



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:15 AM UTC

PDB ID : 7ZA2 / pdb\_00007za2  
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 : 4.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)

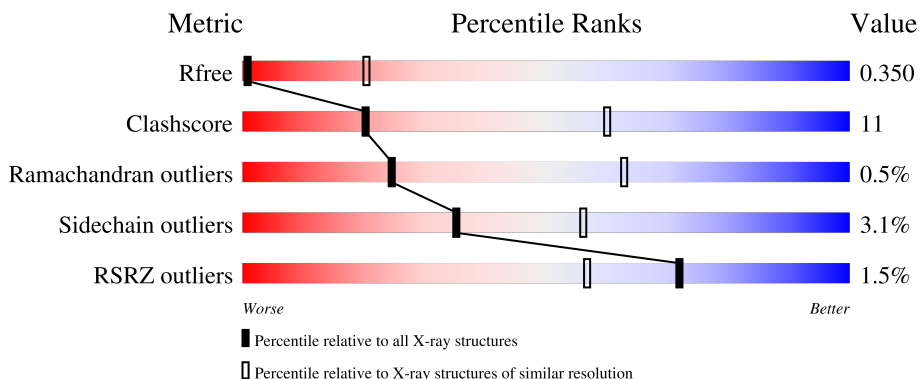
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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  $\geq 3$ , 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	464	 2% 61% 14% 24%
1	B	464	 % 60% 15% 24%
1	C	464	 % 61% 14% 24%
1	D	464	 2% 64% 11% 24%

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Mol	Chain	Length	Quality of chain
2	E	268	 % 65% 26% • 6%
2	F	268	 % 66% 25% • 6%
2	G	268	 % 64% 28% • 6%
2	H	268	 % 67% 26% • 6%
3	I	2	 100%

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	501	-	-	X	-
4	NAG	E	402	-	-	X	-
4	NAG	G	401	-	-	X	-
4	NAG	H	401	-	-	X	-
5	MAN	F	403	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 38653 atoms, of which 19208 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 Glypican-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	351	5631	1791	2825	469	517	29	67	0	0
1	B	351	5630	1791	2824	469	517	29	67	0	0
1	C	351	5631	1791	2825	469	517	29	67	0	0
1	D	351	5631	1791	2825	469	517	29	67	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLU	-	expression tag	UNP Q8CFZ4
A	29	THR	-	expression tag	UNP Q8CFZ4
A	30	GLY	-	expression tag	UNP Q8CFZ4
A	483	GLY	-	expression tag	UNP Q8CFZ4
A	484	THR	-	expression tag	UNP Q8CFZ4
A	485	LYS	-	expression tag	UNP Q8CFZ4
A	486	HIS	-	expression tag	UNP Q8CFZ4
A	487	HIS	-	expression tag	UNP Q8CFZ4
A	488	HIS	-	expression tag	UNP Q8CFZ4
A	489	HIS	-	expression tag	UNP Q8CFZ4
A	490	HIS	-	expression tag	UNP Q8CFZ4
A	491	HIS	-	expression tag	UNP Q8CFZ4
B	28	GLU	-	expression tag	UNP Q8CFZ4
B	29	THR	-	expression tag	UNP Q8CFZ4
B	30	GLY	-	expression tag	UNP Q8CFZ4
B	483	GLY	-	expression tag	UNP Q8CFZ4
B	484	THR	-	expression tag	UNP Q8CFZ4
B	485	LYS	-	expression tag	UNP Q8CFZ4
B	486	HIS	-	expression tag	UNP Q8CFZ4
B	487	HIS	-	expression tag	UNP Q8CFZ4
B	488	HIS	-	expression tag	UNP Q8CFZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	489	HIS	-	expression tag	UNP Q8CFZ4
B	490	HIS	-	expression tag	UNP Q8CFZ4
B	491	HIS	-	expression tag	UNP Q8CFZ4
C	28	GLU	-	expression tag	UNP Q8CFZ4
C	29	THR	-	expression tag	UNP Q8CFZ4
C	30	GLY	-	expression tag	UNP Q8CFZ4
C	483	GLY	-	expression tag	UNP Q8CFZ4
C	484	THR	-	expression tag	UNP Q8CFZ4
C	485	LYS	-	expression tag	UNP Q8CFZ4
C	486	HIS	-	expression tag	UNP Q8CFZ4
C	487	HIS	-	expression tag	UNP Q8CFZ4
C	488	HIS	-	expression tag	UNP Q8CFZ4
C	489	HIS	-	expression tag	UNP Q8CFZ4
C	490	HIS	-	expression tag	UNP Q8CFZ4
C	491	HIS	-	expression tag	UNP Q8CFZ4
D	28	GLU	-	expression tag	UNP Q8CFZ4
D	29	THR	-	expression tag	UNP Q8CFZ4
D	30	GLY	-	expression tag	UNP Q8CFZ4
D	483	GLY	-	expression tag	UNP Q8CFZ4
D	484	THR	-	expression tag	UNP Q8CFZ4
D	485	LYS	-	expression tag	UNP Q8CFZ4
D	486	HIS	-	expression tag	UNP Q8CFZ4
D	487	HIS	-	expression tag	UNP Q8CFZ4
D	488	HIS	-	expression tag	UNP Q8CFZ4
D	489	HIS	-	expression tag	UNP Q8CFZ4
D	490	HIS	-	expression tag	UNP Q8CFZ4
D	491	HIS	-	expression tag	UNP Q8CFZ4

