:124:ASN:HA	2:D:127:ASN:HB2	1.84	0.60
1:G:256:TRP:CE3	1:G:273:ARG:HG2	2.32	0.59
1:F:253:TRP:HZ3	1:F:289:CYS:CB	1.86	0.59
1:F:220:ARG:NH1	2:C:461:GLN:CG	2.66	0.59
1:G:253:TRP:CH2	1:G:289:CYS:CB	2.85	0.59
2:A:90:GLU:OE2	2:A:247:LYS:NZ	2.31	0.59
1:E:76:ARG:HH12	1:E:105:SER:HB2	1.67	0.59
1:F:217:ARG:HB3	1:G:217:ARG:HH12	1.68	0.59
2:A:80:LYS:HA	2:A:83:LEU:HD23	1.84	0.59
1:E:284:ASN:HD21	2:B:468:HIS:CE1	2.20	0.59
1:G:253:TRP:C	1:G:276:THR:O	2.46	0.58
1:F:65:LYS:HB3	2:D:143:GLU:CD	2.28	0.58
1:G:76:ARG:HD3	1:G:109:VAL:HG22	1.85	0.58
1:E:220:ARG:NH2	2:B:461:GLN:CD	2.62	0.58
1:G:256:TRP:CH2	1:G:295:GLN:NE2	2.72	0.58
1:H:256:TRP:CH2	1:H:275:ARG:HD2	2.39	0.58
1:F:76:ARG:HH12	1:F:105:SER:HB2	1.68	0.58
1:H:52:PRO:HG3	1:H:138:SER:HB2	1.83	0.58
1:H:288:PHE:CE1	2:D:158:GLY:HA3	2.39	0.58
2:B:134:TYR:OH	2:B:332:GLN:OE1	2.19	0.58
2:B:385:SER:HA	2:B:388:ARG:HD3	1.86	0.58
1:G:76:ARG:HD2	1:G:107:LEU:HB3	1.84	0.58
2:C:245:HIS:CB	4:K:1:NAG:O6	2.51	0.58
1:E:59:GLU:CD	2:D:87:LEU:HD13	2.28	0.58
1:F:204:GLU:HG2	1:G:204:GLU:CG	2.33	0.58
1:H:282:PRO:HG2	1:H:288:PHE:CD2	2.39	0.58
1:H:76:ARG:HB2	1:H:109:VAL:HG13	1.86	0.58
2:D:80:LYS:HA	2:D:83:LEU:HD23	1.86	0.58
2:D:131:LYS:HZ2	5:D:501:NAG:C8	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ARG:HB2	1:F:109:VAL:HG13	1.86	0.57
1:F:211:ASP:OD2	1:F:213:ASN:ND2	2.37	0.57
2:C:240:ILE:O	2:C:243:THR:OG1	2.17	0.57
2:B:245:HIS:CD2	4:N:1:NAG:C6	2.74	0.57
1:G:253:TRP:CZ2	1:G:289:CYS:CB	2.82	0.57
1:E:175:VAL:HG22	1:E:215:ILE:HG23	1.86	0.57
1:F:65:LYS:C	2:D:143:GLU:HG2	2.29	0.57
1:F:129:ASP:HB3	1:F:151:ARG:HD3	1.86	0.57
1:F:220:ARG:CZ	2:C:461:GLN:HG2	2.35	0.57
1:G:211:ASP:OD2	1:G:213:ASN:ND2	2.38	0.57
2:D:306:LEU:HD11	2:D:476:MET:HB2	1.86	0.56
2:A:134:TYR:OH	2:A:332:GLN:OE1	2.23	0.56
1:E:187:ALA:HB1	1:E:231:ALA:HB1	1.87	0.56
1:H:283:LEU:HD21	2:D:235:LEU:CD1	2.35	0.56
2:C:163:VAL:HA	2:C:166:MET:HE3	1.88	0.56
1:E:160:GLU:HB3	1:E:179:ARG:HB3	1.88	0.56
1:F:199:ASP:HB3	1:F:202:GLN:HB2	1.87	0.56
1:E:211:ASP:OD2	1:E:213:ASN:ND2	2.39	0.56
1:H:76:ARG:HH12	1:H:105:SER:HB2	1.70	0.56
1:F:253:TRP:CZ2	1:F:290:GLU:O	2.59	0.56
1:G:283:LEU:HD21	2:A:235:LEU:CD1	2.36	0.56
1:F:52:PRO:HA	1:F:77:PRO:HD2	1.87	0.55
2:D:131:LYS:HE3	5:D:501:NAG:H81	1.86	0.55
1:G:220:ARG:NH1	2:A:461:GLN:HE21	2.03	0.55
1:E:256:TRP:CD2	1:E:273:ARG:NE	2.74	0.55
1:E:249:VAL:O	1:E:286:GLY:HA3	2.07	0.55
1:H:199:ASP:HB3	1:H:202:GLN:HB2	1.87	0.55
1:H:211:ASP:OD2	1:H:213:ASN:ND2	2.39	0.55
2:A:124:ASN:HA	2:A:127:ASN:HB2	1.89	0.55
1:E:256:TRP:HZ3	1:E:273:ARG:O	1.90	0.55
1:H:70:ALA:HB2	1:H:115:ASN:OD1	2.07	0.54
2:B:250:LYS:HE3	2:B:254:ARG:HH12	1.72	0.54
1:H:249:VAL:O	1:H:286:GLY:HA3	2.07	0.54
2:C:222:SER:HB2	2:C:316:MET:HA	1.90	0.54
2:B:141:ALA:HA	2:B:144:PHE:CZ	2.42	0.54
1:F:171:GLU:OE1	1:F:220:ARG:NE	2.41	0.54
1:E:76:ARG:HD2	1:E:107:LEU:HB3	1.90	0.54
2:A:141:ALA:HA	2:A:144:PHE:CZ	2.43	0.54
2:B:80:LYS:HA	2:B:83:LEU:HD23	1.89	0.54
1:G:76:ARG:HB2	1:G:109:VAL:HG13	1.89	0.53
2:A:222:SER:HB2	2:A:316:MET:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:ALA:HA	2:D:144:PHE:CZ	2.43	0.53
1:E:52:PRO:HA	1:E:77:PRO:HD2	1.90	0.53
6:E:403:MAN:H4	4:N:4:MAN:O2	2.08	0.53
2:A:163:VAL:HA	2:A:166:MET:HE3	1.89	0.53
2:B:163:VAL:HA	2:B:166:MET:HE3	1.89	0.53
2:A:194:ILE:HG12	2:A:349:CYS:HB3	1.90	0.53
2:C:141:ALA:HA	2:C:144:PHE:CZ	2.44	0.53
1:F:254:SER:HB3	1:F:276:THR:O	2.09	0.53
1:G:203:ASP:HB3	1:G:206:ILE:HD12	1.92	0.52
1:F:253:TRP:HH2	1:F:289:CYS:C	2.15	0.52
1:H:205:ASN:HD21	1:H:216:ILE:HG23	1.74	0.52
1:G:205:ASN:HD21	1:G:216:ILE:HG23	1.74	0.52
1:E:76:ARG:HD3	1:E:109:VAL:HG22	1.92	0.52
1:F:195:GLU:OE1	1:F:239:ARG:NH1	2.43	0.52
2:D:128:ALA:HB2	5:D:501:NAG:C7	2.40	0.52
1:H:129:ASP:HB3	1:H:151:ARG:HD3	1.91	0.52
1:H:159:PHE:HA	1:H:181:PRO:HG3	1.91	0.52
1:E:199:ASP:HB3	1:E:202:GLN:HB2	1.90	0.51
1:H:205:ASN:OD1	1:H:217:ARG:HG3	2.10	0.51
1:E:76:ARG:HB2	1:E:109:VAL:HG13	1.91	0.51
2:C:337:ASN:HB3	2:C:341:LEU:HD13	1.92	0.51
1:F:61:ALA:HB3	1:F:150:VAL:HG22	1.92	0.51
1:F:187:ALA:HB1	1:F:231:ALA:HB1	1.93	0.51
1:H:115:ASN:OD1	5:H:404:NAG:O5	2.19	0.51
2:D:222:SER:HB2	2:D:316:MET:HA	1.93	0.51
2:A:432:TYR:CE2	2:A:434:GLN:HG2	2.46	0.51
1:F:203:ASP:HB3	1:F:206:ILE:HD12	1.93	0.51
2:D:456:GLU:N	2:D:457:PRO:HD2	2.26	0.51
1:E:252:GLY:HA3	1:E:280:PRO:HD2	1.92	0.51
1:E:283:LEU:HD22	2:B:468:HIS:HD2	1.76	0.51
1:G:220:ARG:NH2	2:A:461:GLN:NE2	2.59	0.51
1:H:187:ALA:HB1	1:H:231:ALA:HB1	1.91	0.51
2:A:179:TYR:HE1	2:A:342:THR:HA	1.75	0.51
1:E:203:ASP:HB3	1:E:206:ILE:HD12	1.93	0.51
1:F:254:SER:OG	1:F:276:THR:N	2.43	0.51
1:H:52:PRO:HA	1:H:77:PRO:HD2	1.92	0.51
2:B:456:GLU:N	2:B:457:PRO:HD2	2.25	0.51
1:E:278:THR:HG21	2:B:237:ILE:HB	1.93	0.50
1:G:253:TRP:CZ2	1:G:289:CYS:C	2.89	0.50
2:C:394:LYS:O	2:C:397:SER:OG	2.29	0.50
1:F:65:LYS:O	2:D:143:GLU:CD	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASN:OD1	2:C:124:ASN:O	2.28	0.50
1:G:187:ALA:HB1	1:G:231:ALA:HB1	1.93	0.50
1:G:52:PRO:HA	1:G:77:PRO:HD2	1.93	0.50
1:E:61:ALA:HB3	1:E:150:VAL:HG22	1.94	0.50
1:E:220:ARG:NH1	2:B:461:GLN:HG3	2.26	0.50
2:D:163:VAL:HA	2:D:166:MET:HE3	1.93	0.50
2:D:172:ASP:OD2	2:D:203:ARG:NH1	2.43	0.50
1:G:220:ARG:NH1	2:A:461:GLN:CG	2.75	0.49
1:G:131:TRP:HZ3	1:G:133:GLN:HB2	1.77	0.49
1:G:159:PHE:HA	1:G:181:PRO:HG3	1.94	0.49
1:G:220:ARG:NH1	2:A:461:GLN:NE2	2.58	0.49
2:C:172:ASP:OD2	2:C:203:ARG:NH1	2.45	0.49
2:C:456:GLU:N	2:C:457:PRO:HD2	2.27	0.49
2:B:457:PRO:O	2:B:461:GLN:HG3	2.13	0.49
1:G:100:SER:O	1:G:101:LEU:HD22	2.13	0.49
1:G:199:ASP:HB3	1:G:202:GLN:HB2	1.94	0.49
1:E:195:GLU:OE1	1:E:239:ARG:NH1	2.45	0.49
2:A:458:VAL:HA	2:A:461:GLN:NE2	2.27	0.49
2:A:192:LEU:O	2:A:195:ASN:HB2	2.13	0.48
2:B:123:LYS:HE2	2:B:146:GLY:HA2	1.95	0.48
2:A:385:SER:HA	2:A:388:ARG:HD3	1.94	0.48
2:A:456:GLU:N	2:A:457:PRO:HD2	2.27	0.48
2:D:292:ILE:HD11	2:D:459:VAL:HG13	1.94	0.48
1:E:219:ALA:HB1	1:E:247:VAL:HG11	1.95	0.48
1:F:271:GLN:HG2	1:F:297:ILE:O	2.13	0.48
1:G:220:ARG:NH2	2:A:461:GLN:CD	2.72	0.48
2:D:128:ALA:CA	5:D:501:NAG:C8	2.90	0.48
1:G:85:CYS:HA	1:G:132:CYS:HA	1.94	0.48
1:E:66:SER:HB3	2:A:143:GLU:HG2	1.96	0.48
1:E:253:TRP:CH2	1:E:289:CYS:CB	2.90	0.48
1:G:131:TRP:HA	1:G:149:SER:HA	1.95	0.48
2:D:235:LEU:HD11	2:D:465:LYS:HB3	1.95	0.48
2:B:64:VAL:HG22	2:B:254:ARG:HG2	1.96	0.48
1:G:220:ARG:HH22	2:A:461:GLN:NE2	2.12	0.48
2:D:394:LYS:O	2:D:397:SER:OG	2.31	0.48
2:D:333:TYR:O	2:D:336:LYS:HG2	2.14	0.48
1:F:253:TRP:CH2	1:F:289:CYS:CA	2.96	0.48
2:A:303:LEU:HG	2:A:392:ILE:HD11	1.96	0.48
2:B:292:ILE:HD11	2:B:459:VAL:HG13	1.94	0.48
2:B:302:SER:OG	2:B:474:ARG:NH1	2.46	0.48
1:H:256:TRP:CZ3	1:H:275:ARG:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:TRP:HZ3	1:E:133:GLN:HB2	1.79	0.47
1:G:171:GLU:OE1	1:G:220:ARG:NE	2.47	0.47
1:H:195:GLU:OE1	1:H:239:ARG:NH1	2.47	0.47
1:G:271:GLN:HG2	1:G:297:ILE:O	2.15	0.47
2:A:179:TYR:HA	2:A:183:MET:HE3	1.96	0.47
2:D:178:ILE:HG22	2:D:183:MET:HE2	1.95	0.47
1:G:220:ARG:CZ	2:A:461:GLN:CD	2.87	0.47
1:H:85:CYS:HA	1:H:132:CYS:HA	1.95	0.47
1:H:203:ASP:HB3	1:H:206:ILE:HD12	1.96	0.47
1:H:271:GLN:HG2	1:H:297:ILE:O	2.13	0.47
1:H:288:PHE:HZ	2:D:231:GLN:HG2	1.80	0.47
2:C:124:ASN:HA	2:C:127:ASN:HB2	1.96	0.47
1:E:85:CYS:HA	1:E:132:CYS:HA	1.96	0.47
1:F:131:TRP:HA	1:F:149:SER:HA	1.97	0.47
1:F:220:ARG:NH1	2:C:461:GLN:OE1	2.47	0.47
1:F:85:CYS:HA	1:F:132:CYS:HA	1.96	0.47
1:F:220:ARG:NH2	2:C:461:GLN:OE1	2.48	0.47
1:G:253:TRP:HA	1:G:277:CYS:HA	1.97	0.47
1:H:131:TRP:HZ3	1:H:133:GLN:HB2	1.79	0.47
2:D:86:ARG:O	2:D:90:GLU:HG3	2.15	0.47
1:E:284:ASN:CG	2:B:468:HIS:NE2	2.73	0.47
2:A:306:LEU:HD11	2:A:476:MET:HB2	1.97	0.47
