wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2022 – 02:45 am BST

PDB ID	:	7ZA2
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

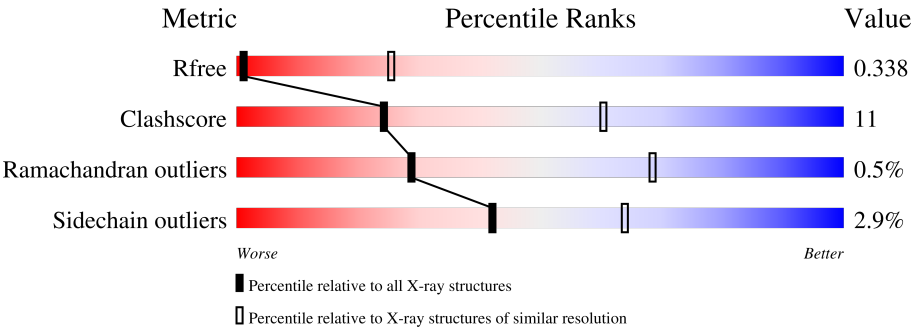
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.60 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}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	464	61% 14% • 24%
1	B	464	61% 14% • 24%
1	C	464	61% 13% • 24%
1	D	464	66% 9% 24%
2	E	268	66% 26% • 6%
2	F	268	67% 25% • 6%

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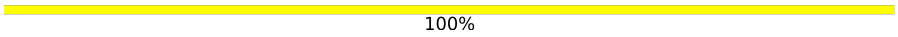
Mol	Chain	Length	Quality of chain
2	G	268	
2	H	268	
3	I	2	

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
1	A	351	Total	C	H	N	O	S	67	0	0
			5631	1791	2825	469	517	29			
1	B	351	Total	C	H	N	O	S	67	0	0
			5630	1791	2824	469	517	29			
1	C	351	Total	C	H	N	O	S	67	0	0
			5631	1791	2825	469	517	29			
1	D	351	Total	C	H	N	O	S	67	0	0
			5631	1791	2825	469	517	29			

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			

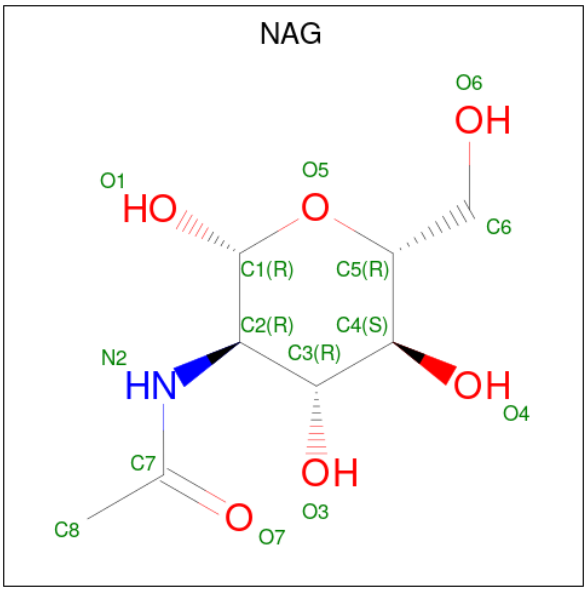
There are 24 discrepancies between the modelled and reference sequences:

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.

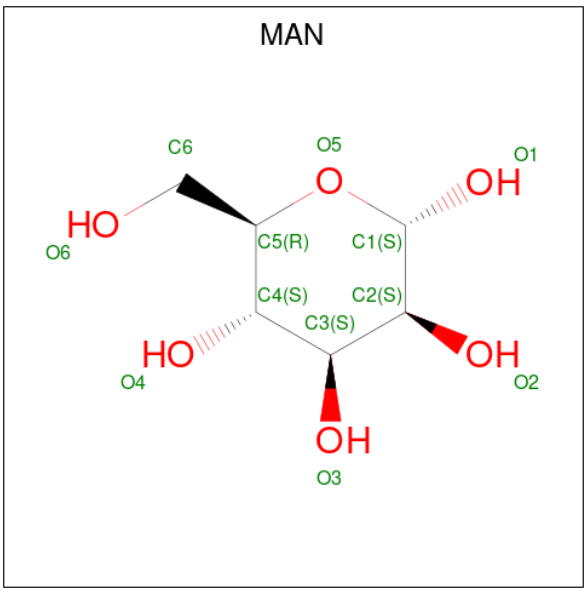
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



