



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:35 PM UTC

PDB ID : 7ZA3 / pdb_00007za3
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 : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

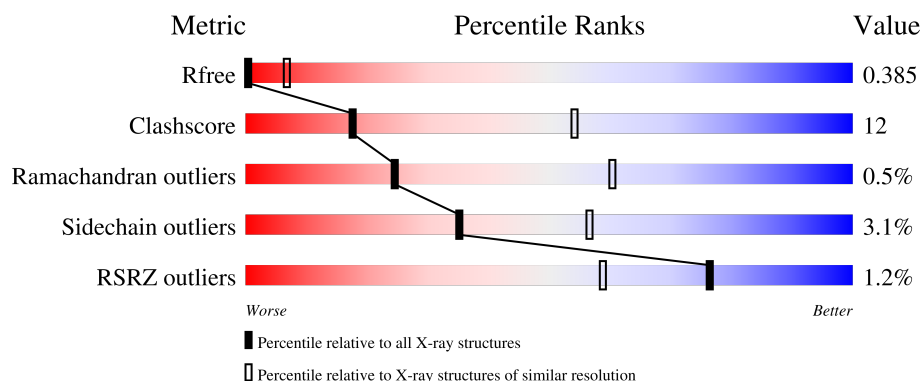
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	A	464	% 59% 16% 24%
1	B	464	59% 16% • 24%
1	C	464	60% 15% • 24%
1	D	464	% 63% 12% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	268	 % 64% 28% • 6%
2	F	268	 3% 62% 29% • 6%
2	G	268	 % 62% 30% • 6%
2	H	268	 % 64% 28% • 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

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

Continued on next page...

Continued from previous page...

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:

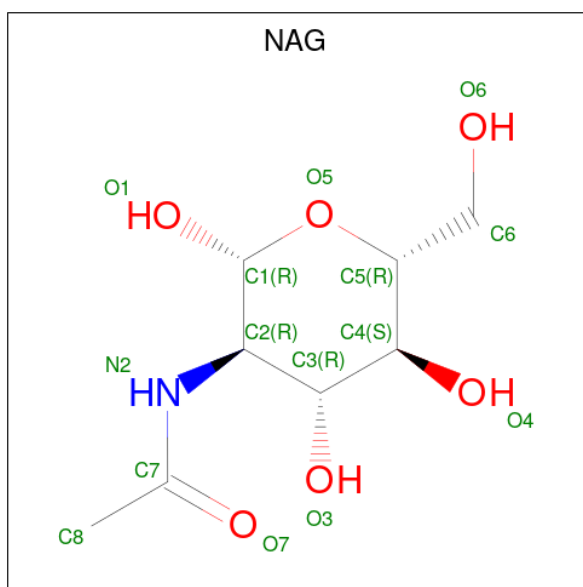
Chain	Residue	Modelled	Actual	Comment	Reference
E	308	HIS	-	expression tag	UNP F1LW30
E	309	HIS	-	expression tag	UNP F1LW30
E	310	HIS	-	expression tag	UNP F1LW30
E	311	HIS	-	expression tag	UNP F1LW30
E	312	HIS	-	expression tag	UNP F1LW30
E	313	HIS	-	expression tag	UNP F1LW30
F	308	HIS	-	expression tag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



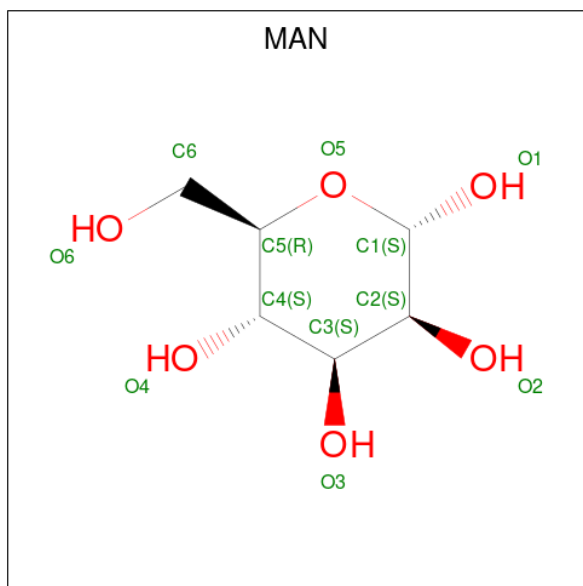
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

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



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 (CCD ID: MAN) (formula: $C_6H_{12}O_6$).

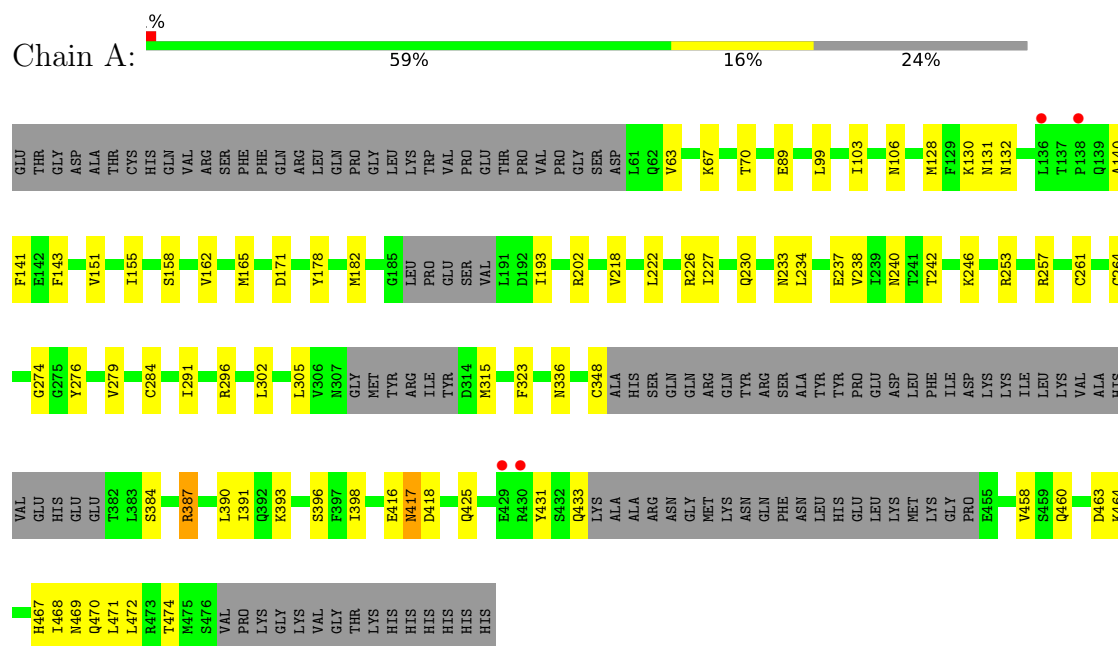


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	4	0
			22	6	11	5		
5	F	1	Total	C	H	O	4	0
			22	6	11	5		
5	G	1	Total	C	H	O	4	0
			22	6	11	5		

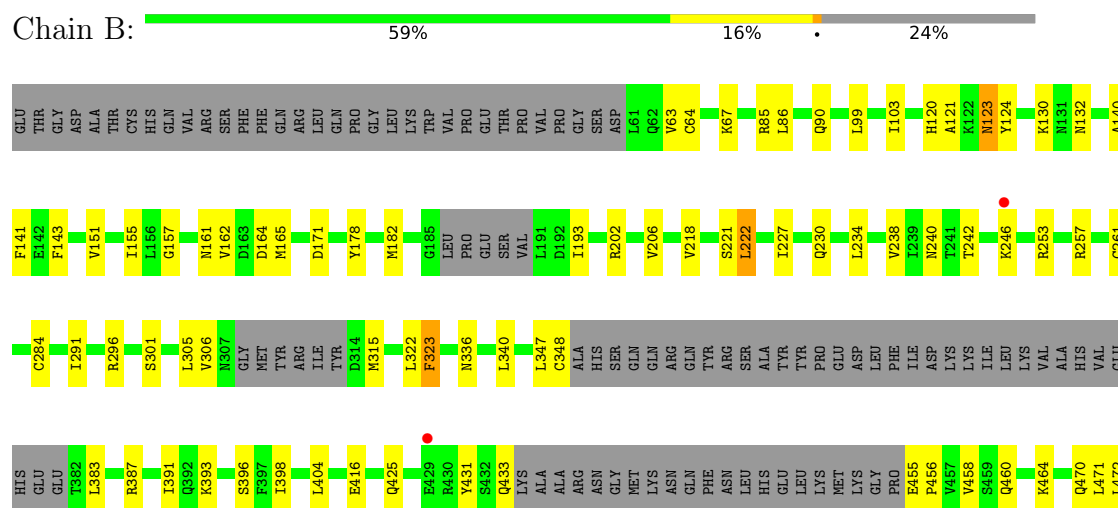
3 Residue-property plots [i](#)

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.