2:C:306:LEU:HD11	2:C:476:MET:HB2	1.96	0.47
2:B:192:LEU:O	2:B:195:ASN:HB2	2.14	0.47
2:D:131:LYS:HZ1	5:D:501:NAG:C8	2.04	0.47
2:B:86:ARG:O	2:B:90:GLU:HG3	2.15	0.47
2:C:179:TYR:HA	2:C:183:MET:HE3	1.96	0.46
2:B:129:MET:HG3	2:B:324:PHE:CD2	2.51	0.46
1:E:284:ASN:ND2	2:B:468:HIS:NE2	2.62	0.46
2:D:239:VAL:O	2:D:243:THR:HG23	2.15	0.46
2:D:302:SER:OG	2:D:474:ARG:NH1	2.48	0.46
1:E:248:TYR:CE1	1:E:286:GLY:HA2	2.51	0.46
1:F:219:ALA:HB1	1:F:247:VAL:HG11	1.97	0.46
1:G:283:LEU:HD21	2:A:235:LEU:HD12	1.97	0.46
2:C:292:ILE:HD11	2:C:459:VAL:HG13	1.98	0.46
2:D:168:ASN:HB3	2:D:203:ARG:HH12	1.80	0.46
1:H:63:ILE:HG22	1:H:152:ILE:HA	1.96	0.46
2:B:459:VAL:O	2:B:463:ILE:HG13	2.15	0.46
1:E:256:TRP:HB3	1:E:273:ARG:HD2	1.98	0.46
1:G:283:LEU:HD12	2:A:465:LYS:HG2	1.98	0.46
2:C:86:ARG:O	2:C:90:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:238:GLU:OE2	2:C:465:LYS:NZ	2.46	0.46
1:E:77:PRO:HB3	1:E:107:LEU:HD21	1.98	0.46
6:F:403:MAN:H4	4:K:4:MAN:C5	2.45	0.46
1:G:160:GLU:HB3	1:G:179:ARG:HB3	1.97	0.46
2:C:235:LEU:HD11	2:C:465:LYS:HB3	1.98	0.46
2:B:179:TYR:HA	2:B:183:MET:HE3	1.98	0.46
1:F:159:PHE:HA	1:F:181:PRO:HG3	1.98	0.45
2:D:238:GLU:OE2	2:D:465:LYS:NZ	2.43	0.45
2:B:268:LEU:HD13	2:B:271:VAL:HG21	1.99	0.45
1:F:189:VAL:HG11	1:F:212:HIS:HB3	1.98	0.45
1:E:253:TRP:CZ3	1:E:289:CYS:CB	2.99	0.45
1:E:271:GLN:HG2	1:E:297:ILE:O	2.16	0.45
2:D:100:LEU:O	2:D:104:ILE:HG13	2.17	0.45
2:D:124:ASN:OD1	2:D:124:ASN:O	2.34	0.45
1:F:168:VAL:HG13	1:F:247:VAL:HG12	1.96	0.45
1:F:288:PHE:CZ	2:C:158:GLY:HA3	2.52	0.45
1:G:249:VAL:O	1:G:286:GLY:HA3	2.16	0.45
2:D:93:LEU:HD23	2:D:409:ILE:HD11	1.98	0.45
1:E:79:MET:HE3	1:E:138:SER:HA	1.98	0.45
1:F:283:LEU:HD23	1:F:283:LEU:HA	1.85	0.45
2:D:459:VAL:O	2:D:463:ILE:HG13	2.17	0.45
1:E:63:ILE:HG22	1:E:152:ILE:HA	1.99	0.45
2:A:333:TYR:O	2:A:336:LYS:HG2	2.17	0.45
1:E:84:LYS:NZ	1:E:87:GLY:O	2.46	0.45
1:E:124:PHE:CZ	1:E:126:GLY:HA3	2.52	0.45
2:C:239:VAL:O	2:C:243:THR:HG23	2.17	0.45
1:F:220:ARG:NH1	2:C:461:GLN:HG3	2.33	0.44
1:H:154:TYR:O	1:H:183:GLY:HA2	2.17	0.44
1:F:84:LYS:NZ	1:F:87:GLY:O	2.45	0.44
1:F:205:ASN:HD21	1:F:216:ILE:HG23	1.82	0.44
1:G:253:TRP:CZ2	1:G:290:GLU:N	2.85	0.44
1:F:249:VAL:HB	1:F:283:LEU:HB2	1.98	0.44
1:G:82:PHE:HZ	1:G:92:GLN:HE22	1.65	0.44
1:H:76:ARG:HG2	1:H:107:LEU:HD23	2.00	0.44
2:C:268:LEU:HD13	2:C:271:VAL:HG21	1.98	0.44
2:B:96:ALA:HB2	2:B:408:TYR:CE1	2.53	0.44
1:F:131:TRP:HZ3	1:F:133:GLN:HB2	1.82	0.44
1:F:220:ARG:NH1	2:C:461:GLN:CD	2.75	0.44
1:H:283:LEU:HD23	1:H:283:LEU:HA	1.74	0.44
2:B:239:VAL:O	2:B:243:THR:HG23	2.17	0.44
1:H:283:LEU:CD1	2:D:465:LYS:HG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASN:OD1	2:C:124:ASN:C	2.60	0.44
2:D:179:TYR:HA	2:D:183:MET:HE3	2.00	0.44
2:D:268:LEU:HD13	2:D:271:VAL:HG21	1.98	0.44
2:D:300:ILE:HD12	2:D:395:LEU:HG	2.00	0.44
2:D:306:LEU:HD11	2:D:476:MET:CB	2.47	0.44
1:H:61:ALA:HB3	1:H:150:VAL:HG22	1.98	0.44
2:A:241:ASN:ND2	4:J:1:NAG:O7	2.51	0.44
1:G:84:LYS:NZ	1:G:87:GLY:O	2.48	0.43
1:G:157:LYS:HE3	2:B:169:GLU:CG	2.44	0.43
1:H:160:GLU:HB3	1:H:179:ARG:HB3	2.00	0.43
2:A:459:VAL:O	2:A:463:ILE:HG13	2.17	0.43
1:E:159:PHE:HA	1:E:181:PRO:HG3	2.00	0.43
1:F:65:LYS:HB3	2:D:143:GLU:OE2	2.18	0.43
2:D:298:GLU:HB3	2:D:470:ASN:ND2	2.33	0.43
2:A:100:LEU:O	2:A:104:ILE:HG13	2.18	0.43
2:C:178:ILE:HG22	2:C:183:MET:HE2	2.00	0.43
2:C:225:VAL:O	2:C:228:ILE:HG22	2.18	0.43
1:G:283:LEU:CD1	2:A:465:LYS:HG2	2.48	0.43
1:H:259:TRP:CE2	1:H:273:ARG:HD3	2.53	0.43
2:B:226:THR:HG21	2:B:316:MET:SD	2.58	0.43
1:E:205:ASN:ND2	1:E:216:ILE:HG23	2.28	0.43
1:F:160:GLU:HB3	1:F:179:ARG:HB3	1.98	0.43
1:G:283:LEU:HD23	1:G:283:LEU:HA	1.82	0.43
2:A:100:LEU:HD21	2:A:296:TRP:CZ2	2.53	0.43
1:G:119:GLN:CD	5:B:501:NAG:H83	2.42	0.43
1:F:119:GLN:CD	5:D:501:NAG:H61	2.27	0.43
2:C:192:LEU:O	2:C:195:ASN:HB2	2.19	0.43
1:F:204:GLU:CG	1:G:204:GLU:HG2	2.48	0.43
1:H:189:VAL:HG11	1:H:212:HIS:HB3	2.01	0.43
2:C:87:LEU:HA	2:C:87:LEU:HD23	1.72	0.43
2:B:179:TYR:HE1	2:B:342:THR:HA	1.83	0.43
2:D:96:ALA:HB2	2:D:408:TYR:CE1	2.54	0.43
1:E:256:TRP:CE3	1:E:273:ARG:NE	2.87	0.42
2:C:385:SER:HA	2:C:388:ARG:HG2	2.01	0.42
2:D:258:ARG:HA	2:D:262:CYS:SG	2.59	0.42
2:B:154:LEU:HD23	2:B:154:LEU:HA	1.81	0.42
1:G:193:LYS:N	1:G:196:GLU:O	2.52	0.42
2:B:333:TYR:O	2:B:336:LYS:HG2	2.18	0.42
1:E:156:ARG:NH1	2:A:154:LEU:HD13	2.34	0.42
1:F:193:LYS:N	1:F:196:GLU:O	2.51	0.42
1:G:253:TRP:CZ3	1:G:289:CYS:CB	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:245:HIS:NE2	4:K:1:NAG:H5	2.34	0.42
1:E:170:ILE:HD13	1:E:170:ILE:HA	1.87	0.42
2:A:258:ARG:HA	2:A:262:CYS:SG	2.59	0.42
1:E:189:VAL:HG11	1:E:212:HIS:HB3	2.01	0.42
2:A:86:ARG:O	2:A:90:GLU:HG3	2.20	0.42
2:A:405:LEU:O	2:A:409:ILE:HG12	2.20	0.42
2:D:64:VAL:O	2:D:258:ARG:NH1	2.52	0.42
1:F:168:VAL:O	1:F:247:VAL:HA	2.20	0.42
1:H:60:ASP:HA	1:H:148:ALA:HB1	2.01	0.42
1:H:278:THR:HG21	2:D:237:ILE:HG21	2.00	0.42
2:A:107:ASN:CG	2:A:391:LEU:HD13	2.44	0.42
1:E:248:TYR:CD1	1:E:286:GLY:HA2	2.55	0.42
1:H:219:ALA:HB1	1:H:247:VAL:HG11	2.02	0.42
2:A:268:LEU:HD13	2:A:271:VAL:HG21	2.01	0.42
2:A:300:ILE:HD12	2:A:395:LEU:HG	2.02	0.42
2:A:457:PRO:O	2:A:461:GLN:HG3	2.20	0.42
1:F:76:ARG:HG2	1:F:107:LEU:HD23	2.01	0.42
1:F:282:PRO:HG2	1:F:288:PHE:CD2	2.55	0.42
4:J:2:NAG:O3	4:J:2:NAG:C7	2.68	0.42
1:G:77:PRO:HB3	1:G:107:LEU:HD21	2.02	0.42
2:A:292:ILE:HD11	2:A:459:VAL:HG13	2.00	0.42
2:D:192:LEU:O	2:D:195:ASN:HB2	2.19	0.42
2:C:405:LEU:O	2:C:409:ILE:HG12	2.20	0.41
1:G:219:ALA:HB1	1:G:247:VAL:HG11	2.02	0.41
1:G:170:ILE:HD13	1:G:170:ILE:HA	1.86	0.41
2:B:405:LEU:O	2:B:409:ILE:HG12	2.20	0.41
2:A:394:LYS:O	2:A:397:SER:OG	2.36	0.41
2:C:107:ASN:CG	2:C:391:LEU:HD13	2.45	0.41
1:E:76:ARG:NH1	1:E:105:SER:HB2	2.36	0.41
2:B:150:THR:O	2:B:154:LEU:HG	2.21	0.41
2:B:155:TYR:HB2	2:B:161:ILE:HB	2.03	0.41
1:E:57:GLU:HG2	1:E:145:SER:HB2	2.03	0.41
1:E:81:ILE:HD12	1:E:110:ARG:HB3	2.02	0.41
1:F:130:TYR:HB3	1:F:150:VAL:O	2.21	0.41
1:G:253:TRP:CZ3	1:G:289:CYS:HB3	2.55	0.41
1:H:84:LYS:NZ	1:H:87:GLY:O	2.47	0.41
2:C:100:LEU:O	2:C:104:ILE:HG13	2.20	0.41
2:C:459:VAL:O	2:C:463:ILE:HG13	2.21	0.41
1:E:256:TRP:CZ2	1:E:295:GLN:NE2	2.89	0.41
2:C:258:ARG:HA	2:C:262:CYS:SG	2.61	0.41
2:D:385:SER:HA	2:D:388:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ILE:HD11	2:B:349:CYS:HB3	2.03	0.41
2:B:258:ARG:HA	2:B:262:CYS:SG	2.61	0.41
2:B:306:LEU:HD11	2:B:476:MET:CB	2.49	0.41
2:B:469:ILE:HD12	2:B:469:ILE:HA	1.93	0.41
1:E:259:TRP:CE2	1:E:273:ARG:HD3	2.56	0.41
2:C:134:TYR:OH	2:C:332:GLN:OE1	2.34	0.41
2:B:219:VAL:HG12	2:B:319:VAL:HG12	2.03	0.41
1:E:65:LYS:O	2:A:143:GLU:OE2	2.39	0.40
1:E:76:ARG:HG2	1:E:107:LEU:HD23	2.02	0.40
1:G:220:ARG:CZ	2:A:461:GLN:NE2	2.84	0.40
2:B:385:SER:HA	2:B:388:ARG:CG	2.52	0.40
2:B:458:VAL:HA	2:B:461:GLN:NE2	2.35	0.40
1:E:66:SER:OG	2:A:143:GLU:OE2	2.39	0.40
1:F:259:TRP:CE2	1:F:273:ARG:HD3	2.57	0.40
1:G:259:TRP:CE2	1:G:273:ARG:HD3	2.57	0.40
2:D:226:THR:HG21	2:D:316:MET:SD	2.60	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	E	249/268 (93%)	238 (96%)	9 (4%)	2 (1%)	16	52
1	F	249/268 (93%)	236 (95%)	11 (4%)	2 (1%)	16	52
1	G	249/268 (93%)	235 (94%)	9 (4%)	5 (2%)	6	33
1	H	249/268 (93%)	237 (95%)	11 (4%)	1 (0%)	30	65
2	A	341/464 (74%)	330 (97%)	11 (3%)	0	100	100
2	B	341/464 (74%)	330 (97%)	11 (3%)	0	100	100
2	C	341/464 (74%)	331 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	341/464 (74%)	331 (97%)	10 (3%)	0	100	100
All	All	2360/2928 (81%)	2268 (96%)	82 (4%)	10 (0%)	30	65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	257	THR
1	G	253	TRP
1	E	130	TYR
1	F	130	TYR
1	G	130	TYR
1	H	130	TYR
1	E	257	THR
1	G	116	VAL
1	G	115	ASN
1	G	224	SER