- Molecule 2 is a protein called Netrin receptor UNC5D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	E	251	Total	C	H	N	O	S	50	0	0
			3904	1237	1913	363	376	15			
2	F	251	Total	C	H	N	O	S	49	0	0
			3904	1237	1913	363	376	15			
2	G	251	Total	C	H	N	O	S	49	0	0
			3904	1237	1913	363	376	15			
2	H	251	Total	C	H	N	O	S	49	0	0
			3905	1237	1914	363	376	15			

There are 24 discrepancies between the modelled and reference sequences:

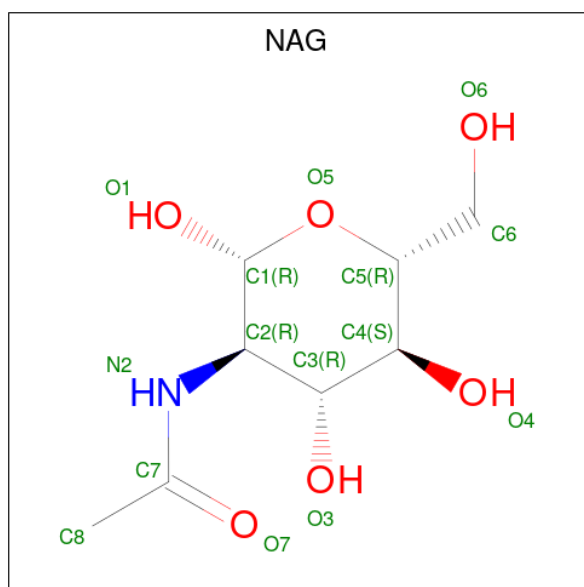
Chain	Residue	Modelled	Actual	Comment	Reference
E	308	HIS	-	expression tag	UNP F1LW30
E	309	HIS	-	expression tag	UNP F1LW30
E	310	HIS	-	expression tag	UNP F1LW30
E	311	HIS	-	expression tag	UNP F1LW30
E	312	HIS	-	expression tag	UNP F1LW30
E	313	HIS	-	expression tag	UNP F1LW30
F	308	HIS	-	expression tag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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



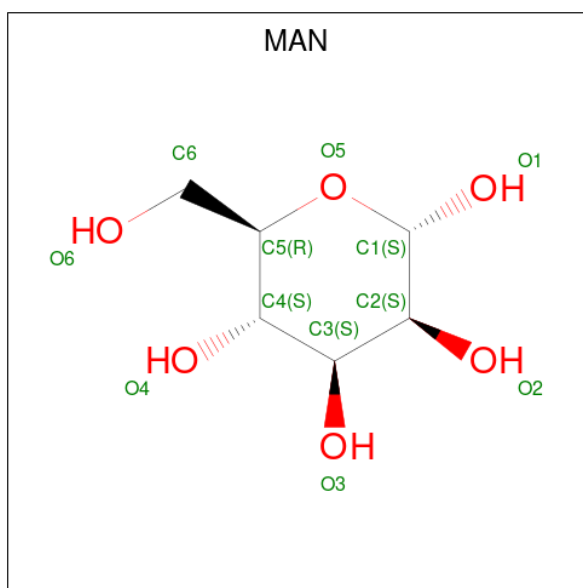
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
3	I	2	55	16	27	2	10	5	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