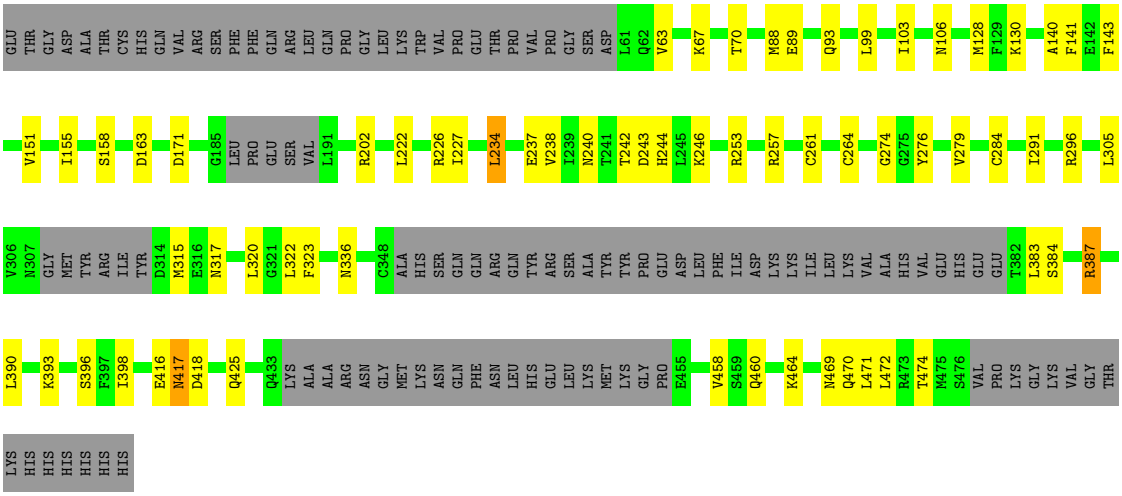
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C H O 22 6 11 5	4	0
5	F	1	Total C H O 22 6 11 5	4	0
5	G	1	Total C H O 22 6 11 5	4	0

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. 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. 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.

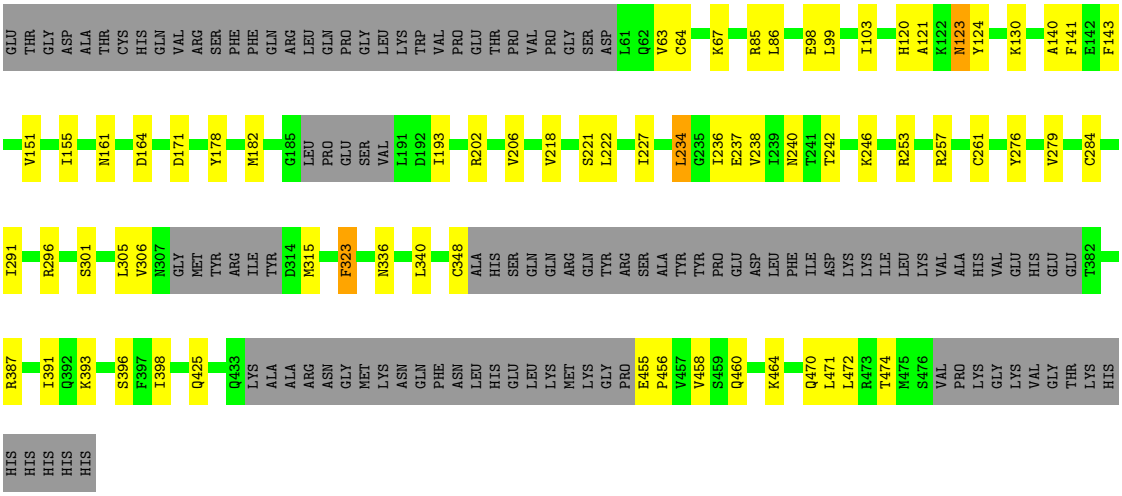
• Molecule 1: Glypican-3

Chain A:



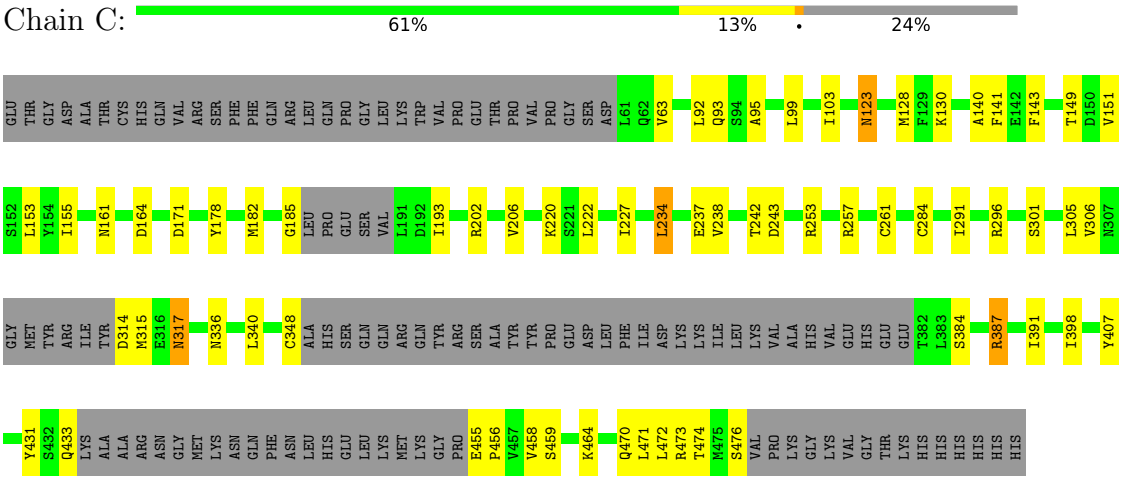
• Molecule 1: Glypican-3

Chain B:



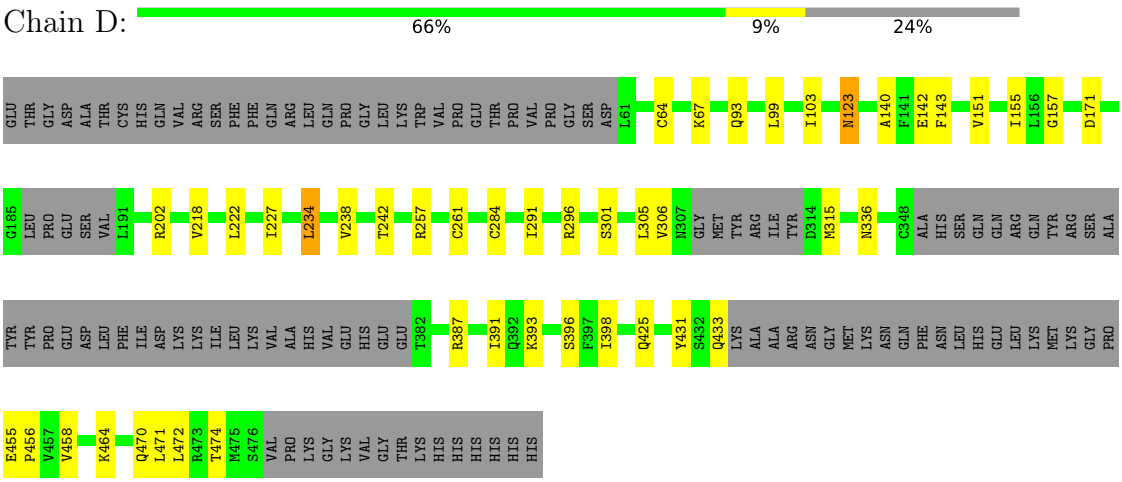
• Molecule 1: Glypican-3

Chain C:



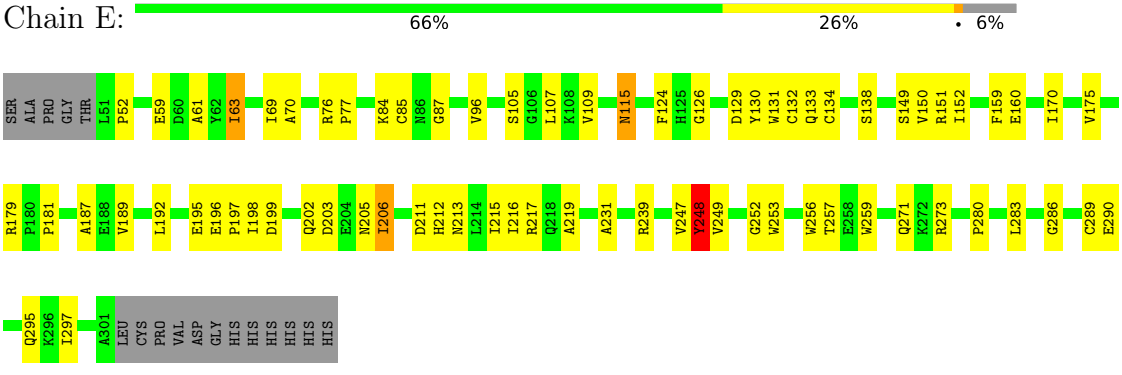
• Molecule 1: Glypican-3

Chain D:



• Molecule 2: Netrin receptor UNC5D

Chain E:

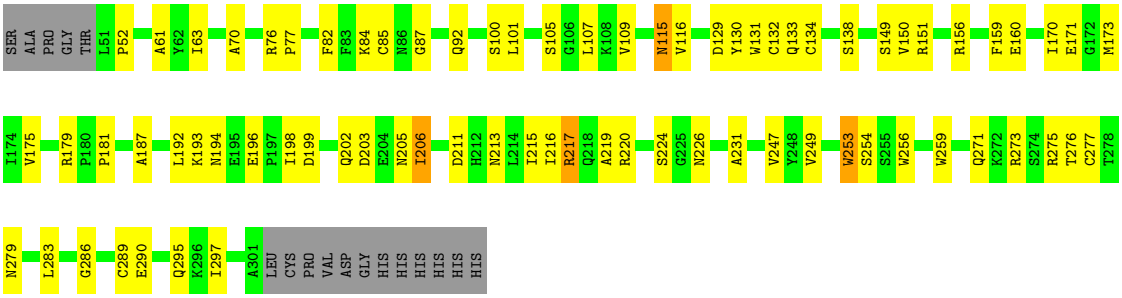


• Molecule 2: Netrin receptor UNC5D

Chain F:

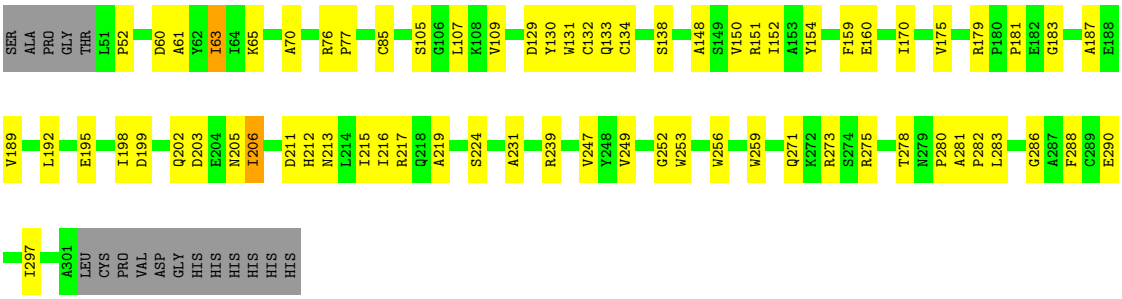
• Molecule 2: Netrin receptor UNC5D

Chain G:



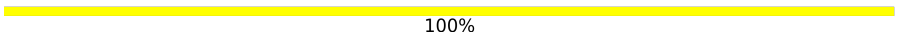
• Molecule 2: Netrin receptor UNC5D

Chain H:



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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.11Å 157.99Å 126.57Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	66.62 – 4.60 66.53 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (66.62-4.60) 99.7 (66.53-4.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 4.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.307 , 0.347 0.298 , 0.338	Depositor DCC
R_{free} test set	1866 reflections (8.55%)	wwPDB-VP
Wilson B-factor (Å^2)	243.1	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	38653	wwPDB-VP
Average B, all atoms (Å^2)	351.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.60	0/2854	0.50	0/3846
1	B	0.60	0/2854	0.49	0/3846
1	C	0.70	1/2854 (0.0%)	0.50	1/3846 (0.0%)
1	D	0.60	0/2854	0.49	0/3846
2	E	0.61	0/2038	0.59	1/2764 (0.0%)
2	F	0.61	0/2038	0.60	0/2764
2	G	0.61	0/2038	0.61	1/2764 (0.0%)
2	H	0.61	0/2038	0.57	0/2764
All	All	0.62	1/19568 (0.0%)	0.54	3/26440 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	GLY	C-O	17.72	1.52	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	217	ARG	CG-CD-NE	-5.40	100.46	111.80
1	C	185	GLY	CA-C-O	-5.32	111.02	120.60
2	E	248	TYR	CA-CB-CG	5.08	123.05	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2806	2825	2814	37	0
1	B	2806	2824	2813	52	0
1	C	2806	2825	2813	40	0
1	D	2806	2825	2815	29	0
2	E	1991	1913	1906	75	0
2	F	1991	1913	1904	73	0
2	G	1991	1913	1906	68	0
2	H	1991	1914	1905	54	0
3	I	28	27	25	0	0
4	A	14	14	13	5	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	9	0
5	G	11	11	10	0	0
All	All	19445	19208	19111	420	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 420 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%)	19	60
2	F	249/268 (93%)	236 (95%)	11 (4%)	2 (1%)	19	60
2	G	249/268 (93%)	235 (94%)	9 (4%)	5 (2%)	7	40
2	H	249/268 (93%)	237 (95%)	10 (4%)	2 (1%)	19	60
All	All	2360/2928 (81%)	2282 (97%)	67 (3%)	11 (0%)	29	68

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%)	309 (97%)	10 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	319/418 (76%)	310 (97%)	9 (3%)	43	65
1	C	319/418 (76%)	311 (98%)	8 (2%)	47	68
1	D	319/418 (76%)	312 (98%)	7 (2%)	52	71
2	E	217/231 (94%)	209 (96%)	8 (4%)	34	59
2	F	217/231 (94%)	211 (97%)	6 (3%)	43	65
2	G	217/231 (94%)	209 (96%)	8 (4%)	34	59
2	H	217/231 (94%)	211 (97%)	6 (3%)	43	65
All	All	2144/2596 (83%)	2082 (97%)	62 (3%)	42	64

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	93	GLN
2	G	206	ILE
2	E	115	ASN
2	G	198	ILE
2	H	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	HIS
1	C	123	ASN
1	D	123	ASN
2	E	295	GLN
2	G	295	GLN