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	E	217/231 (94%)	207 (95%)	10 (5%)	24	47
1	F	217/231 (94%)	207 (95%)	10 (5%)	24	47
1	G	217/231 (94%)	206 (95%)	11 (5%)	21	45
1	H	217/231 (94%)	206 (95%)	11 (5%)	21	45
2	A	319/417 (76%)	313 (98%)	6 (2%)	50	67
2	B	319/417 (76%)	315 (99%)	4 (1%)	61	72
2	C	319/417 (76%)	316 (99%)	3 (1%)	70	76
2	D	317/417 (76%)	313 (99%)	4 (1%)	61	72
All	All	2142/2592 (83%)	2083 (97%)	59 (3%)	38	59

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	63	ILE
1	E	109	VAL
1	E	114	ILE
1	E	134	CYS
1	E	170	ILE
1	E	174	ILE
1	E	192	LEU
1	E	198	ILE
1	E	206	ILE
1	E	298	THR
1	F	63	ILE
1	F	109	VAL
1	F	114	ILE
1	F	134	CYS
1	F	170	ILE
1	F	174	ILE
1	F	192	LEU
1	F	198	ILE
1	F	206	ILE
1	F	298	THR
1	G	63	ILE
1	G	109	VAL
1	G	114	ILE
1	G	134	CYS
1	G	170	ILE
1	G	174	ILE
1	G	192	LEU
1	G	198	ILE
1	G	202	GLN
1	G	206	ILE
1	G	298	THR
1	H	63	ILE
1	H	109	VAL
1	H	114	ILE
1	H	134	CYS
1	H	170	ILE
1	H	174	ILE
1	H	192	LEU
1	H	198	ILE
1	H	202	GLN
1	H	206	ILE
1	H	298	THR
2	A	83	LEU