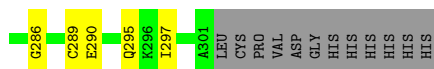
- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



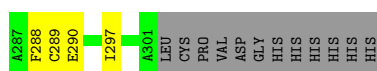
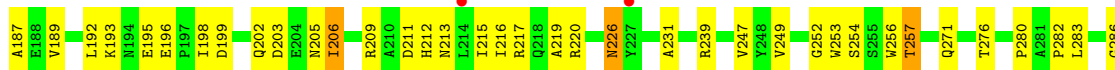
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	E	1	22	6	11	5	4	0
5	F	1	22	6	11	5	4	0
5	G	1	22	6	11	5	4	0



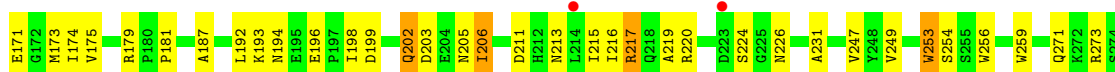




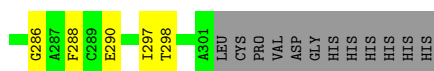
- Molecule 2: Netrin receptor UNC5D



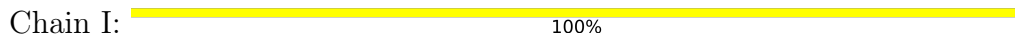
- Molecule 2: Netrin receptor UNC5D



- Molecule 2: Netrin receptor UNC5D



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



MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.11Å 157.99Å 126.57Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	66.62 – 4.60 66.62 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (66.62-4.60) 99.7 (66.62-4.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 4.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.307 , 0.347 0.309 , 0.350	Depositor DCC
$R_{free}$ test set	1866 reflections (8.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	243.1	Xtrriage
Anisotropy	0.290	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 394.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	38653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	351.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, MAN

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	0.84	0/2854	0.84	0/3846
1	B	0.85	0/2854	0.84	0/3846
1	C	0.89	1/2854 (0.0%)	0.84	1/3846 (0.0%)
1	D	0.84	0/2854	0.85	0/3846
2	E	0.85	0/2038	0.79	2/2764 (0.1%)
2	F	0.87	1/2038 (0.0%)	0.81	1/2764 (0.0%)
2	G	0.86	0/2038	0.81	1/2764 (0.0%)
2	H	0.86	0/2038	0.78	0/2764
All	All	0.86	2/19568 (0.0%)	0.82	5/26440 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	GLY	C-O	14.23	1.52	1.23
2	F	257	THR	N-CA	5.06	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	455	GLU	CB-CG-CD	6.18	123.11	112.60
2	F	226	ASN	OD1-CG-ND2	5.34	127.94	122.60
2	E	248	TYR	CB-CA-C	5.32	118.95	109.38
2	G	217	ARG	CG-CD-NE	-5.25	100.46	112.00
2	E	248	TYR	CA-CB-CG	5.08	123.05	113.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2806	2825	2814	39	0
1	B	2806	2824	2813	55	0
1	C	2806	2825	2813	40	0
1	D	2806	2825	2815	33	0
2	E	1991	1913	1906	76	0
2	F	1991	1913	1904	75	0
2	G	1991	1913	1906	69	0
2	H	1991	1914	1905	54	0
3	I	28	27	25	0	0
4	A	14	14	13	4	0
4	B	28	28	26	12	0
4	C	28	28	24	3	0
4	D	28	28	26	3	0
4	E	28	28	26	21	0
4	F	28	28	26	5	0
4	G	28	28	26	10	0
4	H	14	14	13	7	0
5	E	11	11	10	0	0
5	F	11	11	10	10	0
5	G	11	11	10	0	0
All	All	19445	19208	19111	431	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 11.