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	1.05	1 (7%)	17,19,21	1.41	2 (11%)
3	NAG	I	2	3	14,14,15	1.00	0	17,19,21	1.84	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	2.28	1.47	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	2	NAG	C2-N2-C7	4.72	129.62	122.90
3	I	1	NAG	C1-O5-C5	4.22	117.91	112.19
3	I	2	NAG	O5-C1-C2	2.73	115.60	111.29
3	I	2	NAG	O4-C4-C3	-2.36	104.89	110.35
3	I	1	NAG	O3-C3-C2	-2.16	105.00	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

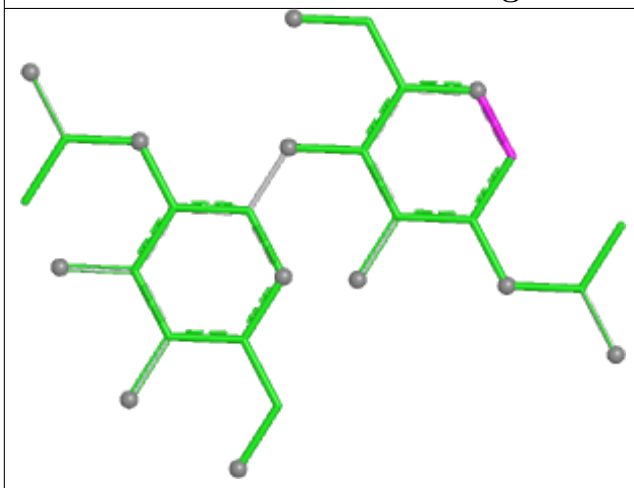
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C4-C5-C6-O6

There are no ring outliers.

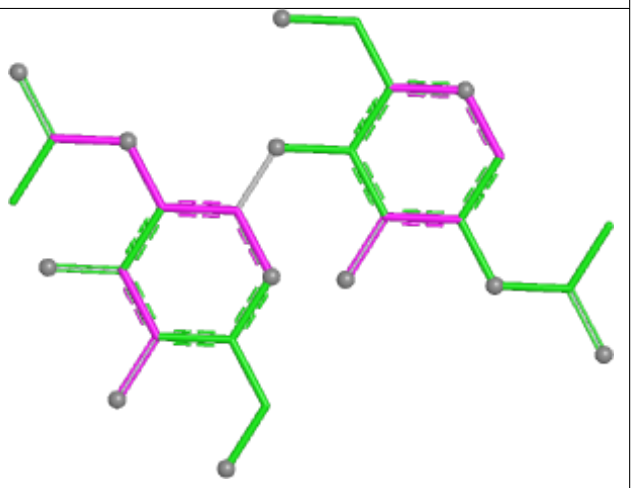
No monomer is involved in short contacts.