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Mol	Chain	Res	Type
2	A	99	GLU
2	A	228	ILE
2	A	306	LEU
2	A	337	ASN
2	A	348	LEU
2	C	83	LEU
2	C	306	LEU
2	C	337	ASN
2	D	83	LEU
2	D	99	GLU
2	D	306	LEU
2	D	337	ASN
2	B	83	LEU
2	B	306	LEU
2	B	337	ASN
2	B	418	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	125	HIS
1	E	271	GLN
1	E	295	GLN
1	F	139	HIS
1	F	161	GLN
1	G	92	GLN
1	G	115	ASN
1	G	119	GLN
1	G	161	GLN
1	G	295	GLN
1	H	279	ASN
2	A	91	GLN
2	A	461	GLN
2	D	245	HIS
2	D	335	GLN
2	B	266	GLN
2	B	335	GLN
2	B	337	ASN
2	B	461	GLN
2	B	468	HIS

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 ⓘ

18 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	NAG	I	1	1,3	14,14,15	0.81	1 (7%)	17,19,21	1.35	3 (17%)
3	NAG	I	2	3	14,14,15	1.02	1 (7%)	17,19,21	1.11	1 (5%)
4	NAG	J	1	2,4	14,14,15	1.15	1 (7%)	17,19,21	1.73	2 (11%)
4	NAG	J	2	4	14,14,15	2.03	3 (21%)	17,19,21	2.50	6 (35%)
4	BMA	J	3	4	11,11,12	1.12	1 (9%)	15,15,17	1.77	3 (20%)
4	MAN	J	4	4	11,11,12	0.73	0	15,15,17	1.42	2 (13%)
4	NAG	K	1	2,4	14,14,15	0.96	2 (14%)	17,19,21	0.99	1 (5%)
4	NAG	K	2	4	14,14,15	1.57	2 (14%)	17,19,21	1.96	6 (35%)
4	BMA	K	3	4	11,11,12	1.29	1 (9%)	15,15,17	1.51	4 (26%)
4	MAN	K	4	4	11,11,12	0.80	0	15,15,17	1.52	1 (6%)
4	NAG	M	1	2,4	14,14,15	0.63	0	17,19,21	1.51	1 (5%)
4	NAG	M	2	4	14,14,15	0.89	1 (7%)	17,19,21	2.01	6 (35%)
4	BMA	M	3	4	11,11,12	1.01	0	15,15,17	1.14	2 (13%)
4	MAN	M	4	4	11,11,12	0.99	1 (9%)	15,15,17	1.07	1 (6%)
4	NAG	N	1	2,4	14,14,15	0.60	0	17,19,21	1.22	2 (11%)
4	NAG	N	2	4	14,14,15	0.37	0	17,19,21	0.57	0
4	BMA	N	3	4	11,11,12	0.27	0	15,15,17	0.65	0
4	MAN	N	4	4	11,11,12	0.33	0	15,15,17	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
4	NAG	J	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	0/2/19/22	0/1/1/1
4	NAG	K	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	1/2/19/22	0/1/1/1
4	NAG	M	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	MAN	M	4	4	-	0/2/19/22	0/1/1/1
4	NAG	N	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	MAN	N	4	4	-	1/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	C1-C2	5.47	1.59	1.52
4	K	2	NAG	C1-C2	4.39	1.58	1.52
4	J	2	NAG	C2-N2	3.58	1.52	1.46
4	K	3	BMA	O5-C1	3.48	1.49	1.43
3	I	2	NAG	C1-C2	2.80	1.56	1.52
4	J	2	NAG	O4-C4	2.79	1.49	1.43
4	J	1	NAG	O4-C4	2.48	1.49	1.43
4	K	2	NAG	O4-C4	2.46	1.49	1.43
4	J	3	BMA	O2-C2	2.19	1.47	1.43
4	M	2	NAG	C1-C2	2.15	1.55	1.52
3	I	1	NAG	C1-C2	2.13	1.55	1.52
4	K	1	NAG	O4-C4	2.07	1.48	1.43
4	M	4	MAN	O5-C1	2.01	1.47	1.43
4	K	1	NAG	C4-C5	2.01	1.57	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	C1-C2-N2	6.48	120.65	110.43
4	M	1	NAG	C1-O5-C5	5.50	119.56	112.19
4	J	1	NAG	C1-O5-C5	4.93	118.80	112.19
4	K	4	MAN	C1-O5-C5	4.83	118.66	112.19
4	J	2	NAG	O7-C7-N2	4.48	129.90	121.98
4	K	2	NAG	O7-C7-N2	4.31	129.59	121.98
4	J	4	MAN	C1-O5-C5	4.29	117.93	112.19
4	M	2	NAG	C8-C7-N2	-4.19	109.17	116.12
4	J	1	NAG	O5-C1-C2	-3.89	105.27	111.29
4	J	3	BMA	O2-C2-C1	3.80	117.92	109.22
4	J	2	NAG	C2-N2-C7	3.61	127.74	122.90
4	M	2	NAG	C2-N2-C7	-3.57	118.12	122.90
4	J	3	BMA	C1-C2-C3	-3.53	104.50	109.64
4	M	2	NAG	C1-C2-N2	3.46	115.89	110.43
4	J	2	NAG	O5-C1-C2	-3.44	105.96	111.29
4	J	3	BMA	O5-C1-C2	-3.39	102.70	110.79
4	K	3	BMA	O2-C2-C1	3.26	116.70	109.22
4	K	2	NAG	C1-O5-C5	-3.12	108.00	112.19
3	I	2	NAG	C2-N2-C7	3.10	127.05	122.90
3	I	1	NAG	C1-O5-C5	2.96	116.16	112.19
4	K	2	NAG	O7-C7-C8	-2.87	116.95	122.05
4	M	2	NAG	O7-C7-C8	2.83	127.09	122.05
4	N	1	NAG	C1-O5-C5	2.75	115.87	112.19
4	K	2	NAG	C2-N2-C7	2.72	126.55	122.90
4	K	2	NAG	C1-C2-N2	2.60	114.54	110.43
4	K	3	BMA	C2-C3-C4	2.58	115.39	110.86
4	M	4	MAN	C1-O5-C5	2.57	115.64	112.19
4	M	2	NAG	C4-C3-C2	-2.50	107.35	111.02
4	K	3	BMA	O5-C1-C2	-2.49	104.84	110.79
4	K	3	BMA	C1-C2-C3	-2.46	106.06	109.64
4	J	2	NAG	O7-C7-C8	-2.45	117.69	122.05
4	M	2	NAG	C1-O5-C5	2.36	115.34	112.19
4	J	2	NAG	C8-C7-N2	-2.35	112.22	116.12
4	M	3	BMA	C2-C3-C4	2.34	114.98	110.86
3	I	1	NAG	C8-C7-N2	2.23	119.81	116.12
4	M	3	BMA	O3-C3-C4	2.22	115.61	110.38
4	N	1	NAG	O3-C3-C2	-2.20	104.82	109.40
4	K	2	NAG	O5-C1-C2	-2.12	108.02	111.29
4	K	1	NAG	O4-C4-C3	-2.10	105.42	110.38
3	I	1	NAG	O7-C7-C8	-2.09	118.34	122.05
4	J	4	MAN	C3-C4-C5	2.05	113.94	110.23

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
4	K	1	NAG	C1-C2-N2-C7
4	M	2	NAG	C8-C7-N2-C2
4	J	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	K	3	BMA	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	N	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	K	3	BMA	O5-C5-C6-O6
4	K	2	NAG	O7-C7-N2-C2
4	K	1	NAG	O5-C5-C6-O6
4	N	4	MAN	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	N	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C1-C2-N2-C7
4	N	1	NAG	C1-C2-N2-C7
4	J	3	BMA	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	J	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C1-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
4	N	1	NAG	C3-C2-N2-C7
3	I	1	NAG	O5-C5-C6-O6
4	K	4	MAN	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 18 short contacts:

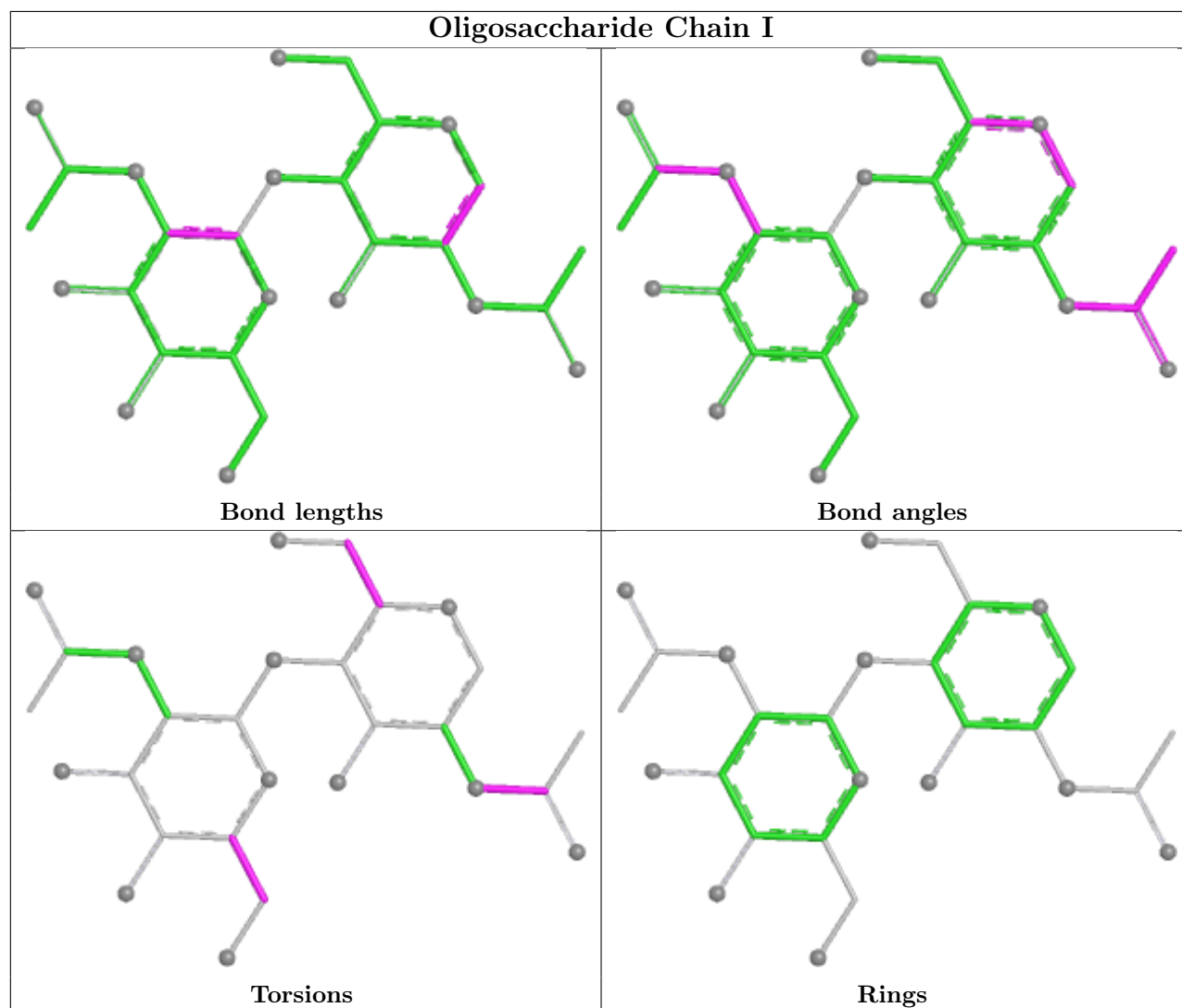
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	4	MAN	2	0
4	K	1	NAG	7	0

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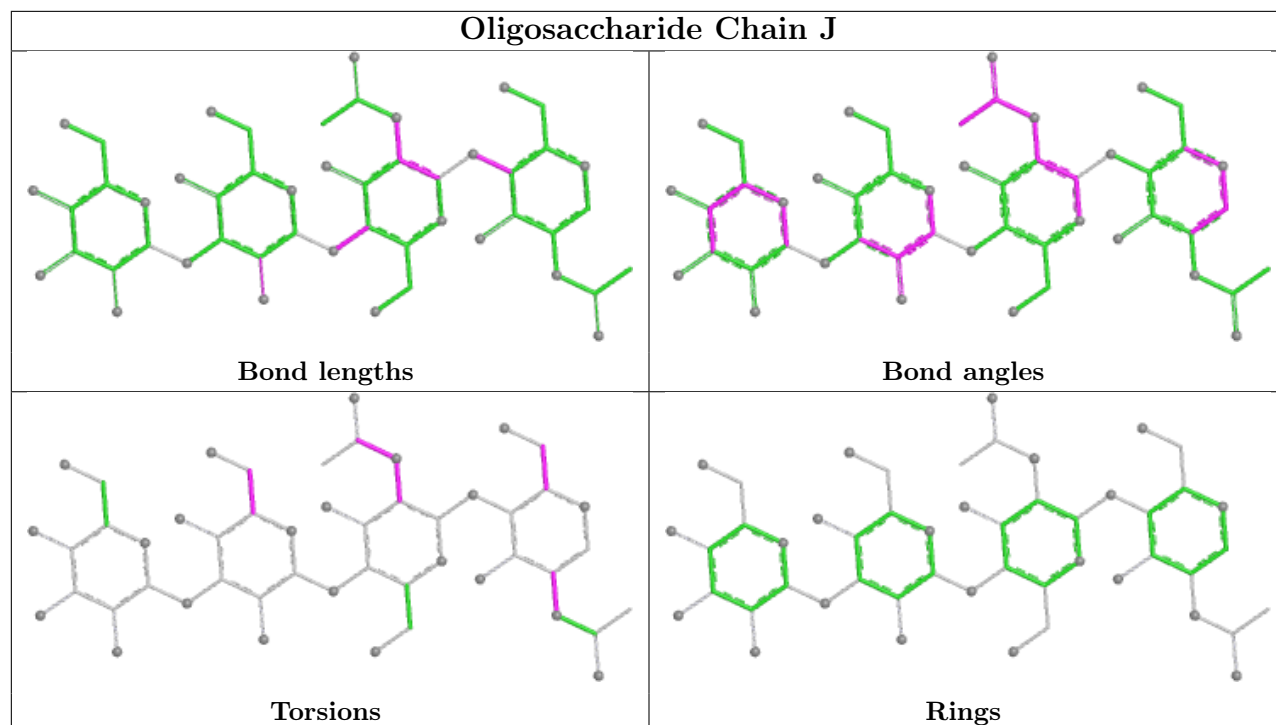
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	2	NAG	1	0
4	J	1	NAG	1	0
4	M	1	NAG	2	0
4	N	1	NAG	3	0
4	N	4	MAN	1	0
4	M	2	NAG	1	0

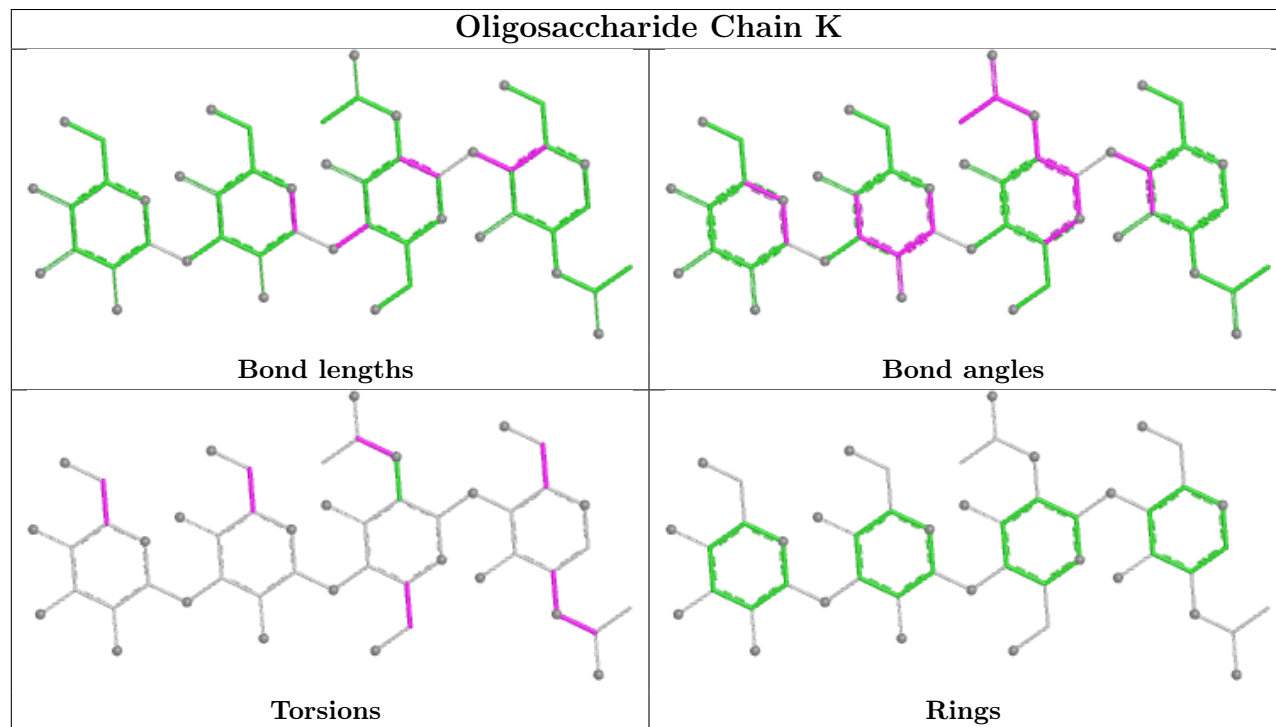
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