The worst 5 of 431 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)
2:F:253:TRP:CZ3	2:F:289:CYS:HB3	1.19	1.62
2:E:70:ALA:HB2	4:E:402:NAG:C7	1.23	1.55
1:D:123:ASN:HD21	4:D:501:NAG:C1	1.31	1.43
2:F:256:TRP:HD1	5:F:403:MAN:C1	1.13	1.37
2:F:253:TRP:CZ3	2:F:289:CYS:CB	2.09	1.33

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/464 (74%)	334 (98%)	7 (2%)	0	100	100
1	B	341/464 (74%)	334 (98%)	7 (2%)	0	100	100
1	C	341/464 (74%)	334 (98%)	7 (2%)	0	100	100
1	D	341/464 (74%)	334 (98%)	7 (2%)	0	100	100
2	E	249/268 (93%)	238 (96%)	9 (4%)	2 (1%)	16	53
2	F	249/268 (93%)	236 (95%)	11 (4%)	2 (1%)	16	53
2	G	249/268 (93%)	235 (94%)	9 (4%)	5 (2%)	6	31
2	H	249/268 (93%)	237 (95%)	10 (4%)	2 (1%)	16	53
All	All	2360/2928 (81%)	2282 (97%)	67 (3%)	11 (0%)	24	63

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	257	THR
2	G	253	TRP
2	E	130	TYR
2	F	130	TYR
2	E	257	THR

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/418 (76%)	313 (98%)	6 (2%)	50	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	319/418 (76%)	311 (98%)	8 (2%)	42	62
1	C	319/418 (76%)	312 (98%)	7 (2%)	45	64
1	D	319/418 (76%)	315 (99%)	4 (1%)	61	72
2	E	217/231 (94%)	206 (95%)	11 (5%)	21	43
2	F	217/231 (94%)	208 (96%)	9 (4%)	27	49
2	G	217/231 (94%)	205 (94%)	12 (6%)	19	42
2	H	217/231 (94%)	207 (95%)	10 (5%)	24	46
All	All	2144/2596 (83%)	2077 (97%)	67 (3%)	35	56

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	63	ILE
2	H	114	ILE
2	H	206	ILE
1	D	387	ARG
1	D	336	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	336	ASN
2	G	161	GLN
1	D	194	ASN
2	F	161	GLN
1	D	123	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates i

2 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	2,3	14,14,15	1.04	1 (7%)	17,19,21	1.41	2 (11%)
3	NAG	I	2	3	14,14,15	1.03	0	17,19,21	1.90	4 (23%)

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	2,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	O5-C1	2.18	1.47	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C2-N2-C7	5.02	129.62	122.90
3	I	1	NAG	C1-O5-C5	4.27	117.91	112.19
3	I	2	NAG	O5-C1-C2	2.79	115.60	111.29
3	I	2	NAG	O4-C4-C3	-2.33	104.89	110.38
3	I	2	NAG	C1-C2-N2	2.24	113.97	110.43

There are no chirality outliers.