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

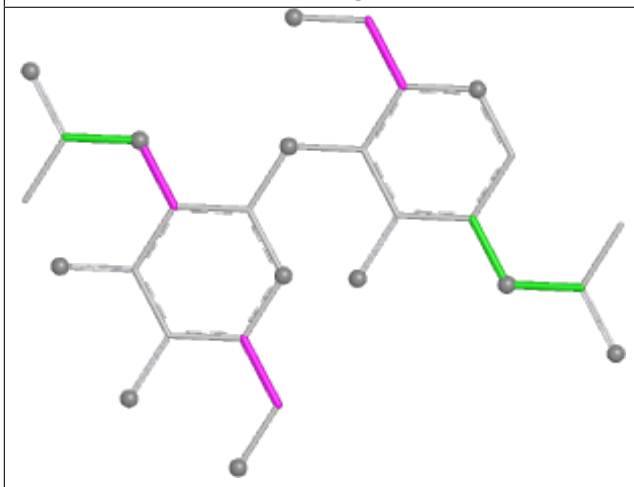
Oligosaccharide Chain I



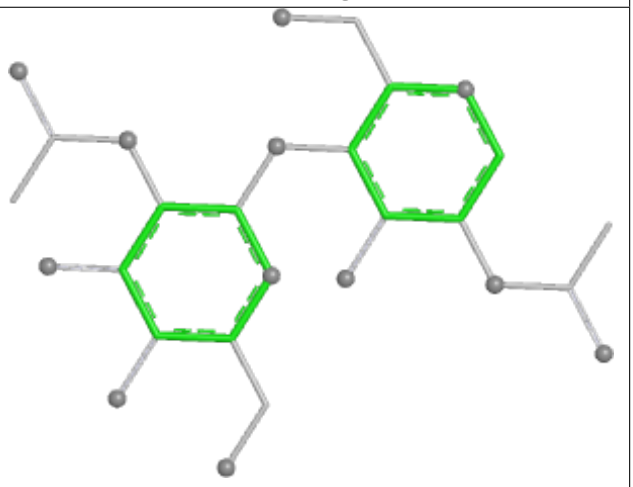
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	NAG	H	401	2	14,14,15	0.44	0	17,19,21	1.07	1 (5%)
4	NAG	G	401	2	14,14,15	1.27	3 (21%)	17,19,21	2.95	8 (47%)
4	NAG	F	402	2	14,14,15	1.18	1 (7%)	17,19,21	1.94	3 (17%)
4	NAG	C	502	1	14,14,15	1.33	2 (14%)	17,19,21	3.67	10 (58%)
5	MAN	G	403	2	11,11,12	1.46	2 (18%)	15,15,17	2.78	6 (40%)
4	NAG	A	501	1	14,14,15	1.24	2 (14%)	17,19,21	2.94	6 (35%)
4	NAG	G	402	2	14,14,15	1.66	3 (21%)	17,19,21	3.08	8 (47%)
4	NAG	D	502	1	14,14,15	1.68	3 (21%)	17,19,21	2.77	7 (41%)
5	MAN	E	401	2	11,11,12	1.59	4 (36%)	15,15,17	2.37	8 (53%)
4	NAG	B	502	1	14,14,15	0.88	0	17,19,21	2.25	6 (35%)
4	NAG	E	403	2	14,14,15	1.41	2 (14%)	17,19,21	1.87	2 (11%)
4	NAG	C	501	1	14,14,15	0.92	1 (7%)	17,19,21	1.30	3 (17%)
4	NAG	F	401	2	14,14,15	1.91	4 (28%)	17,19,21	1.56	2 (11%)
4	NAG	D	501	1	14,14,15	0.64	0	17,19,21	1.37	1 (5%)
4	NAG	B	501	1	14,14,15	0.93	1 (7%)	17,19,21	1.43	3 (17%)
5	MAN	F	403	2	11,11,12	0.88	0	15,15,17	2.52	5 (33%)
4	NAG	E	402	2	14,14,15	0.94	0	17,19,21	2.28	8 (47%)

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

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

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	502	NAG	C1-C2	4.53	1.59	1.52
4	F	401	NAG	C2-N2	4.41	1.53	1.46
4	F	402	NAG	C1-C2	3.96	1.58	1.52
4	G	402	NAG	C1-C2	3.57	1.57	1.52
4	E	403	NAG	O5-C5	3.47	1.50	1.43

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	NAG	O5-C5-C6	9.25	121.71	107.20
4	G	401	NAG	C2-N2-C7	8.57	135.11	122.90
4	C	502	NAG	C2-N2-C7	7.99	134.28	122.90
4	G	402	NAG	C2-N2-C7	7.68	133.84	122.90
4	C	502	NAG	O5-C5-C6	6.78	117.83	107.20

There are no chirality outliers.

5 of 32 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
4	H	401	NAG	7	0
4	G	401	NAG	7	0
4	F	402	NAG	1	0
4	C	502	NAG	1	0
4	A	501	NAG	5	0
4	G	402	NAG	3	0
4	D	502	NAG	1	0
4	B	502	NAG	1	0
4	E	403	NAG	1	0
4	C	501	NAG	2	0
4	F	401	NAG	4	0
4	D	501	NAG	2	0
4	B	501	NAG	11	0
5	F	403	MAN	9	0
4	E	402	NAG	20	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

Unable to reproduce the depositors R factor - this section is therefore empty.