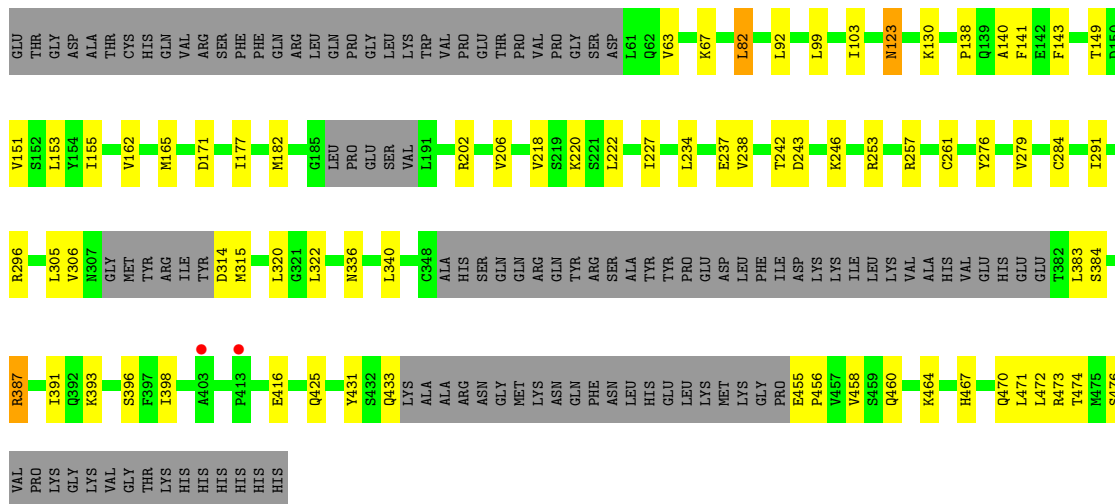
• Molecule 1: Glypican-3



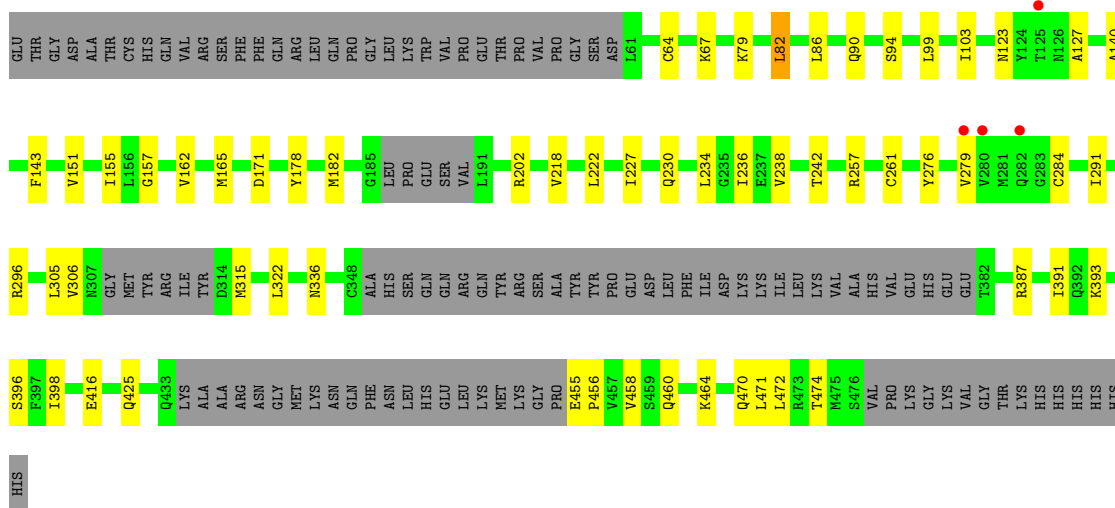
• Molecule 1: Glypican-3



- Molecule 1: Glypican-3

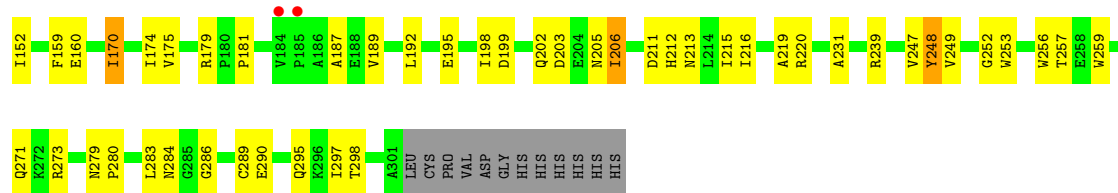


- Molecule 1: Glypican-3

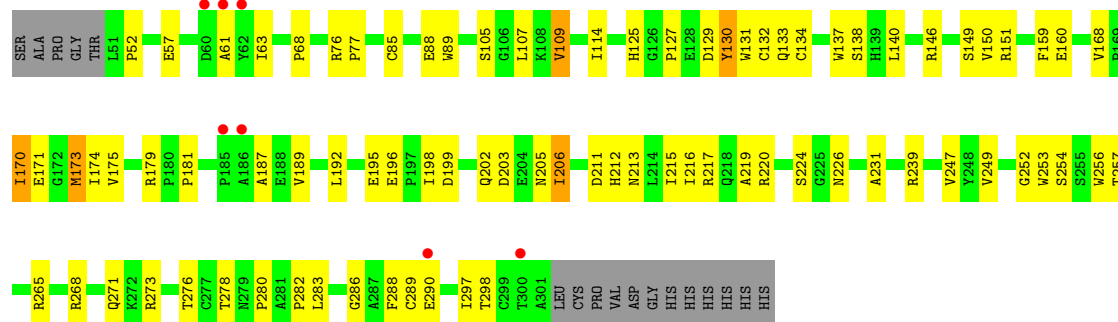


- Molecule 2: Netrin receptor UNC5D

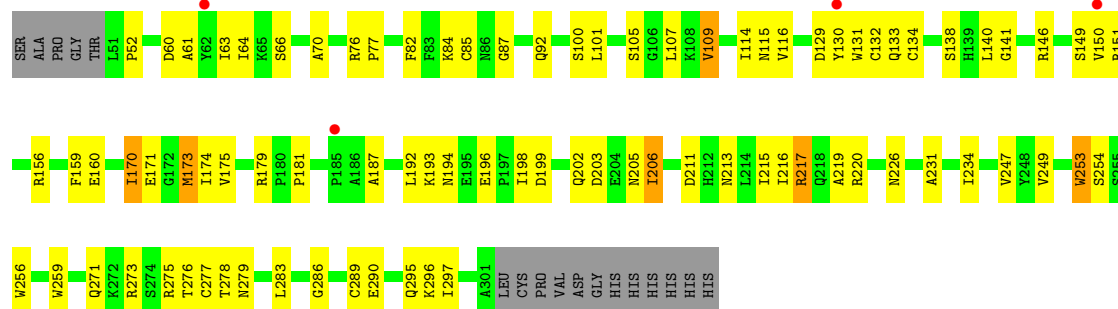




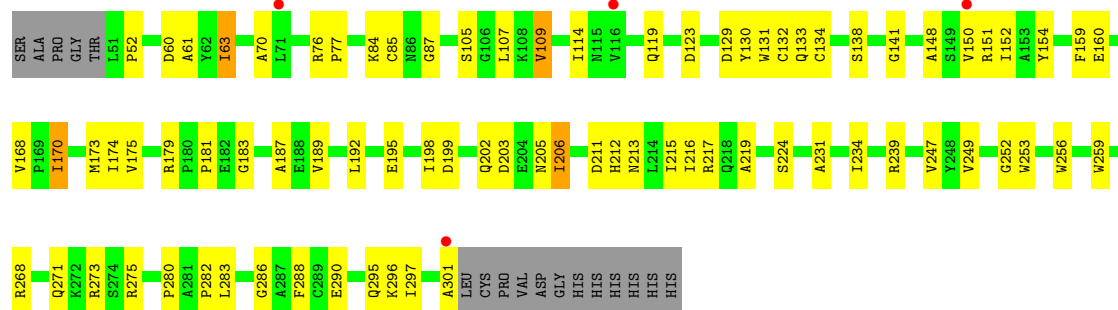
• Molecule 2: Netrin receptor UNC5D



• 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

Chain I:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	119.58Å 119.58Å 257.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.88 – 4.00 80.88 – 4.00	Depositor EDS
% Data completeness (in resolution range)	74.8 (80.88-4.00) 74.8 (80.88-4.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.355 , 0.385 0.353 , 0.385	Depositor DCC
R_{free} test set	1333 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	210.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 933.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.418 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	38653	wwPDB-VP
Average B, all atoms (Å ²)	319.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	0.86	0/2854	0.95	0/3846
1	B	0.88	0/2854	0.98	0/3846
1	C	0.87	0/2854	0.95	0/3846
1	D	0.87	0/2854	0.94	0/3846
2	E	0.88	0/2038	0.87	1/2764 (0.0%)
2	F	0.90	0/2038	0.91	1/2764 (0.0%)
2	G	0.88	0/2038	0.87	1/2764 (0.0%)
2	H	0.89	0/2038	0.86	0/2764
All	All	0.88	0/19568	0.93	3/26440 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	217	ARG	CG-CD-NE	-7.53	95.44	112.00
2	E	248	TYR	CB-CA-C	5.97	120.13	109.38
2	F	226	ASN	OD1-CG-ND2	5.37	127.97	122.60

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	48	4
1	B	2806	2824	2813	62	4
1	C	2806	2825	2813	55	0
1	D	2806	2825	2815	46	0
2	E	1991	1913	1906	77	1
2	F	1991	1913	1904	89	30
2	G	1991	1913	1906	88	26
2	H	1991	1914	1906	66	3
3	I	28	27	25	0	0
4	A	14	14	13	4	0
4	B	28	28	26	11	0
4	C	28	28	24	4	0
4	D	28	28	26	3	0
4	E	28	28	26	11	0
4	F	28	28	26	4	0
4	G	28	28	26	9	0
4	H	14	14	13	7	0
5	E	11	11	10	0	0
5	F	11	11	10	8	0
5	G	11	11	10	0	0
All	All	19445	19208	19112	474	35