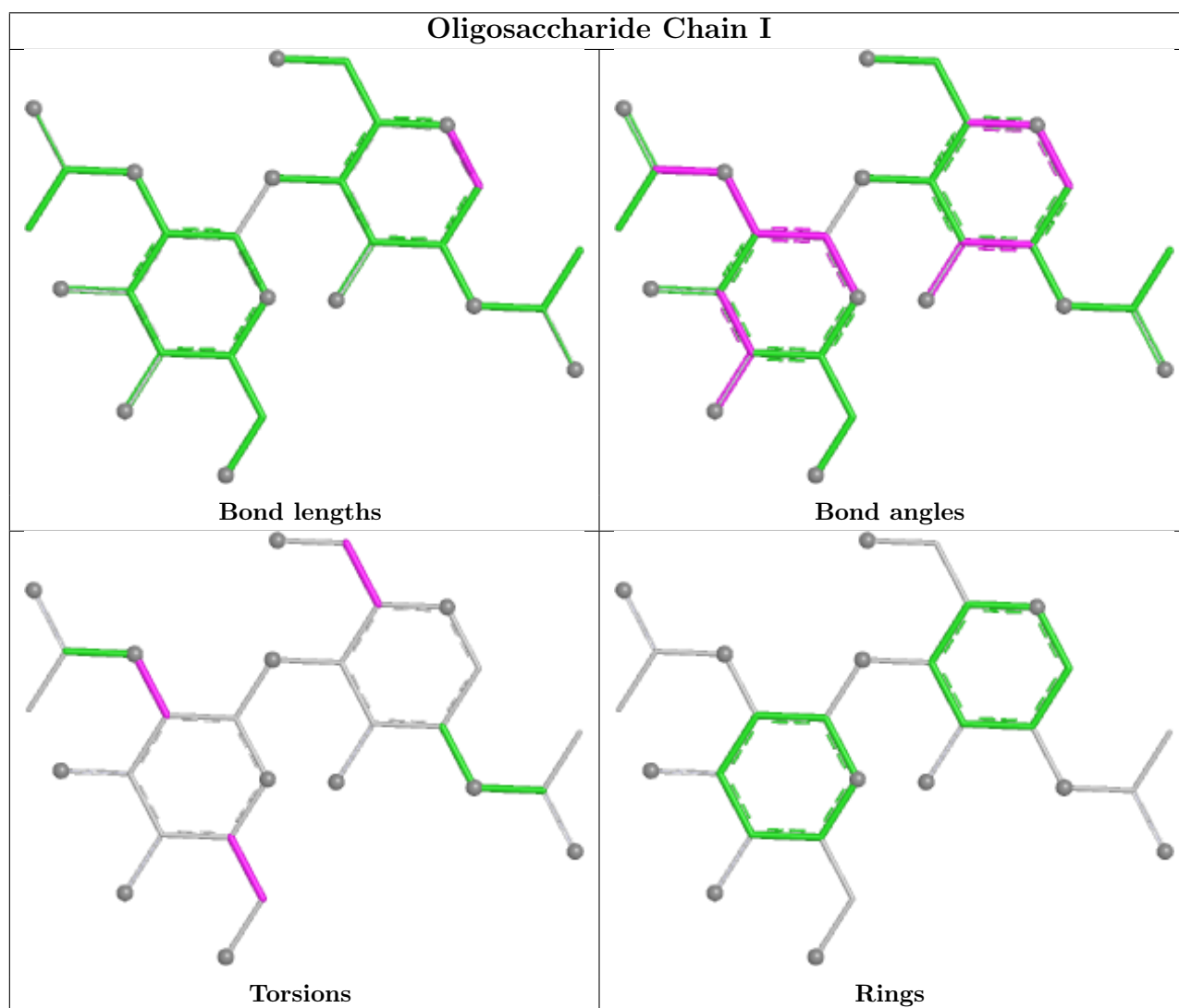
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C1-C2-N2-C7
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

17 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	MAN	E	401	2	11,11,12	1.56	2 (18%)	15,15,17	2.23	7 (46%)
5	MAN	F	403	2	11,11,12	0.86	0	15,15,17	2.21	5 (33%)
4	NAG	D	502	1	14,14,15	1.75	3 (21%)	17,19,21	2.59	7 (41%)
4	NAG	H	401	2	14,14,15	0.44	0	17,19,21	1.09	1 (5%)
4	NAG	C	502	1	14,14,15	1.34	1 (7%)	17,19,21	3.63	10 (58%)
4	NAG	C	501	1	14,14,15	0.91	1 (7%)	17,19,21	1.23	2 (11%)
4	NAG	A	501	1	14,14,15	1.26	2 (14%)	17,19,21	2.58	6 (35%)
4	NAG	E	403	2	14,14,15	1.46	2 (14%)	17,19,21	1.74	3 (17%)
4	NAG	D	501	1	14,14,15	0.65	0	17,19,21	1.46	1 (5%)
4	NAG	G	401	2	14,14,15	1.28	3 (21%)	17,19,21	3.04	8 (47%)
4	NAG	G	402	2	14,14,15	1.72	3 (21%)	17,19,21	3.21	8 (47%)
4	NAG	F	402	2	14,14,15	1.27	1 (7%)	17,19,21	2.03	3 (17%)
4	NAG	B	502	1	14,14,15	0.88	0	17,19,21	2.03	6 (35%)
4	NAG	F	401	2	14,14,15	1.93	3 (21%)	17,19,21	1.57	2 (11%)
4	NAG	E	402	2	14,14,15	0.96	0	17,19,21	2.23	8 (47%)
4	NAG	B	501	1	14,14,15	0.91	1 (7%)	17,19,21	1.34	3 (17%)
5	MAN	G	403	2	11,11,12	1.45	2 (18%)	15,15,17	2.56	6 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	E	401	2	-	1/2/19/22	0/1/1/1
5	MAN	F	403	2	-	1/2/19/22	0/1/1/1
4	NAG	D	502	1	-	1/6/23/26	0/1/1/1
4	NAG	H	401	2	-	1/6/23/26	0/1/1/1
4	NAG	C	502	1	-	1/6/23/26	0/1/1/1
4	NAG	C	501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	501	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	403	2	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	2/6/23/26	0/1/1/1
4	NAG	G	401	2	-	3/6/23/26	0/1/1/1
4	NAG	G	402	2	-	5/6/23/26	0/1/1/1
4	NAG	F	402	2	-	3/6/23/26	0/1/1/1
4	NAG	B	502	1	-	1/6/23/26	0/1/1/1
4	NAG	F	401	2	-	4/6/23/26	0/1/1/1
4	NAG	E	402	2	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
5	MAN	G	403	2	-	2/2/19/22	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	502	NAG	C1-C2	4.96	1.59	1.52
4	F	401	NAG	C2-N2	4.57	1.53	1.46
4	F	402	NAG	C1-C2	4.34	1.58	1.52
4	G	402	NAG	C1-C2	3.92	1.57	1.52
4	E	403	NAG	O5-C5	3.61	1.50	1.43