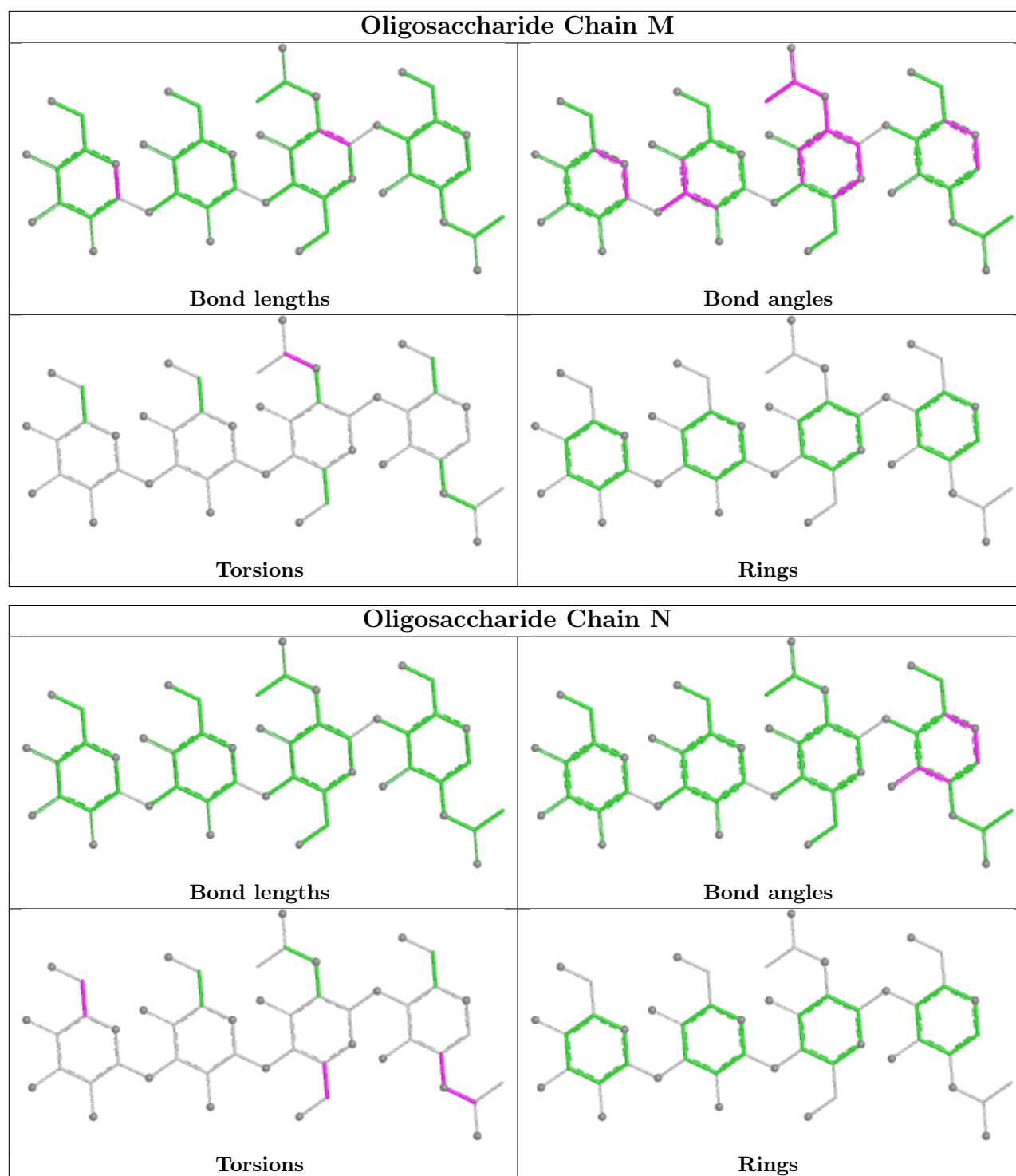


Oligosaccharide Chain J



Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

18 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
5	NAG	B	501	2	14,14,15	1.21	1 (7%)	17,19,21	0.72	0
6	MAN	H	402	1	11,11,12	0.96	0	15,15,17	2.01	4 (26%)
5	NAG	H	401	1	14,14,15	0.68	0	17,19,21	0.94	1 (5%)
5	NAG	E	402	1	14,14,15	0.70	1 (7%)	17,19,21	1.11	2 (11%)
5	NAG	B	502	2	14,14,15	0.74	0	17,19,21	1.34	3 (17%)
5	NAG	A	501	2	14,14,15	0.98	1 (7%)	17,19,21	2.24	3 (17%)
6	MAN	F	403	1	11,11,12	0.70	0	15,15,17	1.40	3 (20%)
5	NAG	D	501	2	14,14,15	1.17	2 (14%)	17,19,21	1.50	2 (11%)
5	NAG	A	502	2	14,14,15	1.61	2 (14%)	17,19,21	1.83	4 (23%)
5	NAG	F	401	1	14,14,15	0.78	0	17,19,21	1.00	2 (11%)
6	MAN	E	404	1	11,11,12	0.61	0	15,15,17	1.68	1 (6%)
5	NAG	F	404	1	14,14,15	0.46	0	17,19,21	1.15	2 (11%)
6	MAN	H	403	1	11,11,12	0.53	0	15,15,17	1.95	3 (20%)
5	NAG	H	404	1	14,14,15	1.08	2 (14%)	17,19,21	2.10	4 (23%)
6	MAN	F	402	1	11,11,12	0.49	0	15,15,17	1.69	1 (6%)
6	MAN	E	403	1	11,11,12	0.84	0	15,15,17	1.85	4 (26%)
5	NAG	C	501	2	14,14,15	0.96	2 (14%)	17,19,21	1.32	2 (11%)
5	NAG	E	401	1	14,14,15	0.50	0	17,19,21	0.94	1 (5%)

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
5	NAG	B	501	2	-	0/6/23/26	0/1/1/1
6	MAN	H	402	1	-	2/2/19/22	0/1/1/1
5	NAG	H	401	1	-	0/6/23/26	0/1/1/1
5	NAG	E	402	1	-	2/6/23/26	0/1/1/1
5	NAG	B	502	2	-	1/6/23/26	0/1/1/1
5	NAG	A	501	2	-	4/6/23/26	0/1/1/1
6	MAN	F	403	1	-	2/2/19/22	0/1/1/1
5	NAG	D	501	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	502	2	-	0/6/23/26	0/1/1/1
5	NAG	F	401	1	-	0/6/23/26	0/1/1/1
6	MAN	E	404	1	-	0/2/19/22	0/1/1/1
5	NAG	F	404	1	-	2/6/23/26	0/1/1/1
6	MAN	H	403	1	-	2/2/19/22	0/1/1/1
5	NAG	H	404	1	-	4/6/23/26	0/1/1/1
6	MAN	F	402	1	-	2/2/19/22	0/1/1/1
6	MAN	E	403	1	-	2/2/19/22	0/1/1/1
5	NAG	C	501	2	-	4/6/23/26	0/1/1/1
5	NAG	E	401	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	NAG	O5-C1	-4.60	1.36	1.43
5	B	501	NAG	C1-C2	3.84	1.57	1.52
5	A	502	NAG	C1-C2	3.02	1.56	1.52
5	D	501	NAG	O5-C5	2.80	1.48	1.43
5	H	404	NAG	O5-C5	2.47	1.48	1.43
5	A	501	NAG	O5-C5	2.45	1.48	1.43
5	H	404	NAG	C1-C2	2.42	1.55	1.52
5	D	501	NAG	O5-C1	2.32	1.47	1.43
5	E	402	NAG	C1-C2	2.26	1.55	1.52
5	C	501	NAG	C1-C2	2.23	1.55	1.52
5	C	501	NAG	O5-C1	-2.01	1.40	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	NAG	C2-N2-C7	6.73	131.92	122.90
5	H	404	NAG	C1-O5-C5	6.20	120.50	112.19
6	H	403	MAN	C1-O5-C5	6.09	120.35	112.19
6	F	402	MAN	C1-O5-C5	5.74	119.88	112.19
5	A	502	NAG	C1-O5-C5	5.58	119.66	112.19
6	E	404	MAN	C1-O5-C5	5.18	119.13	112.19
6	H	402	MAN	C1-O5-C5	5.08	119.00	112.19
5	D	501	NAG	C2-N2-C7	4.20	128.53	122.90
6	E	403	MAN	C1-O5-C5	3.95	117.48	112.19
5	B	502	NAG	C2-N2-C7	3.87	128.08	122.90
5	A	501	NAG	C1-C2-N2	-3.79	104.46	110.43
5	C	501	NAG	C1-O5-C5	3.65	117.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	404	NAG	C1-O5-C5	3.46	116.82	112.19
6	E	403	MAN	C3-C4-C5	3.35	116.30	110.23
6	H	402	MAN	O3-C3-C2	3.12	116.41	110.05
6	F	403	MAN	C3-C4-C5	3.10	115.86	110.23
6	E	403	MAN	C6-C5-C4	3.10	120.64	113.02
5	H	401	NAG	C1-O5-C5	3.03	116.25	112.19
5	H	404	NAG	C8-C7-N2	3.00	121.10	116.12
6	H	402	MAN	C3-C4-C5	2.98	115.64	110.23
5	H	404	NAG	C3-C4-C5	2.86	115.42	110.23
5	A	501	NAG	O7-C7-N2	2.86	127.03	121.98
5	C	501	NAG	C1-C2-N2	2.85	114.93	110.43
5	E	402	NAG	C2-N2-C7	2.81	126.67	122.90
5	A	502	NAG	O5-C1-C2	2.72	115.50	111.29
5	D	501	NAG	C1-O5-C5	2.69	115.79	112.19
5	A	502	NAG	C1-C2-N2	2.64	114.59	110.43
5	F	401	NAG	C1-O5-C5	2.64	115.72	112.19
6	F	403	MAN	O5-C5-C6	2.63	112.78	107.66
5	A	502	NAG	C2-N2-C7	2.54	126.30	122.90
5	E	401	NAG	C1-O5-C5	2.47	115.49	112.19
5	F	404	NAG	O5-C1-C2	-2.39	107.60	111.29
6	E	403	MAN	C1-C2-C3	-2.21	106.42	109.64
6	H	403	MAN	O5-C5-C6	2.21	111.97	107.66
6	H	403	MAN	C1-C2-C3	2.20	112.85	109.64
5	B	502	NAG	O5-C1-C2	2.17	114.66	111.29
5	B	502	NAG	C1-C2-N2	2.14	113.81	110.43
6	F	403	MAN	C1-C2-C3	2.12	112.73	109.64
5	H	404	NAG	O3-C3-C2	-2.11	105.01	109.40
6	H	402	MAN	O5-C5-C6	2.10	111.74	107.66
5	F	401	NAG	O5-C1-C2	-2.07	108.09	111.29
5	E	402	NAG	O7-C7-N2	2.01	125.54	121.98