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 (474) 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	1.23	1.65
2:F:256:TRP:HD1	5:F:403:MAN:C1	1.17	1.43
1:D:123:ASN:HD21	4:D:501:NAG:C1	1.31	1.41
2:F:253:TRP:CZ3	2:F:289:CYS:CB	2.15	1.28
2:G:70:ALA:HB2	4:G:401:NAG:O7	1.35	1.25
2:F:253:TRP:CH2	2:F:289:CYS:HB3	1.71	1.23
1:C:123:ASN:HD21	4:C:501:NAG:C1	1.54	1.21
1:C:82:LEU:HD22	2:H:234:ILE:HD13	1.29	1.10
1:D:82:LEU:HD22	2:G:234:ILE:HD13	1.10	1.08
2:E:70:ALA:N	4:E:402:NAG:H81	1.68	1.06
2:F:127:PRO:HG3	2:H:296:LYS:O	1.55	1.05
1:C:138:PRO:HG3	2:G:66:SER:OG	1.54	1.05
1:B:123:ASN:HB2	4:B:501:NAG:O7	1.56	1.05
2:G:253:TRP:CZ2	2:G:289:CYS:HB3	1.96	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:ALA:HB3	4:H:401:NAG:C7	1.91	1.00
1:B:90:GLN:OE1	2:E:146:ARG:NH1	1.95	1.00
2:G:253:TRP:CE2	2:G:289:CYS:HB3	1.97	0.99
2:H:70:ALA:CB	4:H:401:NAG:C7	2.41	0.99
2:E:256:TRP:CE3	2:E:273:ARG:HG2	2.00	0.96
1:D:82:LEU:CD2	2:G:234:ILE:HD13	1.95	0.96
1:B:123:ASN:CB	4:B:501:NAG:O7	2.13	0.96
2:F:256:TRP:CD1	5:F:403:MAN:C2	2.49	0.94
1:C:82:LEU:HD22	2:H:234:ILE:CD1	1.96	0.93
2:E:256:TRP:HE3	2:E:273:ARG:HG2	1.32	0.91
2:F:127:PRO:CG	2:H:296:LYS:O	2.18	0.90
2:H:70:ALA:HB3	4:H:401:NAG:C8	2.02	0.90
2:F:127:PRO:HD3	2:H:296:LYS:O	1.72	0.89
2:E:256:TRP:CH2	2:E:295:GLN:HB2	2.08	0.89
2:E:253:TRP:CH2	2:E:289:CYS:HB3	2.09	0.88
1:D:82:LEU:HD22	2:G:234:ILE:CD1	2.01	0.87
2:F:253:TRP:HZ3	2:F:289:CYS:HB3	1.30	0.87
1:B:157:GLY:O	2:H:288:PHE:CE1	2.26	0.87
2:H:253:TRP:CZ3	2:H:275:ARG:HD3	2.11	0.86
2:F:127:PRO:CD	2:H:296:LYS:O	2.27	0.83
1:A:227:ILE:HD11	1:A:471:LEU:HB3	1.60	0.81
1:D:305:LEU:HD22	1:D:472:LEU:HD23	1.64	0.79
2:E:70:ALA:N	4:E:402:NAG:C8	2.45	0.79
2:F:256:TRP:HE1	5:F:403:MAN:H2	1.47	0.79
2:F:256:TRP:NE1	5:F:403:MAN:C1	2.45	0.78
1:C:305:LEU:HD22	1:C:472:LEU:HD23	1.66	0.78
1:C:234:LEU:HD11	1:C:464:LYS:HB3	1.66	0.78
2:F:127:PRO:HB3	2:H:295:GLN:HG3	1.66	0.78
2:G:256:TRP:HE3	2:G:273:ARG:HG2	1.47	0.78
1:B:305:LEU:HD22	1:B:472:LEU:HD23	1.65	0.76
1:D:94:SER:OG	2:G:146:ARG:NH2	2.18	0.76
1:A:305:LEU:HD22	1:A:472:LEU:HD23	1.67	0.76
2:G:70:ALA:HB2	4:G:401:NAG:C7	2.13	0.75
2:G:70:ALA:CB	4:G:401:NAG:H81	2.16	0.75
4:A:501:NAG:C8	2:G:279:ASN:HB2	2.17	0.74
1:B:227:ILE:HD11	1:B:471:LEU:HB3	1.70	0.74
2:F:253:TRP:CH2	2:F:290:GLU:N	2.56	0.74
1:C:227:ILE:HD11	1:C:471:LEU:HB3	1.70	0.73
1:B:120:HIS:HA	4:B:501:NAG:O7	1.88	0.73
2:E:69:ILE:C	4:E:402:NAG:H81	2.13	0.73
2:G:253:TRP:CH2	2:G:289:CYS:HB3	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:253:TRP:CE3	2:F:289:CYS:SG	2.82	0.73
2:H:253:TRP:HZ2	2:H:290:GLU:O	1.70	0.72
2:G:253:TRP:HZ2	2:G:290:GLU:C	1.98	0.72
2:E:129:ASP:HB3	2:E:151:ARG:HD3	1.72	0.71
2:F:256:TRP:NE1	5:F:403:MAN:C2	2.53	0.71
1:A:233:ASN:HB3	2:G:278:THR:HG22	1.73	0.70
2:E:253:TRP:HZ2	2:E:290:GLU:O	1.75	0.70
1:A:234:LEU:HD11	1:A:464:LYS:HB3	1.74	0.70
2:G:254:SER:OG	2:G:276:THR:N	2.25	0.70
2:H:70:ALA:CB	4:H:401:NAG:O7	2.39	0.69
2:G:129:ASP:HB3	2:G:151:ARG:HD3	1.74	0.69
1:C:138:PRO:CG	2:G:66:SER:OG	2.38	0.69
1:D:227:ILE:HD11	1:D:471:LEU:HB3	1.73	0.69
2:G:226:ASN:ND2	4:G:402:NAG:H82	2.07	0.68
2:E:205:ASN:HD21	2:E:216:ILE:HG23	1.59	0.68
2:G:70:ALA:CB	4:G:401:NAG:O7	2.28	0.68
1:A:70:THR:OG1	1:A:264:CYS:SG	2.52	0.67
1:C:220:LYS:NZ	1:C:314:ASP:OD1	2.22	0.67
2:F:256:TRP:CD1	5:F:403:MAN:HO2	2.12	0.67
2:E:96:VAL:HG11	4:E:402:NAG:C6	2.25	0.67
1:B:155:ILE:HD11	1:B:222:LEU:HD22	1.75	0.67
1:D:79:LYS:HE2	2:G:64:ILE:HD13	1.75	0.67
1:D:230:GLN:HE21	2:F:288:PHE:HZ	1.42	0.66
1:B:123:ASN:HB2	4:B:501:NAG:C7	2.25	0.66
1:B:123:ASN:HB3	4:B:501:NAG:O7	1.95	0.66
1:C:473:ARG:O	1:C:476:SER:OG	2.11	0.66
2:E:253:TRP:HZ2	2:E:290:GLU:C	2.04	0.66
1:A:417:ASN:OD1	1:A:417:ASN:N	2.27	0.66
2:H:253:TRP:CE3	2:H:275:ARG:NE	2.64	0.66
2:G:70:ALA:HB1	4:G:401:NAG:H81	1.76	0.66
1:B:123:ASN:CB	4:B:501:NAG:C7	2.73	0.66
1:B:234:LEU:HD11	1:B:464:LYS:HB3	1.78	0.65
1:D:236:ILE:HG21	2:F:278:THR:HG21	1.78	0.65
2:E:52:PRO:HG3	2:E:138:SER:HB2	1.78	0.65
2:G:256:TRP:CZ3	2:G:295:GLN:HB2	2.32	0.65
1:D:236:ILE:CG2	2:F:278:THR:HG21	2.26	0.65
2:F:253:TRP:CH2	2:F:289:CYS:CB	2.60	0.65
2:F:252:GLY:HA3	2:F:280:PRO:HD2	1.79	0.65
1:D:155:ILE:HD11	1:D:222:LEU:HD22	1.78	0.65
2:E:96:VAL:HG21	4:E:402:NAG:H62	1.78	0.64
1:A:291:ILE:HD11	1:A:458:VAL:HG13	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:175:VAL:HG22	2:G:215:ILE:HG23	1.78	0.64
2:H:76:ARG:HD3	2:H:109:VAL:HG22	1.80	0.64
2:G:256:TRP:CE3	2:G:273:ARG:NE	2.66	0.64
2:H:70:ALA:HB2	4:H:401:NAG:C7	2.25	0.64
2:E:253:TRP:CZ2	2:E:289:CYS:HB3	2.34	0.63
2:G:61:ALA:HB3	2:G:150:VAL:HG22	1.80	0.63
1:A:463:ASP:OD2	2:G:220:ARG:HB3	1.99	0.63
1:A:155:ILE:HD11	1:A:222:LEU:HD22	1.80	0.63
2:G:253:TRP:C	2:G:276:THR:O	2.42	0.62
2:F:76:ARG:HD3	2:F:109:VAL:HG22	1.81	0.62
2:F:76:ARG:HD2	2:F:107:LEU:HB3	1.82	0.62
1:A:230:GLN:OE1	2:G:283:LEU:HD23	1.99	0.62
1:C:291:ILE:HD11	1:C:458:VAL:HG13	1.82	0.62
2:F:68:PRO:O	4:F:401:NAG:H3	1.99	0.62
2:F:249:VAL:O	2:F:286:GLY:HA3	1.99	0.62
1:C:153:LEU:HD11	2:G:156:ARG:HH12	1.64	0.61
1:D:157:GLY:HA3	2:F:288:PHE:CE1	2.35	0.61
1:D:123:ASN:CG	4:D:501:NAG:C1	2.73	0.61
2:E:253:TRP:CZ2	2:E:290:GLU:O	2.53	0.61
1:C:155:ILE:HD11	1:C:222:LEU:HD22	1.81	0.61
2:E:253:TRP:CZ3	2:E:289:CYS:HB3	2.34	0.61
2:F:253:TRP:CH2	2:F:289:CYS:C	2.79	0.61
1:D:234:LEU:HD11	1:D:464:LYS:HB3	1.82	0.61
2:F:205:ASN:OD1	2:F:217:ARG:HG3	2.01	0.61
2:G:253:TRP:CD2	2:G:289:CYS:HB3	2.35	0.60
2:H:76:ARG:HD2	2:H:107:LEU:HB3	1.81	0.60
1:A:171:ASP:OD2	1:A:202:ARG:NH1	2.34	0.60
2:E:131:TRP:HA	2:E:149:SER:HA	1.83	0.60
2:H:252:GLY:HA3	2:H:280:PRO:HD2	1.84	0.60
2:E:256:TRP:CE3	2:E:273:ARG:CG	2.81	0.60
2:E:187:ALA:HB1	2:E:231:ALA:HB1	1.83	0.60
2:G:52:PRO:HG3	2:G:138:SER:HB2	1.84	0.59
2:G:253:TRP:CH2	2:G:289:CYS:CB	2.84	0.59
2:G:256:TRP:HZ3	2:G:295:GLN:HB2	1.67	0.59
2:H:175:VAL:HG22	2:H:215:ILE:HG23	1.84	0.59
1:A:296:ARG:HG2	1:A:398:ILE:HG12	1.84	0.59
1:C:162:VAL:HA	1:C:165:MET:HE3	1.85	0.59
2:E:125:HIS:O	2:G:296:LYS:HE3	2.03	0.59
2:G:76:ARG:HD2	2:G:107:LEU:HB3	1.84	0.59
2:F:76:ARG:HB2	2:F:109:VAL:HG13	1.85	0.59
2:F:253:TRP:HH2	2:F:290:GLU:N	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:76:ARG:HD3	2:G:109:VAL:HG22	1.84	0.58
2:F:211:ASP:OD2	2:F:213:ASN:ND2	2.36	0.58
2:H:282:PRO:HG2	2:H:288:PHE:CD2	2.38	0.58
2:F:217:ARG:NH2	2:G:217:ARG:HE	2.02	0.58
1:C:305:LEU:HD11	1:C:472:LEU:O	2.04	0.58
2:G:254:SER:OG	2:G:275:ARG:HA	2.02	0.58
2:G:76:ARG:HH12	2:G:105:SER:HB2	1.68	0.58
1:B:171:ASP:OD2	1:B:202:ARG:NH1	2.36	0.58
2:G:256:TRP:CE3	2:G:273:ARG:HG2	2.36	0.58
1:B:86:LEU:HD13	2:E:59:GLU:CD	2.28	0.58
2:F:175:VAL:HG22	2:F:215:ILE:HG23	1.85	0.58
2:H:199:ASP:HB3	2:H:202:GLN:HB2	1.86	0.57
2:E:76:ARG:HH12	2:E:105:SER:HB2	1.69	0.57
2:F:253:TRP:CZ3	2:F:289:CYS:SG	2.97	0.57
2:G:211:ASP:OD2	2:G:213:ASN:ND2	2.36	0.57
1:B:120:HIS:HA	4:B:501:NAG:H81	1.86	0.57
2:F:256:TRP:NE1	5:F:403:MAN:H2	2.12	0.57
1:B:305:LEU:HD11	1:B:472:LEU:O	2.04	0.57
2:F:76:ARG:HH12	2:F:105:SER:HB2	1.70	0.57
1:D:162:VAL:HA	1:D:165:MET:HE3	1.87	0.57
2:F:199:ASP:HB3	2:F:202:GLN:HB2	1.87	0.57
2:H:249:VAL:O	2:H:286:GLY:HA3	2.04	0.57
1:B:296:ARG:HG2	1:B:398:ILE:HG12	1.87	0.57
2:H:76:ARG:HB2	2:H:109:VAL:HG13	1.85	0.57
2:H:253:TRP:CZ3	2:H:275:ARG:CD	2.86	0.57
2:F:129:ASP:HB3	2:F:151:ARG:HD3	1.86	0.57
1:B:157:GLY:O	2:H:288:PHE:CD1	2.57	0.56
2:E:211:ASP:OD2	2:E:213:ASN:ND2	2.38	0.56
2:F:253:TRP:CZ2	2:F:290:GLU:O	2.58	0.56
2:H:253:TRP:CE3	2:H:275:ARG:CD	2.87	0.56
1:B:120:HIS:HA	4:B:501:NAG:C7	2.35	0.56
2:G:256:TRP:CH2	2:G:295:GLN:NE2	2.74	0.56
2:H:52:PRO:HG3	2:H:138:SER:HB2	1.87	0.56
1:D:305:LEU:HD11	1:D:472:LEU:O	2.05	0.56
1:B:124:TYR:HB3	1:B:323:PHE:CE1	2.40	0.56
2:E:96:VAL:HG11	4:E:402:NAG:H62	1.88	0.56
2:H:211:ASP:OD2	2:H:213:ASN:ND2	2.39	0.56
1:A:416:GLU:H	1:A:416:GLU:CD	2.12	0.56
1:C:431:TYR:CE2	1:C:433:GLN:HG2	2.40	0.56
2:E:249:VAL:O	2:E:286:GLY:HA3	2.06	0.55
1:B:130:LYS:HG3	1:B:141:PHE:HZ	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:70:ALA:CB	4:G:401:NAG:C7	2.83	0.55
2:E:160:GLU:HB3	2:E:179:ARG:HB3	1.87	0.55
2:E:256:TRP:HZ3	2:E:273:ARG:O	1.90	0.55
1:C:130:LYS:HG3	1:C:141:PHE:HZ	1.71	0.55
2:G:70:ALA:CB	4:G:401:NAG:C8	2.84	0.55
1:A:237:GLU:OE2	1:A:464:LYS:NZ	2.40	0.55
2:G:253:TRP:CZ2	2:G:289:CYS:CB	2.83	0.55
2:H:129:ASP:HB3	2:H:151:ARG:HD3	1.88	0.55
1:B:157:GLY:HA3	2:H:288:PHE:CZ	2.42	0.55
2:E:70:ALA:N	4:E:402:NAG:C7	2.64	0.55
2:F:52:PRO:HG3	2:F:138:SER:HB2	1.88	0.55
1:D:171:ASP:OD2	1:D:202:ARG:NH1	2.40	0.54
2:E:76:ARG:HD2	2:E:107:LEU:HB3	1.89	0.54
2:E:175:VAL:HG22	2:E:215:ILE:HG23	1.89	0.54
2:H:205:ASN:HD21	2:H:216:ILE:HG23	1.72	0.54
2:G:76:ARG:HB2	2:G:109:VAL:HG13	1.88	0.54
2:F:187:ALA:HB1	2:F:231:ALA:HB1	1.89	0.54
2:G:205:ASN:HD21	2:G:216:ILE:HG23	1.73	0.54
2:F:127:PRO:CB	2:H:295:GLN:HG3	2.35	0.54
2:F:254:SER:OG	2:F:276:THR:N	2.40	0.54
1:B:162:VAL:HA	1:B:165:MET:HE3	1.88	0.54
4:C:502:NAG:H61	2:E:279:ASN:ND2	2.22	0.54
1:D:296:ARG:HG2	1:D:398:ILE:HG12	1.89	0.54
2:E:76:ARG:HD3	2:E:109:VAL:HG22	1.89	0.54
2:F:52:PRO:HA	2:F:77:PRO:HD2	1.88	0.54
2:E:199:ASP:HB3	2:E:202:GLN:HB2	1.90	0.54
2:E:256:TRP:CD2	2:E:273:ARG:NE	2.76	0.54
2:F:253:TRP:CE3	2:F:289:CYS:CB	2.88	0.54
1:B:230:GLN:HE21	2:H:288:PHE:HZ	1.56	0.54
1:C:99:LEU:O	1:C:103:ILE:HG13	2.08	0.54
1:B:291:ILE:HD11	1:B:458:VAL:HG13	1.88	0.53
2:G:194:ASN:OD1	4:G:402:NAG:H81	2.08	0.53
4:A:501:NAG:O4	4:A:501:NAG:O6	2.21	0.53
2:F:125:HIS:O	2:H:296:LYS:HE3	2.08	0.53
2:H:70:ALA:HB3	4:H:401:NAG:O7	2.03	0.53
2:E:253:TRP:CH2	2:E:289:CYS:CB	2.89	0.53
1:B:123:ASN:HB3	4:B:501:NAG:H2	1.90	0.53
2:H:76:ARG:HH12	2:H:105:SER:HB2	1.73	0.53
2:H:253:TRP:HZ3	2:H:275:ARG:HD3	1.71	0.53
1:A:467:HIS:HD2	2:G:283:LEU:HD13	1.74	0.53
2:H:205:ASN:OD1	2:H:217:ARG:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ASN:C	1:D:123:ASN:HD22	2.15	0.53
2:E:76:ARG:HB2	2:E:109:VAL:HG13	1.90	0.52
1:B:151:VAL:O	1:B:155:ILE:HG12	2.09	0.52
2:E:52:PRO:HA	2:E:77:PRO:HD2	1.92	0.52
1:A:384:SER:HA	1:A:387:ARG:HD3	1.90	0.52
2:E:252:GLY:HA3	2:E:280:PRO:HD2	1.92	0.52
1:A:151:VAL:O	1:A:155:ILE:HG12	2.10	0.52
2:G:199:ASP:HB3	2:G:202:GLN:HB2	1.92	0.52
1:D:291:ILE:HD11	1:D:458:VAL:HG13	1.91	0.52
1:A:162:VAL:HA	1:A:165:MET:HE3	1.91	0.52
1:C:467:HIS:NE2	2:E:284:ASN:ND2	2.58	0.52
1:B:99:LEU:O	1:B:103:ILE:HG13	2.09	0.51
1:D:151:VAL:O	1:D:155:ILE:HG12	2.09	0.51
2:F:61:ALA:HB3	2:F:150:VAL:HG22	1.92	0.51
1:B:123:ASN:HB3	4:B:501:NAG:C2	2.41	0.51
2:E:70:ALA:H	4:E:402:NAG:C8	2.22	0.51
1:A:99:LEU:O	1:A:103:ILE:HG13	2.11	0.51