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	NAG	C2-N2-C7	9.11	135.11	122.90
4	C	502	NAG	C2-N2-C7	8.49	134.28	122.90
4	G	402	NAG	C2-N2-C7	8.17	133.84	122.90
4	A	501	NAG	O5-C5-C6	7.22	121.71	107.66
4	C	502	NAG	O7-C7-N2	5.85	132.32	121.98

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	403	NAG	C3-C2-N2-C7
4	F	402	NAG	C1-C2-N2-C7
4	G	401	NAG	C1-C2-N2-C7
4	G	402	NAG	C1-C2-N2-C7
4	A	501	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	403	MAN	10	0
4	D	502	NAG	1	0
4	H	401	NAG	7	0
4	C	502	NAG	1	0
4	C	501	NAG	2	0
4	A	501	NAG	4	0
4	E	403	NAG	1	0
4	D	501	NAG	2	0
4	G	401	NAG	7	0
4	G	402	NAG	3	0
4	F	402	NAG	1	0
4	B	502	NAG	1	0
4	F	401	NAG	4	0
4	E	402	NAG	20	0
4	B	501	NAG	11	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	351/464 (75%)	-0.23	7 (1%) 65 51	166, 294, 412, 464	0
1	B	351/464 (75%)	-0.22	4 (1%) 78 62	255, 427, 584, 695	0
1	C	351/464 (75%)	-0.12	6 (1%) 69 55	152, 298, 446, 609	0
1	D	351/464 (75%)	-0.16	9 (2%) 57 45	213, 331, 492, 560	0
2	E	251/268 (93%)	-0.21	2 (0%) 82 68	181, 321, 413, 473	0
2	F	251/268 (93%)	-0.28	2 (0%) 82 68	249, 392, 545, 618	0
2	G	251/268 (93%)	-0.13	2 (0%) 82 68	185, 344, 439, 484	0
2	H	251/268 (93%)	-0.03	4 (1%) 70 55	228, 359, 491, 570	0
All	All	2408/2928 (82%)	-0.17	36 (1%) 72 57	152, 338, 520, 695	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	214	LEU	5.0
1	D	136	LEU	4.9
1	D	176	VAL	4.7
1	D	173	LEU	4.5
1	B	394	LEU	4.0