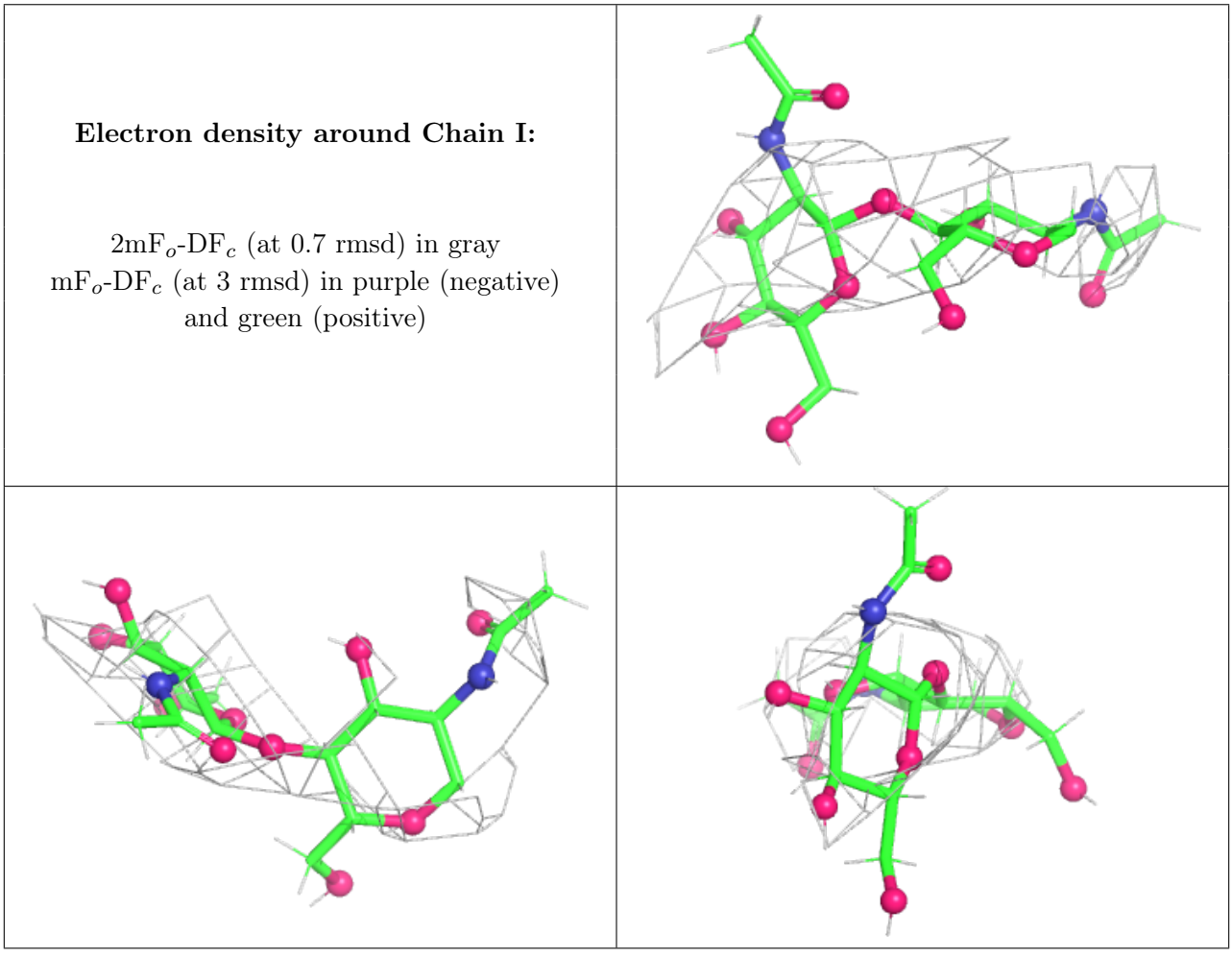
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.