1:C:296:ARG:HG2	1:C:398:ILE:HG12	1.92	0.51
2:H:187:ALA:HB1	2:H:231:ALA:HB1	1.90	0.51
1:D:99:LEU:O	1:D:103:ILE:HG13	2.10	0.51
4:A:501:NAG:HO6	4:A:501:NAG:HO4	1.57	0.51
1:A:140:ALA:HA	1:A:143:PHE:CZ	2.46	0.51
1:C:138:PRO:HG3	2:G:66:SER:CB	2.40	0.51
2:F:171:GLU:OE1	2:F:220:ARG:NE	2.43	0.51
2:F:195:GLU:OE1	2:F:239:ARG:NH1	2.45	0.50
2:G:203:ASP:HB3	2:G:206:ILE:HD12	1.92	0.50
1:B:120:HIS:HA	4:B:501:NAG:C8	2.41	0.50
1:C:140:ALA:HA	1:C:143:PHE:CZ	2.46	0.50
2:H:159:PHE:HA	2:H:181:PRO:HG3	1.93	0.50
1:A:140:ALA:HA	1:A:143:PHE:CE2	2.46	0.50
1:C:151:VAL:O	1:C:155:ILE:HG12	2.10	0.50
2:H:52:PRO:HA	2:H:77:PRO:HD2	1.93	0.50
2:F:217:ARG:CZ	2:G:217:ARG:HE	2.25	0.50
1:A:130:LYS:HG3	1:A:141:PHE:HZ	1.75	0.50
1:C:384:SER:HA	1:C:387:ARG:HD3	1.93	0.50
1:D:238:VAL:O	1:D:242:THR:HG23	2.12	0.50
1:B:90:GLN:HE22	2:E:146:ARG:HH22	1.60	0.50
2:G:85:CYS:HA	2:G:132:CYS:HA	1.94	0.50
2:E:115:ASN:N	2:E:115:ASN:HD22	2.09	0.49
4:E:403:NAG:O7	4:E:403:NAG:H3	2.12	0.49
1:B:140:ALA:HA	1:B:143:PHE:CE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:217:ARG:NE	2:G:217:ARG:NE	2.60	0.49
2:G:187:ALA:HB1	2:G:231:ALA:HB1	1.94	0.49
2:G:253:TRP:CZ2	2:G:289:CYS:C	2.90	0.49
1:C:257:ARG:HA	1:C:261:CYS:HB2	1.95	0.49
2:E:219:ALA:HB1	2:E:247:VAL:HG11	1.94	0.49
2:G:159:PHE:HA	2:G:181:PRO:HG3	1.95	0.49
1:A:431:TYR:CE2	1:A:433:GLN:HG3	2.48	0.49
1:D:140:ALA:HA	1:D:143:PHE:CZ	2.48	0.49
2:F:68:PRO:HD2	4:F:401:NAG:O6	2.13	0.49
2:F:85:CYS:HA	2:F:132:CYS:HA	1.95	0.49
2:H:85:CYS:HA	2:H:132:CYS:HA	1.94	0.49
2:H:271:GLN:HG2	2:H:297:ILE:O	2.13	0.49
1:B:206:VAL:HG12	1:B:340:LEU:HD11	1.94	0.49
1:A:238:VAL:O	1:A:242:THR:HG23	2.13	0.49
2:G:131:TRP:HZ3	2:G:133:GLN:HB2	1.77	0.48
1:B:315:MET:O	1:B:315:MET:HG2	2.13	0.48
2:G:52:PRO:HA	2:G:77:PRO:HD2	1.95	0.48
2:H:195:GLU:OE1	2:H:239:ARG:NH1	2.47	0.48
2:F:256:TRP:CD1	5:F:403:MAN:O2	2.65	0.48
2:F:271:GLN:HG2	2:F:297:ILE:O	2.13	0.48
2:G:131:TRP:HA	2:G:149:SER:HA	1.96	0.48
1:A:63:VAL:HG22	1:A:253:ARG:HG2	1.96	0.48
1:B:140:ALA:HA	1:B:143:PHE:CZ	2.48	0.48
1:B:460:GLN:HG2	1:B:464:LYS:HE3	1.94	0.48
2:F:254:SER:HB3	2:F:276:THR:O	2.14	0.48
1:C:140:ALA:HA	1:C:143:PHE:CE2	2.49	0.48
1:C:206:VAL:HG12	1:C:340:LEU:HD11	1.95	0.48
4:C:502:NAG:H61	2:E:279:ASN:CG	2.39	0.48
1:D:393:LYS:O	1:D:396:SER:OG	2.31	0.48
2:E:61:ALA:HB3	2:E:150:VAL:HG22	1.95	0.48
2:F:68:PRO:HD2	4:F:401:NAG:H5	1.96	0.48
2:H:154:TYR:O	2:H:183:GLY:HA2	2.13	0.48
1:A:305:LEU:HD11	1:A:472:LEU:O	2.14	0.48
2:E:203:ASP:HB3	2:E:206:ILE:HD12	1.96	0.48
2:E:256:TRP:HB3	2:E:273:ARG:HD2	1.96	0.48
1:A:89:GLU:OE2	1:A:246:LYS:NZ	2.46	0.47
1:B:63:VAL:HG22	1:B:253:ARG:HG2	1.96	0.47
2:G:249:VAL:O	2:G:286:GLY:HA3	2.13	0.47
1:D:306:VAL:HG11	1:D:391:ILE:HG13	1.96	0.47
2:E:85:CYS:HA	2:E:132:CYS:HA	1.95	0.47
2:F:253:TRP:HH2	2:F:289:CYS:C	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:100:SER:O	2:G:101:LEU:HD22	2.14	0.47
1:B:238:VAL:O	1:B:242:THR:HG23	2.13	0.47
2:F:168:VAL:HG13	2:F:247:VAL:HG12	1.95	0.47
2:F:189:VAL:HG11	2:F:212:HIS:HB3	1.96	0.47
1:C:455:GLU:N	1:C:456:PRO:HD2	2.30	0.47
1:D:140:ALA:HA	1:D:143:PHE:CE2	2.49	0.47
1:A:158:SER:O	1:A:226:ARG:NH2	2.48	0.47
1:B:121:ALA:O	1:B:323:PHE:HE1	1.97	0.47
2:H:131:TRP:HZ3	2:H:133:GLN:HB2	1.80	0.47
4:A:501:NAG:H83	4:A:501:NAG:H2	1.76	0.47
2:F:170:ILE:HG12	2:F:249:VAL:HG22	1.96	0.47
1:B:455:GLU:N	1:B:456:PRO:HD2	2.30	0.47
2:F:219:ALA:HB1	2:F:247:VAL:HG11	1.96	0.47
1:A:106:ASN:CG	1:A:390:LEU:HD13	2.40	0.46
1:B:193:ILE:HD11	1:B:348:CYS:HB3	1.96	0.46
1:D:86:LEU:HD13	2:G:60:ASP:OD2	2.16	0.46
2:E:131:TRP:HZ3	2:E:133:GLN:HB2	1.79	0.46
2:F:68:PRO:HB2	4:F:401:NAG:H5	1.97	0.46
2:F:203:ASP:HB3	2:F:206:ILE:HD12	1.97	0.46
2:E:96:VAL:HG11	4:E:402:NAG:O6	2.16	0.46
2:E:271:GLN:HG2	2:E:297:ILE:O	2.15	0.46
2:G:271:GLN:HG2	2:G:297:ILE:O	2.14	0.46
1:A:128:MET:HG3	1:A:323:PHE:CD2	2.51	0.46
1:A:460:GLN:HB2	2:G:220:ARG:CZ	2.45	0.46
2:F:131:TRP:HA	2:F:149:SER:HA	1.98	0.46
1:D:257:ARG:HA	1:D:261:CYS:HB2	1.98	0.46
2:E:79:MET:HE3	2:E:138:SER:HA	1.96	0.46
2:H:63:ILE:HG22	2:H:152:ILE:HA	1.96	0.46
1:A:67:LYS:HD2	1:A:425:GLN:HB2	1.98	0.46
1:D:67:LYS:HE3	1:D:425:GLN:HB2	1.97	0.46
2:F:205:ASN:HD21	2:F:216:ILE:HG23	1.81	0.46
1:B:257:ARG:HA	1:B:261:CYS:HB2	1.98	0.46
1:C:63:VAL:HG22	1:C:253:ARG:HG2	1.96	0.46
2:E:70:ALA:H	4:E:402:NAG:C7	2.29	0.46
2:G:171:GLU:OE1	2:G:220:ARG:NE	2.49	0.46
2:E:84:LYS:NZ	2:E:87:GLY:O	2.47	0.46
2:F:168:VAL:O	2:F:247:VAL:HA	2.15	0.46
2:G:253:TRP:HA	2:G:277:CYS:HA	1.97	0.46
2:E:195:GLU:OE1	2:E:239:ARG:NH1	2.49	0.45
2:E:253:TRP:CZ3	2:E:289:CYS:CB	2.99	0.45
2:E:205:ASN:ND2	2:E:216:ILE:HG23	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:VAL:O	1:C:242:THR:HG23	2.15	0.45
2:H:170:ILE:HD13	2:H:170:ILE:HA	1.86	0.45
1:B:86:LEU:HD13	2:E:59:GLU:CG	2.47	0.45
1:B:86:LEU:CD1	2:E:59:GLU:CD	2.89	0.45
1:B:393:LYS:O	1:B:396:SER:OG	2.29	0.45
1:C:171:ASP:OD2	1:C:202:ARG:NH1	2.50	0.45
1:D:470:GLN:O	1:D:474:THR:HG23	2.17	0.45
1:C:474:THR:C	1:C:476:SER:H	2.24	0.45
2:F:125:HIS:O	2:H:296:LYS:CE	2.65	0.45
1:B:67:LYS:HE3	1:B:425:GLN:HB2	1.99	0.45
1:C:237:GLU:OE2	1:C:464:LYS:NZ	2.50	0.45
1:D:90:GLN:OE1	2:G:146:ARG:HD2	2.17	0.45
1:A:460:GLN:HB2	2:G:220:ARG:NH1	2.32	0.45
1:C:306:VAL:HG11	1:C:391:ILE:HG13	1.99	0.45
1:C:322:LEU:HD23	1:C:322:LEU:HA	1.85	0.44
2:G:170:ILE:HD13	2:G:170:ILE:HA	1.86	0.44
2:H:189:VAL:HG11	2:H:212:HIS:HB3	2.00	0.44
1:C:470:GLN:O	1:C:474:THR:HG23	2.17	0.44
1:D:178:TYR:HD1	1:D:182:MET:HE3	1.82	0.44
1:D:416:GLU:CD	1:D:416:GLU:H	2.25	0.44
2:F:217:ARG:NE	2:G:217:ARG:CZ	2.81	0.44
2:F:249:VAL:HB	2:F:283:LEU:HB2	1.99	0.44
1:B:416:GLU:CD	1:B:416:GLU:H	2.25	0.44
1:C:234:LEU:CD1	2:E:283:LEU:HD11	2.47	0.44
1:C:416:GLU:CD	1:C:416:GLU:H	2.25	0.44
2:F:160:GLU:HB3	2:F:179:ARG:HB3	1.98	0.44
1:A:460:GLN:HG2	1:A:464:LYS:HE3	2.00	0.44
1:B:470:GLN:O	1:B:474:THR:HG23	2.18	0.44
2:E:63:ILE:HG22	2:E:152:ILE:HA	2.00	0.44
2:E:124:PHE:CZ	2:E:126:GLY:HA3	2.52	0.44
2:H:203:ASP:HB3	2:H:206:ILE:HD12	2.00	0.44
2:H:283:LEU:HA	2:H:283:LEU:HD23	1.75	0.44
1:C:315:MET:O	1:C:315:MET:HG2	2.18	0.44
1:D:234:LEU:HD13	2:F:283:LEU:HD21	1.99	0.44
1:D:236:ILE:CB	2:F:278:THR:HG21	2.48	0.44
1:D:455:GLU:N	1:D:456:PRO:HD2	2.32	0.44
2:G:253:TRP:CZ2	2:G:290:GLU:N	2.86	0.44
2:H:61:ALA:HB3	2:H:150:VAL:HG22	1.98	0.44
1:D:90:GLN:OE1	2:G:146:ARG:CD	2.65	0.43
2:E:77:PRO:HB3	2:E:107:LEU:HD21	1.99	0.43
2:G:84:LYS:NZ	2:G:87:GLY:O	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:TRP:HZ3	2:F:133:GLN:HB2	1.82	0.43
2:G:160:GLU:HB3	2:G:179:ARG:HB3	2.00	0.43
2:F:217:ARG:CZ	2:G:217:ARG:NE	2.81	0.43
1:B:218:VAL:O	1:B:222:LEU:HG	2.18	0.43
1:B:85:ARG:NH2	1:B:246:LYS:HD2	2.33	0.43
2:G:283:LEU:HD23	2:G:283:LEU:HA	1.81	0.43
1:C:149:THR:O	1:C:153:LEU:HG	2.19	0.43
1:B:306:VAL:HG11	1:B:391:ILE:HG13	2.01	0.43
1:D:236:ILE:HB	2:F:278:THR:HG21	2.00	0.43
1:A:393:LYS:O	1:A:396:SER:OG	2.31	0.43
2:H:219:ALA:HB1	2:H:247:VAL:HG11	2.01	0.43
1:A:257:ARG:HA	1:A:261:CYS:HB2	2.00	0.43
2:E:248:TYR:CE1	2:E:286:GLY:HA2	2.53	0.43
1:A:178:TYR:HD1	1:A:182:MET:HE3	1.83	0.43
1:A:315:MET:O	1:A:315:MET:HG2	2.17	0.43
1:C:82:LEU:CD2	2:H:234:ILE:HD13	2.22	0.43
2:F:159:PHE:HA	2:F:181:PRO:HG3	2.01	0.43
1:C:177:ILE:HG22	1:C:182:MET:HE2	2.01	0.42
2:E:189:VAL:HG11	2:E:212:HIS:HB3	2.00	0.42
2:F:282:PRO:HG2	2:F:288:PHE:CD2	2.54	0.42
1:D:315:MET:O	1:D:315:MET:HG2	2.18	0.42
1:C:460:GLN:HB2	2:E:220:ARG:NH1	2.33	0.42
2:E:256:TRP:CE3	2:E:273:ARG:NE	2.88	0.42
2:F:76:ARG:HG2	2:F:107:LEU:HD23	2.01	0.42
2:G:253:TRP:CZ3	2:G:289:CYS:HB3	2.54	0.42
1:B:221:SER:HB2	1:B:315:MET:HB2	2.01	0.42
1:A:469:ASN:HA	1:A:472:LEU:HD12	2.01	0.42
1:B:161:ASN:HB3	1:B:164:ASP:HB2	2.01	0.42
1:C:393:LYS:O	1:C:396:SER:OG	2.36	0.42
1:D:460:GLN:HG2	1:D:464:LYS:HE3	2.02	0.42
1:C:467:HIS:CE1	2:E:284:ASN:HD21	2.37	0.42
1:D:322:LEU:HD23	1:D:322:LEU:HA	1.86	0.42
2:G:77:PRO:HB3	2:G:107:LEU:HD21	2.01	0.42
2:G:253:TRP:CZ3	2:G:289:CYS:CB	3.02	0.42
2:H:84:LYS:NZ	2:H:87:GLY:O	2.48	0.42
2:H:256:TRP:CE3	2:H:273:ARG:NE	2.87	0.42
2:H:259:TRP:CE2	2:H:273:ARG:HD3	2.54	0.42
1:A:431:TYR:CD2	1:A:433:GLN:HG3	2.55	0.42
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.86	0.42
1:C:467:HIS:NE2	2:E:284:ASN:CG	2.78	0.42
2:G:219:ALA:HB1	2:G:247:VAL:HG11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:GLU:OE2	2:H:268:ARG:HD3	2.20	0.41
1:A:193:ILE:HD11	1:A:348:CYS:HB3	2.01	0.41
1:A:218:VAL:O	1:A:222:LEU:HG	2.20	0.41
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.94	0.41
1:A:234:LEU:HD22	1:A:468:ILE:HG21	2.03	0.41
1:C:92:LEU:HB3	1:C:243:ASP:HA	2.01	0.41
1:C:218:VAL:O	1:C:222:LEU:HG	2.21	0.41
1:C:383:LEU:HD23	1:C:383:LEU:HA	1.92	0.41
1:D:218:VAL:O	1:D:222:LEU:HG	2.20	0.41
1:A:230:GLN:OE1	2:G:283:LEU:CD2	2.67	0.41
1:B:178:TYR:HD1	1:B:182:MET:HE3	1.85	0.41
2:E:170:ILE:HD13	2:E:170:ILE:HA	1.87	0.41
2:F:253:TRP:CH2	2:F:289:CYS:CA	3.03	0.41
2:F:253:TRP:HZ2	2:F:290:GLU:O	2.03	0.41
1:A:470:GLN:O	1:A:474:THR:HG23	2.20	0.41
1:B:86:LEU:HD13	2:E:59:GLU:HG3	2.02	0.41
1:C:123:ASN:HD22	4:C:501:NAG:C1	2.21	0.41
1:D:127:ALA:HA	4:D:501:NAG:O7	2.20	0.41
2:E:159:PHE:HA	2:E:181:PRO:HG3	2.02	0.41
2:E:259:TRP:CE2	2:E:273:ARG:HD3	2.55	0.41
2:H:160:GLU:HB3	2:H:179:ARG:HB3	2.01	0.41
1:A:302:LEU:HG	1:A:391:ILE:HD11	2.03	0.41
1:B:86:LEU:CD1	2:E:59:GLU:OE1	2.69	0.41
2:F:170:ILE:HD13	2:F:170:ILE:HA	1.87	0.41
2:G:82:PHE:HZ	2:G:92:GLN:HE22	1.66	0.41
1:A:276:TYR:HA	1:A:279:VAL:HG22	2.02	0.41
1:C:67:LYS:HE3	1:C:425:GLN:HB2	2.02	0.41
2:E:76:ARG:HG2	2:E:107:LEU:HD23	2.02	0.41
2:F:173:MET:CE	2:G:173:MET:HE1	2.50	0.41
2:G:193:LYS:N	2:G:196:GLU:O	2.54	0.41
1:B:301:SER:HB2	1:B:472:LEU:HD13	2.03	0.41
1:B:404:LEU:HD12	1:B:404:LEU:HA	1.96	0.40
1:C:246:LYS:HA	1:C:246:LYS:HD3	1.90	0.40
1:C:320:LEU:HD23	1:C:320:LEU:HA	1.92	0.40
2:H:70:ALA:HB3	4:H:401:NAG:H81	1.97	0.40
2:H:119:GLN:HG2	2:H:123:ASP:OD2	2.21	0.40
1:C:257:ARG:HA	1:C:261:CYS:CB	2.51	0.40
1:D:276:TYR:HA	1:D:279:VAL:HG22	2.04	0.40
2:G:259:TRP:CE2	2:G:273:ARG:HD3	2.57	0.40
1:B:85:ARG:HH22	1:B:246:LYS:HD2	1.86	0.40
2:F:253:TRP:HZ3	2:F:289:CYS:CB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:VAL:HG13	2:H:247:VAL:HG12	2.02	0.40
1:A:274:GLY:N	1:A:418:ASP:OD1	2.54	0.40
1:B:431:TYR:CD2	1:B:433:GLN:HG3	2.57	0.40
1:C:276:TYR:HA	1:C:279:VAL:HG22	2.03	0.40
2:F:130:TYR:HB3	2:F:150:VAL:O	2.22	0.40
2:F:256:TRP:CE3	2:F:273:ARG:NE	2.89	0.40
2:H:60:ASP:HA	2:H:148:ALA:HB1	2.03	0.40
2:F:57:GLU:OE1	2:F:146:ARG:HG3	2.22	0.40
2:H:76:ARG:HG2	2:H:107:LEU:HD23	2.02	0.40