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

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

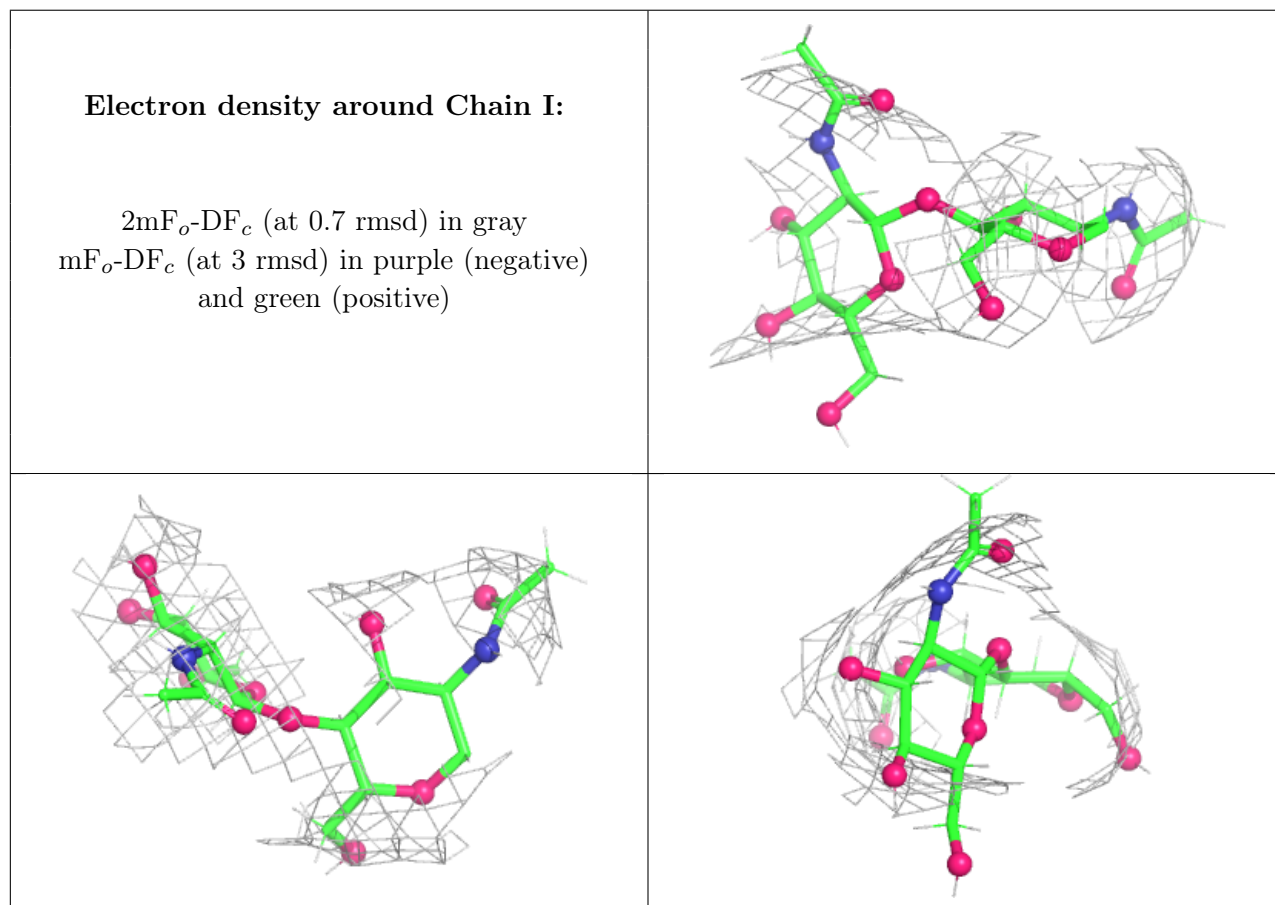
### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	I	2	14/15	0.48	0.12	30,395,413,426	3
3	NAG	I	1	14/15	0.89	0.06	30,323,357,381	2

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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	H	401	14/15	0.09	0.10	30,397,431,442	3
4	NAG	E	402	14/15	0.11	0.12	30,438,487,495	3
4	NAG	D	501	14/15	0.27	0.10	30,420,457,486	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	401	14/15	0.43	0.13	30,351,369,378	3
4	NAG	F	401	14/15	0.46	0.15	30,564,594,608	3
5	MAN	F	403	11/12	0.47	0.14	30,368,378,383	4
5	MAN	E	401	11/12	0.53	0.21	30,451,484,508	4
5	MAN	G	403	11/12	0.54	0.12	30,394,405,425	4
4	NAG	C	502	14/15	0.59	0.18	30,322,407,425	3
4	NAG	G	402	14/15	0.61	0.11	30,237,256,259	3
4	NAG	B	502	14/15	0.63	0.13	30,331,340,344	3
4	NAG	D	502	14/15	0.67	0.13	30,281,287,288	3
4	NAG	B	501	14/15	0.68	0.09	30,504,585,611	3
4	NAG	A	501	14/15	0.83	0.14	30,271,288,307	3
4	NAG	E	403	14/15	0.84	0.09	30,271,306,318	3
4	NAG	C	501	14/15	0.86	0.07	30,371,393,412	3
4	NAG	F	402	14/15	0.92	0.07	30,306,320,326	3

## 6.5 Other polymers [i](#)

There are no such residues in this entry.