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	404	NAG	C8-C7-N2-C2
5	H	404	NAG	O7-C7-N2-C2
5	A	501	NAG	C3-C2-N2-C7
5	D	501	NAG	C8-C7-N2-C2
5	D	501	NAG	O7-C7-N2-C2
5	C	501	NAG	O5-C5-C6-O6
6	F	402	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	501	NAG	C4-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	F	404	NAG	O5-C5-C6-O6
5	H	404	NAG	C4-C5-C6-O6
5	C	501	NAG	C8-C7-N2-C2
6	F	402	MAN	C4-C5-C6-O6
6	H	402	MAN	C4-C5-C6-O6
5	H	404	NAG	O5-C5-C6-O6
5	C	501	NAG	O7-C7-N2-C2
6	F	403	MAN	C4-C5-C6-O6
6	E	403	MAN	C4-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
6	H	403	MAN	C4-C5-C6-O6
5	F	404	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
6	F	403	MAN	O5-C5-C6-O6
5	E	402	NAG	C1-C2-N2-C7
5	E	402	NAG	C3-C2-N2-C7
6	H	402	MAN	O5-C5-C6-O6
6	E	403	MAN	O5-C5-C6-O6
5	A	501	NAG	C8-C7-N2-C2
6	H	403	MAN	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	NAG	3	0
6	F	403	MAN	2	0
5	D	501	NAG	22	0
5	H	404	NAG	1	0
6	E	403	MAN	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	E	251/268 (93%)	0.27	6 (2%)	59	45	102, 172, 251, 290	0
1	F	251/268 (93%)	0.21	7 (2%)	55	41	136, 234, 364, 416	0
1	G	251/268 (93%)	0.34	10 (3%)	42	33	111, 178, 241, 286	0
1	H	251/268 (93%)	0.35	10 (3%)	42	33	115, 201, 284, 315	0
2	A	351/464 (75%)	0.17	10 (2%)	55	41	78, 156, 243, 289	0
2	B	351/464 (75%)	0.26	15 (4%)	40	32	80, 161, 249, 338	0
2	C	351/464 (75%)	0.20	14 (3%)	42	33	105, 193, 294, 348	0
2	D	351/464 (75%)	0.18	7 (1%)	65	49	144, 248, 341, 402	0
All	All	2408/2928 (82%)	0.24	79 (3%)	49	37	78, 186, 307, 416	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	465	LYS	4.7
2	C	174	LEU	4.1
1	H	176	LEU	3.9
2	D	177	VAL	3.9
2	D	174	LEU	3.5
2	C	137	LEU	3.5
1	H	214	LEU	3.4
1	E	64	ILE	3.3
2	A	323	LEU	3.2
1	H	135	VAL	3.1
1	E	288	PHE	3.0
1	F	214	LEU	3.0
1	G	114	ILE	3.0
2	C	315	ASP	2.9
1	H	191	TRP	2.9
2	C	327	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	104	ILE	2.8
1	F	227	TYR	2.8
2	C	144	PHE	2.7
2	B	470	ASN	2.7
1	H	301	ALA	2.7
2	C	177	VAL	2.7
1	E	187	ALA	2.6
1	G	127	PRO	2.6
2	A	223	LEU	2.6
2	D	80	LYS	2.6
2	A	433	SER	2.6
1	H	206	ILE	2.6
2	B	132	ASN	2.6
1	F	223	ASP	2.5
2	C	180	THR	2.5
2	C	215	ILE	2.5
2	C	323	LEU	2.5
1	H	116	VAL	2.5
2	B	465	LYS	2.5
2	D	179	TYR	2.5
1	G	241	LEU	2.5
2	B	308	ASN	2.5
1	E	223	ASP	2.4
2	C	214	LEU	2.4
2	C	130	PHE	2.4
1	G	220	ARG	2.4
1	H	223	ASP	2.4
2	A	341	LEU	2.4
2	B	300	ILE	2.4
2	B	399	ILE	2.4
1	G	283	LEU	2.4
2	D	315	ASP	2.3
2	B	323	LEU	2.3
1	E	153	ALA	2.3
2	A	320	LEU	2.3
2	D	412	HIS	2.3
2	B	349	CYS	2.2
2	B	240	ILE	2.2
2	A	256	LEU	2.2
1	G	106	GLY	2.2
1	G	214	LEU	2.2
1	F	198	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	257	THR	2.2
1	G	176	LEU	2.1
1	G	223	ASP	2.1
2	D	137	LEU	2.1
2	A	89	MET	2.1
1	E	234	ILE	2.1
1	H	94	GLU	2.1
2	B	477	SER	2.1
1	F	291	GLY	2.1
2	A	308	ASN	2.1
2	B	401	PHE	2.1
2	B	235	LEU	2.0
2	B	299	TYR	2.0
1	F	215	ILE	2.0
1	F	132	CYS	2.0
2	C	210	ASN	2.0
1	G	135	VAL	2.0
2	B	301	LEU	2.0
2	A	163	VAL	2.0
2	A	219	VAL	2.0
2	C	433	SER	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.

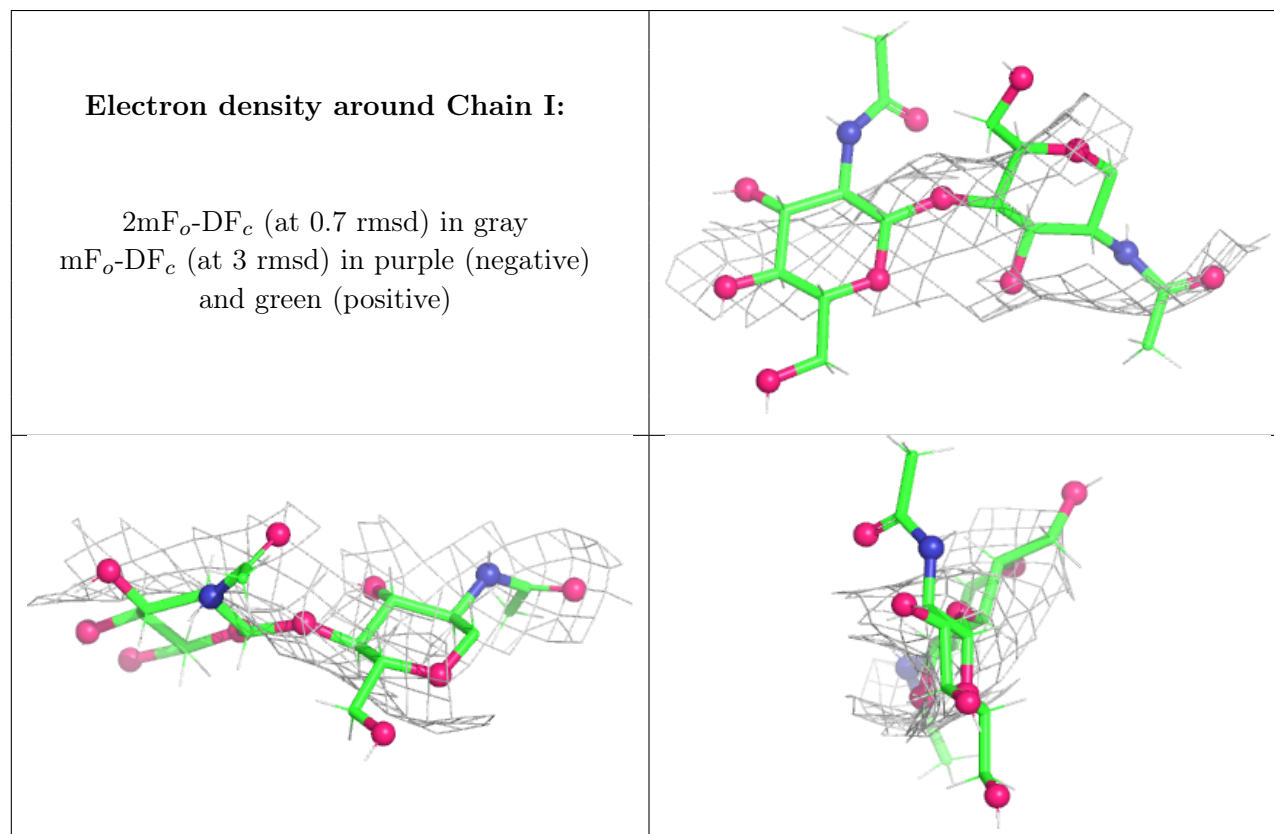
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	M	3	11/12	0.48	0.15	30,222,225,228	3
4	NAG	J	2	14/15	0.50	0.15	30,138,148,152	2
4	BMA	K	3	11/12	0.66	0.15	30,206,214,216	3
4	BMA	J	3	11/12	0.67	0.12	30,156,175,178	3
3	NAG	I	2	14/15	0.68	0.17	30,291,297,302	3
4	NAG	K	2	14/15	0.68	0.16	30,182,194,198	2
4	MAN	K	4	11/12	0.69	0.12	30,221,239,251	4