All (35) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:LEU:CG	2:G:141:GLY:N[1_665]	0.90	1.30
2:F:140:LEU:CG	2:G:141:GLY:CA[1_665]	0.98	1.22
2:F:140:LEU:CD2	2:G:141:GLY:N[1_665]	1.15	1.05
2:F:140:LEU:HG	2:G:141:GLY:CA[1_665]	0.64	0.96
2:F:140:LEU:CD1	2:G:140:LEU:C[1_665]	1.42	0.78
2:F:140:LEU:HG	2:G:141:GLY:HA3[1_665]	0.86	0.74
2:F:140:LEU:CG	2:G:140:LEU:C[1_665]	1.57	0.63
2:F:137:TRP:HH2	2:F:265:ARG:HH12[1_665]	1.04	0.56
2:F:140:LEU:CD1	2:G:141:GLY:N[1_665]	1.64	0.56
1:A:131:ASN:C	1:B:132:ASN:OD1[2_655]	1.66	0.54
2:F:140:LEU:HD22	2:G:141:GLY:H[1_665]	1.06	0.54
2:F:140:LEU:HB3	2:G:141:GLY:HA2[1_665]	1.15	0.45
2:F:140:LEU:CB	2:G:141:GLY:CA[1_665]	1.75	0.45
2:F:140:LEU:HD13	2:G:140:LEU:C[1_665]	1.16	0.44
1:A:131:ASN:O	1:B:132:ASN:OD1[2_655]	1.77	0.43
2:F:140:LEU:CD2	2:G:141:GLY:CA[1_665]	1.83	0.37
2:F:140:LEU:CD1	2:G:140:LEU:O[1_665]	1.83	0.37
2:F:268:ARG:NH2	2:H:301:ALA:O[1_445]	1.86	0.34
2:F:140:LEU:CD2	2:G:140:LEU:C[1_665]	1.88	0.32
2:E:140:LEU:HG	2:H:141:GLY:HA2[1_665]	1.30	0.30
2:F:140:LEU:CG	2:G:141:GLY:HA3[1_665]	1.30	0.30
2:F:268:ARG:HH22	2:H:301:ALA:O[1_445]	1.30	0.30
2:F:140:LEU:HD13	2:G:140:LEU:O[1_665]	1.31	0.29
1:A:132:ASN:N	1:B:132:ASN:OD1[2_655]	1.95	0.25
2:F:140:LEU:HD22	2:G:141:GLY:N[1_665]	1.36	0.24
2:F:140:LEU:CB	2:G:141:GLY:HA2[1_665]	1.39	0.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:LEU:HB2	2:G:140:LEU:O[1_665]	1.41	0.19
2:F:140:LEU:CB	2:G:140:LEU:O[1_665]	2.01	0.19
2:F:140:LEU:HG	2:G:141:GLY:N[1_665]	1.43	0.17
2:F:140:LEU:CG	2:G:140:LEU:O[1_665]	2.04	0.16
2:F:140:LEU:CG	2:G:141:GLY:HA2[1_665]	1.51	0.09
1:A:131:ASN:OD1	1:B:132:ASN:ND2[2_655]	2.13	0.07
2:F:89:TRP:CH2	2:F:265:ARG:NH1[1_665]	2.13	0.07
2:F:140:LEU:CD2	2:G:141:GLY:H[1_665]	1.54	0.06
2:F:140:LEU:HG	2:G:141:GLY:C[1_665]	1.59	0.01

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	52
2	F	249/268 (93%)	236 (95%)	10 (4%)	3 (1%)	10	42
2	G	249/268 (93%)	235 (94%)	10 (4%)	4 (2%)	7	37
2	H	249/268 (93%)	237 (95%)	10 (4%)	2 (1%)	16	52
All	All	2360/2928 (81%)	2282 (97%)	67 (3%)	11 (0%)	24	60

All (11) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	130	TYR
2	G	130	TYR
2	H	130	TYR
2	E	257	THR
2	F	224	SER
2	G	115	ASN
2	G	116	VAL
2	H	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	A	319/418 (76%)	314 (98%)	5 (2%)	55	70
1	B	319/418 (76%)	310 (97%)	9 (3%)	38	60
1	C	319/418 (76%)	314 (98%)	5 (2%)	55	70
1	D	319/418 (76%)	314 (98%)	5 (2%)	55	70
2	E	217/231 (94%)	206 (95%)	11 (5%)	21	45
2	F	217/231 (94%)	205 (94%)	12 (6%)	19	44
2	G	217/231 (94%)	207 (95%)	10 (5%)	24	47
2	H	217/231 (94%)	207 (95%)	10 (5%)	24	47
All	All	2144/2596 (83%)	2077 (97%)	67 (3%)	35	56

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	284	CYS
1	A	336	ASN
1	A	387	ARG
1	A	417	ASN
1	B	64	CYS
1	B	123	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	LEU
1	B	240	ASN
1	B	284	CYS
1	B	323	PHE
1	B	336	ASN
1	B	347	LEU
1	B	387	ARG
1	C	82	LEU
1	C	123	ASN
1	C	284	CYS
1	C	336	ASN
1	C	387	ARG
1	D	64	CYS
1	D	82	LEU
1	D	284	CYS
1	D	336	ASN
1	D	387	ARG
2	E	63	ILE
2	E	109	VAL
2	E	114	ILE
2	E	115	ASN
2	E	134	CYS
2	E	170	ILE
2	E	174	ILE
2	E	192	LEU
2	E	198	ILE
2	E	206	ILE
2	E	298	THR
2	F	63	ILE
2	F	109	VAL
2	F	114	ILE
2	F	134	CYS
2	F	170	ILE
2	F	173	MET
2	F	174	ILE
2	F	192	LEU
2	F	196	GLU
2	F	198	ILE
2	F	206	ILE
2	F	298	THR
2	G	63	ILE
2	G	109	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	114	ILE
2	G	134	CYS
2	G	170	ILE
2	G	173	MET
2	G	174	ILE
2	G	192	LEU
2	G	198	ILE
2	G	206	ILE
2	H	63	ILE
2	H	109	VAL
2	H	114	ILE
2	H	134	CYS
2	H	170	ILE
2	H	173	MET
2	H	174	ILE
2	H	192	LEU
2	H	198	ILE
2	H	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	336	ASN
1	A	467	HIS
1	B	81	GLN
1	B	131	ASN
1	B	230	GLN
1	B	244	HIS
1	B	334	GLN
1	C	90	GLN
1	C	123	ASN
1	C	194	ASN
1	C	334	GLN
1	C	336	ASN
1	D	81	GLN
1	D	123	ASN
1	D	194	ASN
1	D	230	GLN
1	D	233	ASN
1	D	334	GLN
2	E	295	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	139	HIS
2	F	161	GLN
2	F	218	GLN
2	F	271	GLN
2	G	92	GLN
2	G	161	GLN
2	G	295	GLN
2	H	139	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 ⓘ

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	1.17	2 (14%)	17,19,21	1.21	1 (5%)
3	NAG	I	2	3	14,14,15	0.95	1 (7%)	17,19,21	1.57	6 (35%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	O5-C1	2.38	1.47	1.43
3	I	2	NAG	C1-C2	2.15	1.55	1.52
3	I	1	NAG	O4-C4	2.01	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	O5-C1-C2	3.18	116.22	111.29
3	I	1	NAG	C1-O5-C5	2.87	116.04	112.19
3	I	2	NAG	C2-N2-C7	2.72	126.55	122.90
3	I	2	NAG	O4-C4-C3	-2.61	104.22	110.38
3	I	2	NAG	C1-C2-N2	2.25	113.98	110.43
3	I	2	NAG	O4-C4-C5	2.07	114.42	109.32
3	I	2	NAG	C4-C3-C2	2.02	113.97	111.02

There are no chirality outliers.