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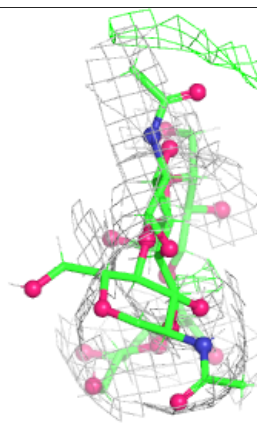
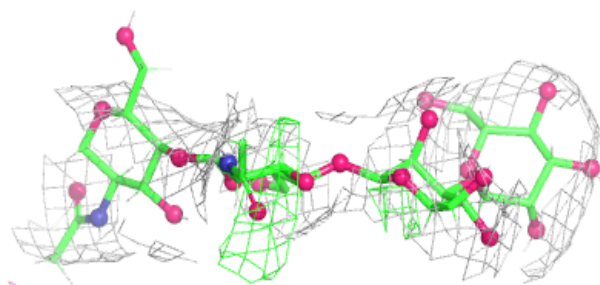
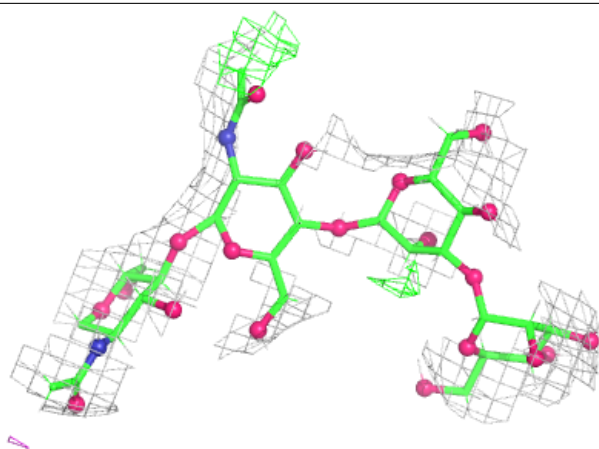
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	M	2	14/15	0.76	0.14	30,200,206,210	2
4	MAN	J	4	11/12	0.78	0.11	30,156,167,174	4
4	MAN	M	4	11/12	0.78	0.10	30,228,232,236	4
3	NAG	I	1	14/15	0.83	0.12	30,192,218,242	2
4	NAG	K	1	14/15	0.89	0.12	30,152,165,167	2
4	NAG	M	1	14/15	0.93	0.15	30,188,198,202	2
4	NAG	J	1	14/15	0.93	0.19	30,97,111,119	2
4	NAG	N	1	14/15	-	-	30,150,165,167	2
4	NAG	N	2	14/15	-	-	30,174,181,186	2
4	BMA	N	3	11/12	-	-	30,193,200,205	3
4	MAN	N	4	11/12	-	-	30,199,207,209	4

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.



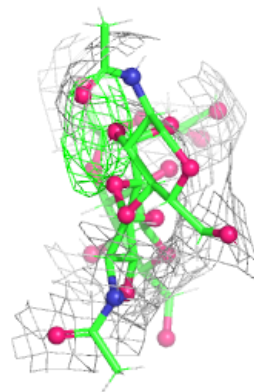
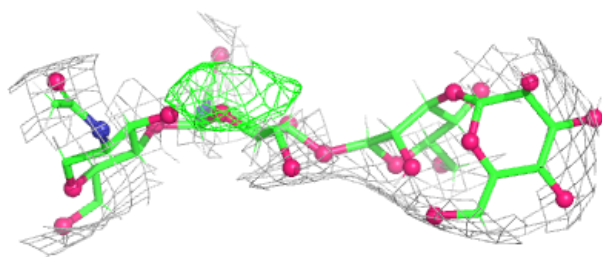
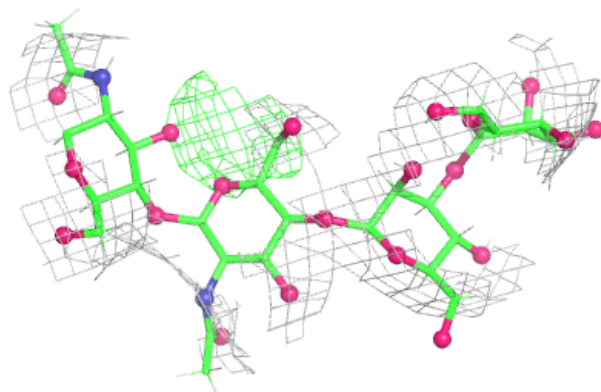
Electron density around Chain J:

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

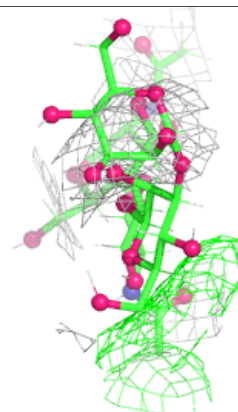
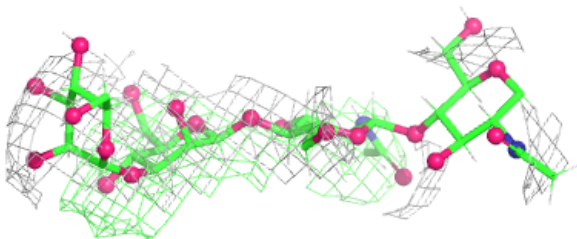
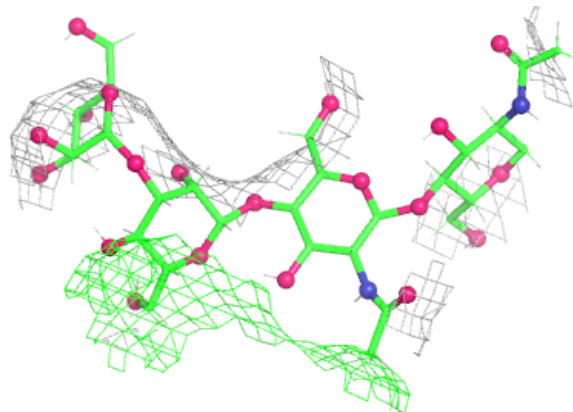


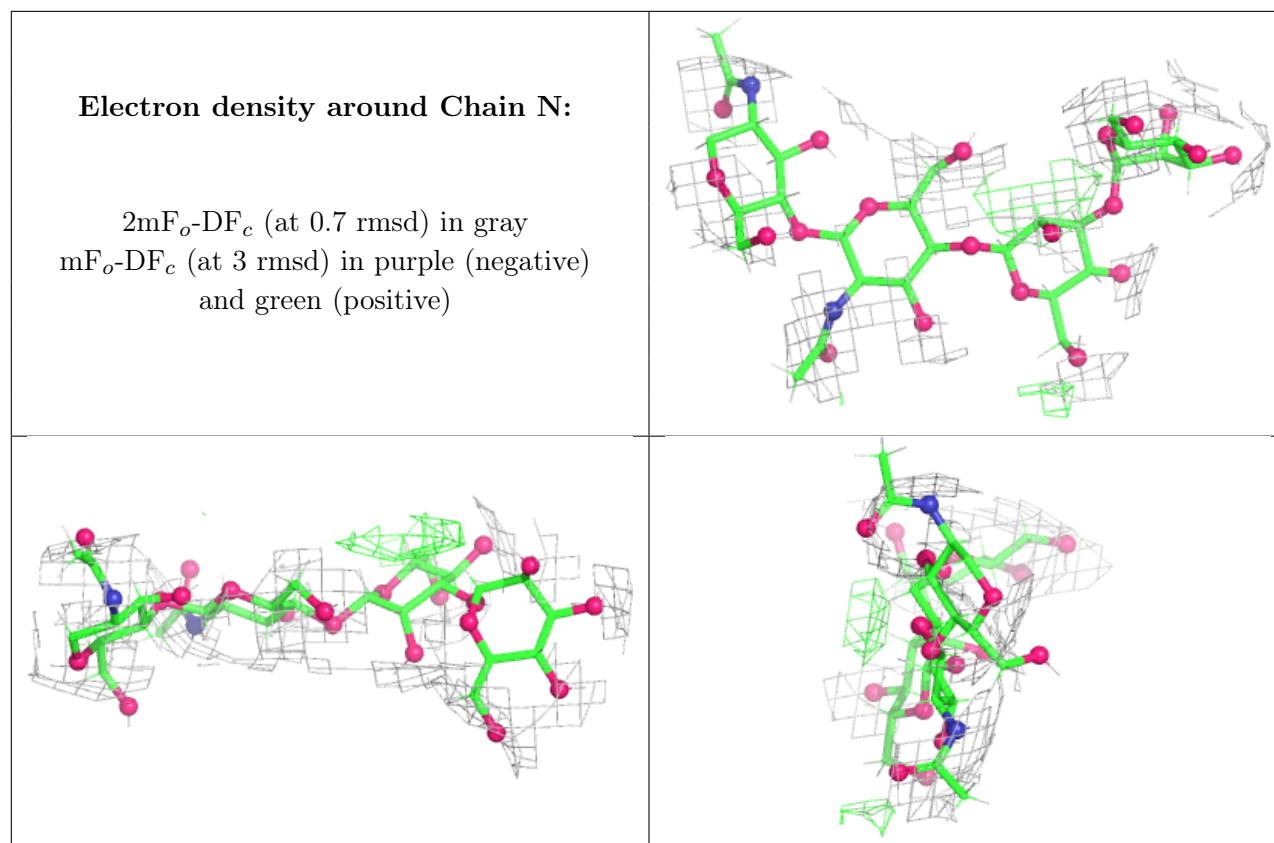
Electron density around Chain K:

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

**Electron density around Chain M:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	D	501	14/15	0.04	0.17	30,346,363,365	3
5	NAG	H	404	14/15	0.47	0.14	30,226,229,233	3
5	NAG	F	401	14/15	0.51	0.14	30,193,200,203	3
5	NAG	A	501	14/15	0.60	0.14	30,219,235,243	3
5	NAG	B	502	14/15	0.61	0.14	30,294,312,314	3
5	NAG	F	404	14/15	0.62	0.10	30,274,281,283	3
5	NAG	A	502	14/15	0.63	0.23	30,308,324,338	3
5	NAG	C	501	14/15	0.68	0.13	30,273,282,289	3
5	NAG	E	402	14/15	0.71	0.10	30,198,202,204	3
6	MAN	H	402	11/12	0.72	0.15	30,296,306,308	4
5	NAG	H	401	14/15	0.78	0.11	30,155,164,170	3
6	MAN	F	403	11/12	0.79	0.16	30,311,314,316	4
5	NAG	E	401	14/15	0.80	0.13	30,137,153,155	3
6	MAN	H	403	11/12	0.80	0.09	30,203,205,206	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	501	14/15	0.81	0.12	30,205,212,216	3
6	MAN	E	403	11/12	0.86	0.11	30,269,275,279	4
6	MAN	E	404	11/12	0.88	0.08	30,138,143,145	4
6	MAN	F	402	11/12	0.89	0.09	30,207,218,224	4

6.5 Other polymers [i](#)

There are no such residues in this entry.