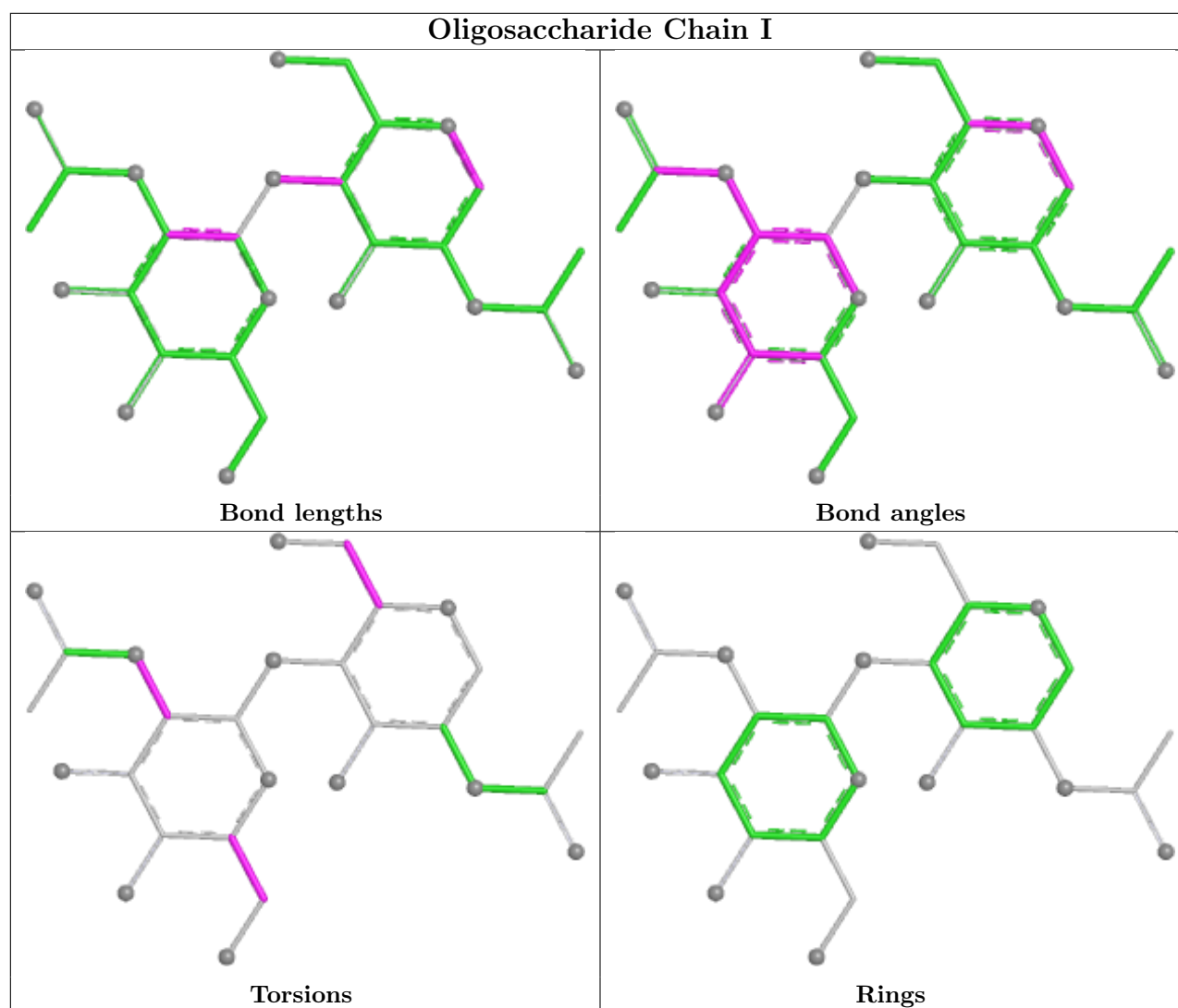
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C3-C2-N2-C7
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.



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	$\# Z > 2$
4	NAG	C	501	1	14,14,15	0.99	1 (7%)	17,19,21	0.97	2 (11%)
4	NAG	D	501	1	14,14,15	0.77	0	17,19,21	2.11	5 (29%)
4	NAG	F	401	2	14,14,15	1.80	3 (21%)	17,19,21	1.56	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	403	2	14,14,15	1.66	3 (21%)	17,19,21	1.81	5 (29%)
4	NAG	E	402	2	14,14,15	0.94	0	17,19,21	2.04	6 (35%)
4	NAG	G	401	2	14,14,15	1.26	1 (7%)	17,19,21	2.98	9 (52%)
4	NAG	B	502	1	14,14,15	1.13	1 (7%)	17,19,21	1.82	3 (17%)
4	NAG	F	402	2	14,14,15	1.26	1 (7%)	17,19,21	2.19	4 (23%)
5	MAN	G	403	2	11,11,12	1.27	0	15,15,17	2.46	5 (33%)
4	NAG	C	502	1	14,14,15	1.23	2 (14%)	17,19,21	3.62	11 (64%)
4	NAG	H	401	2	14,14,15	0.39	0	17,19,21	0.88	0
5	MAN	F	403	2	11,11,12	0.83	0	15,15,17	2.20	5 (33%)
4	NAG	B	501	1	14,14,15	0.76	0	17,19,21	1.22	3 (17%)
5	MAN	E	401	2	11,11,12	1.38	1 (9%)	15,15,17	2.32	7 (46%)
4	NAG	A	501	1	14,14,15	1.30	1 (7%)	17,19,21	2.27	7 (41%)
4	NAG	D	502	1	14,14,15	1.64	4 (28%)	17,19,21	2.84	5 (29%)
4	NAG	G	402	2	14,14,15	1.68	3 (21%)	17,19,21	2.91	9 (52%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	402	2	-	5/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	402	NAG	C1-C2	4.18	1.58	1.52
4	F	401	NAG	C2-N2	4.18	1.53	1.46
4	E	403	NAG	O5-C1	3.73	1.50	1.43
4	G	402	NAG	C1-C2	3.71	1.57	1.52
4	D	502	NAG	C1-C2	3.50	1.57	1.52
4	E	403	NAG	O5-C5	3.40	1.50	1.43
4	F	401	NAG	C3-C2	3.04	1.58	1.52
4	B	502	NAG	C1-C2	2.96	1.56	1.52
4	D	502	NAG	O5-C5	2.88	1.49	1.43
4	A	501	NAG	C1-C2	2.85	1.56	1.52
4	G	402	NAG	C4-C5	2.63	1.58	1.53
4	E	403	NAG	C1-C2	2.45	1.55	1.52
4	C	501	NAG	O5-C1	-2.45	1.39	1.43
4	D	502	NAG	C3-C2	2.42	1.57	1.52
4	G	402	NAG	C3-C2	2.40	1.57	1.52
4	C	502	NAG	C8-C7	-2.27	1.45	1.50
4	D	502	NAG	O5-C1	2.23	1.47	1.43
4	C	502	NAG	C2-N2	2.23	1.49	1.46
5	E	401	MAN	C4-C5	2.18	1.57	1.53
4	F	401	NAG	C4-C3	2.05	1.57	1.52
4	G	401	NAG	O5-C5	2.01	1.47	1.43

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	NAG	C2-N2-C7	8.42	134.18	122.90
4	C	502	NAG	C2-N2-C7	7.96	133.56	122.90
4	D	502	NAG	C1-O5-C5	7.43	122.15	112.19
4	G	402	NAG	C2-N2-C7	7.35	132.75	122.90
4	C	502	NAG	O7-C7-N2	6.49	133.45	121.98
4	A	501	NAG	O5-C5-C6	6.05	119.44	107.66
4	D	502	NAG	O5-C1-C2	-5.78	102.34	111.29
4	F	402	NAG	C1-C2-N2	5.75	119.49	110.43
5	G	403	MAN	C1-O5-C5	5.55	119.62	112.19
4	B	502	NAG	O5-C5-C6	5.51	118.39	107.66
4	D	501	NAG	C1-C2-N2	5.49	119.09	110.43
4	G	402	NAG	C8-C7-N2	5.25	124.82	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	NAG	O5-C1-C2	5.24	119.40	111.29
4	F	402	NAG	C1-O5-C5	5.21	119.17	112.19
4	C	502	NAG	O5-C5-C6	5.05	117.49	107.66
4	E	402	NAG	C1-O5-C5	4.84	118.67	112.19
5	F	403	MAN	O5-C5-C6	4.75	116.91	107.66
5	E	401	MAN	O3-C3-C2	4.69	119.62	110.05
4	E	403	NAG	O5-C5-C6	4.47	116.37	107.66
5	G	403	MAN	O3-C3-C2	4.46	119.16	110.05
4	F	401	NAG	O3-C3-C2	4.46	118.66	109.40
4	C	502	NAG	C8-C7-N2	-4.43	108.77	116.12
5	E	401	MAN	C1-O5-C5	4.36	118.03	112.19
4	G	402	NAG	C1-C2-N2	4.11	116.90	110.43
4	G	401	NAG	C1-C2-N2	4.06	116.83	110.43
5	G	403	MAN	C3-C4-C5	3.86	117.23	110.23
5	F	403	MAN	C1-O5-C5	3.84	117.34	112.19
4	C	502	NAG	C1-C2-N2	-3.71	104.58	110.43
4	G	401	NAG	C1-O5-C5	3.69	117.13	112.19
5	E	401	MAN	C3-C4-C5	3.62	116.79	110.23
4	C	502	NAG	C6-C5-C4	-3.58	104.23	113.02
4	D	502	NAG	O5-C5-C6	3.56	114.58	107.66
4	A	501	NAG	O5-C1-C2	-3.47	105.92	111.29
4	D	502	NAG	C1-C2-N2	3.44	115.86	110.43
5	F	403	MAN	C3-C4-C5	3.43	116.44	110.23
4	G	401	NAG	C8-C7-N2	-3.41	110.46	116.12
4	C	502	NAG	C1-O5-C5	-3.26	107.81	112.19
4	G	401	NAG	O5-C1-C2	3.25	116.33	111.29
5	G	403	MAN	O5-C5-C6	3.20	113.89	107.66
4	C	502	NAG	O4-C4-C5	-3.16	101.53	109.32
4	E	402	NAG	C1-C2-N2	-3.15	105.46	110.43
4	E	402	NAG	C3-C4-C5	3.08	115.81	110.23
4	G	402	NAG	O3-C3-C2	3.07	115.77	109.40
4	E	403	NAG	O5-C1-C2	-3.04	106.58	111.29
4	A	501	NAG	C6-C5-C4	-3.04	105.55	113.02
4	F	402	NAG	O5-C1-C2	-2.98	106.69	111.29
5	F	403	MAN	O3-C3-C4	2.95	117.33	110.38
4	G	402	NAG	O4-C4-C5	2.93	116.54	109.32
5	E	401	MAN	O4-C4-C3	-2.90	103.54	110.38
4	D	502	NAG	C6-C5-C4	-2.87	105.98	113.02
4	C	502	NAG	C3-C4-C5	2.82	115.34	110.23
4	F	402	NAG	C2-N2-C7	2.75	126.58	122.90
4	C	502	NAG	O7-C7-C8	-2.68	117.28	122.05
4	G	402	NAG	O7-C7-N2	-2.67	117.26	121.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	402	NAG	C1-O5-C5	2.66	115.75	112.19
4	F	401	NAG	C4-C3-C2	-2.59	107.22	111.02
4	E	402	NAG	O5-C5-C6	2.59	112.70	107.66
5	E	401	MAN	C6-C5-C4	2.58	119.35	113.02
4	D	501	NAG	C1-O5-C5	2.48	115.50	112.19
4	C	502	NAG	O4-C4-C3	2.47	116.20	110.38
4	E	403	NAG	C1-C2-N2	2.46	114.30	110.43
4	B	502	NAG	C2-N2-C7	2.37	126.08	122.90
4	A	501	NAG	O7-C7-C8	-2.37	117.83	122.05
5	F	403	MAN	C1-C2-C3	2.36	113.09	109.64
4	B	501	NAG	C8-C7-N2	2.35	120.01	116.12
4	G	402	NAG	O7-C7-C8	-2.33	117.91	122.05
4	B	501	NAG	O5-C1-C2	2.32	114.88	111.29
4	E	402	NAG	O3-C3-C4	2.31	115.82	110.38
4	E	403	NAG	C1-O5-C5	2.24	115.19	112.19
4	C	501	NAG	O5-C5-C6	2.24	112.01	107.66
4	G	401	NAG	O7-C7-N2	2.23	125.92	121.98
4	G	401	NAG	C4-C3-C2	-2.21	107.77	111.02
4	G	402	NAG	C4-C3-C2	-2.21	107.78	111.02
5	E	401	MAN	C1-C2-C3	2.21	112.86	109.64
4	A	501	NAG	C3-C4-C5	-2.18	106.28	110.23
4	G	401	NAG	O3-C3-C4	-2.16	105.28	110.38
4	A	501	NAG	O3-C3-C4	-2.15	105.32	110.38
4	A	501	NAG	O4-C4-C3	2.14	115.41	110.38
5	G	403	MAN	O2-C2-C1	2.13	114.09	109.22
4	E	402	NAG	O4-C4-C5	-2.12	104.11	109.32
4	G	401	NAG	O3-C3-C2	2.12	113.80	109.40
4	B	502	NAG	O5-C1-C2	2.12	114.57	111.29
4	B	501	NAG	O5-C5-C6	2.11	111.78	107.66
4	D	501	NAG	C2-N2-C7	2.09	125.70	122.90
5	E	401	MAN	O4-C4-C5	2.06	114.39	109.32
4	E	403	NAG	C4-C3-C2	2.05	114.03	111.02
4	D	501	NAG	O7-C7-C8	-2.01	118.47	122.05
4	C	501	NAG	O5-C1-C2	2.01	114.40	111.29

There are no chirality outliers.

All (34) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	402	NAG	C1-C2-N2-C7
4	A	501	NAG	C8-C7-N2-C2
4	A	501	NAG	O7-C7-N2-C2
5	G	403	MAN	O5-C5-C6-O6
4	D	501	NAG	O7-C7-N2-C2
4	G	402	NAG	O5-C5-C6-O6
4	D	502	NAG	O5-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
5	F	403	MAN	O5-C5-C6-O6
4	C	501	NAG	C4-C5-C6-O6
4	D	502	NAG	C4-C5-C6-O6
4	F	401	NAG	O5-C5-C6-O6
4	G	402	NAG	C4-C5-C6-O6
5	G	403	MAN	C4-C5-C6-O6
4	G	401	NAG	C4-C5-C6-O6
4	D	501	NAG	C8-C7-N2-C2
4	F	401	NAG	C8-C7-N2-C2
4	F	401	NAG	O7-C7-N2-C2
4	G	402	NAG	C8-C7-N2-C2
4	G	402	NAG	O7-C7-N2-C2
4	G	401	NAG	O5-C5-C6-O6
4	F	401	NAG	C4-C5-C6-O6
4	C	502	NAG	O5-C5-C6-O6
4	B	502	NAG	O5-C5-C6-O6
4	E	403	NAG	O5-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	H	401	NAG	C4-C5-C6-O6
4	F	402	NAG	C4-C5-C6-O6
4	F	402	NAG	O5-C5-C6-O6
5	F	403	MAN	C4-C5-C6-O6
5	E	401	MAN	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	NAG	2	0
4	D	501	NAG	3	0
4	F	401	NAG	4	0
4	E	403	NAG	1	0
4	E	402	NAG	10	0
4	G	401	NAG	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	NAG	2	0
4	H	401	NAG	7	0
5	F	403	MAN	8	0
4	B	501	NAG	11	0
4	A	501	NAG	4	0
4	G	402	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	351/464 (75%)	-0.15	4 (1%)	78 60	157, 332, 462, 578	0
1	B	351/464 (75%)	-0.03	2 (0%)	85 71	224, 359, 494, 629	0
1	C	351/464 (75%)	-0.26	2 (0%)	85 71	152, 280, 392, 478	0
1	D	351/464 (75%)	-0.09	4 (1%)	78 60	178, 309, 438, 503	0
2	E	251/268 (93%)	-0.16	3 (1%)	76 59	166, 296, 432, 470	0
2	F	251/268 (93%)	-0.22	7 (2%)	55 40	168, 327, 489, 583	0
2	G	251/268 (93%)	-0.15	4 (1%)	70 52	146, 290, 513, 657	0
2	H	251/268 (93%)	-0.25	4 (1%)	70 52	145, 284, 452, 543	0
All	All	2408/2928 (82%)	-0.16	30 (1%)	76 59	145, 312, 467, 657	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	282	GLN	5.6
2	E	185	PRO	4.5
2	F	300	THR	4.4
2	F	62	TYR	4.3
2	G	150	VAL	3.5
2	G	62	TYR	3.5
2	F	61	ALA	3.3
1	A	136	LEU	2.8
1	A	429	GLU	2.8
1	D	279	VAL	2.7
2	F	186	ALA	2.7
1	B	429	GLU	2.7
2	H	71	LEU	2.6
2	F	60	ASP	2.5
2	H	301	ALA	2.5
2	H	116	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	290	GLU	2.5
2	F	185	PRO	2.4
2	E	184	VAL	2.4
1	A	430	ARG	2.4
1	A	138	PRO	2.4
1	C	403	ALA	2.4
1	D	125	THR	2.3
1	D	280	VAL	2.3
2	G	130	TYR	2.2
2	E	67	ASN	2.2
2	G	185	PRO	2.1
1	C	413	PRO	2.1
2	H	150	VAL	2.1
1	B	246	LYS	2.1

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

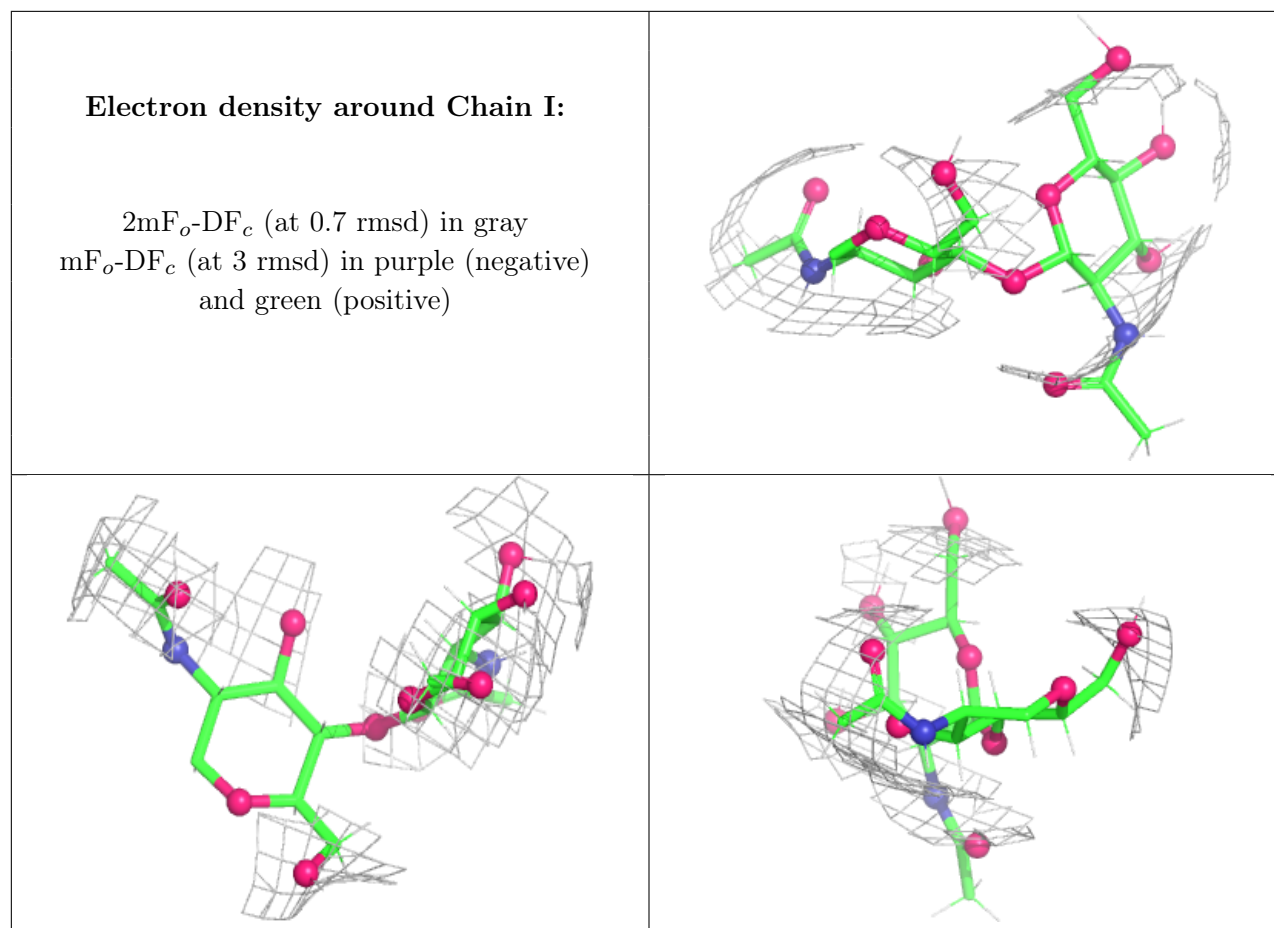
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	NAG	I	1	14/15	0.98	0.05	30,256,268,270	2
3	NAG	I	2	14/15	0.98	0.06	30,262,268,275	3

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 ⓘ

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	MAN	F	403	11/12	0.90	0.09	30,330,336,336	4
4	NAG	D	501	14/15	0.91	0.09	30,440,496,498	3
4	NAG	G	401	14/15	0.92	0.07	30,432,449,462	3
5	MAN	G	403	11/12	0.92	0.10	30,361,387,418	4
4	NAG	C	501	14/15	0.94	0.07	30,338,366,378	3
4	NAG	H	401	14/15	0.95	0.09	30,312,330,333	3
5	MAN	E	401	11/12	0.95	0.10	30,430,436,440	4
4	NAG	B	501	14/15	0.96	0.10	30,436,449,453	3
4	NAG	G	402	14/15	0.96	0.08	30,234,282,284	3
4	NAG	E	402	14/15	0.96	0.09	30,403,417,426	3
4	NAG	E	403	14/15	0.97	0.07	30,283,309,320	3
4	NAG	F	401	14/15	0.97	0.08	30,600,677,694	3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	402	14/15	0.97	0.08	30,293,359,371	3
4	NAG	B	502	14/15	0.98	0.08	30,267,285,288	3
4	NAG	D	502	14/15	0.98	0.07	30,244,263,266	3
4	NAG	C	502	14/15	0.98	0.09	30,258,339,354	3
4	NAG	A	501	14/15	0.99	0.07	30,220,237,248	3

6.5 Other polymers [i](#)

There are no such residues in this entry.