



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:17 AM UTC

PDB ID : 3HUI / pdb_00003hui
Title : Crystal structure of human CD1d-alpha-Galactosylceramide in complex with semi-invariant NKT cell receptor
Authors : Pang, S.S.
Deposited on : 2009-06-14
Resolution : 2.50 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

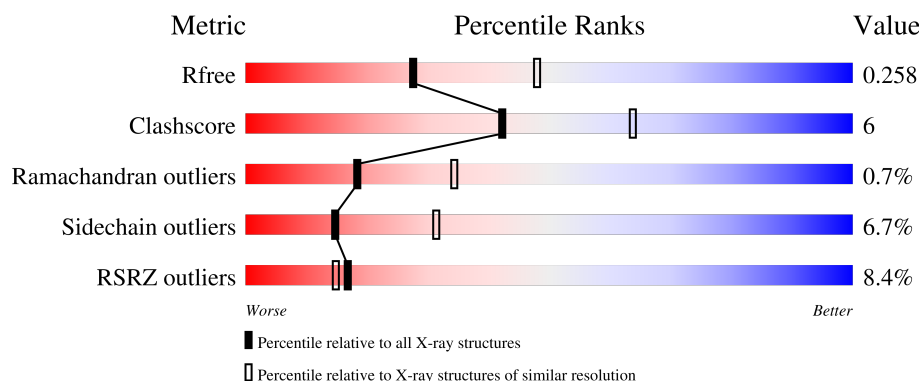
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	284	7% 76% 19% ..
1	C	284	13% 77% 18% ..
2	B	99	82% 15% ..
2	D	99	% 82% 15% .
3	E	209	11% 80% 11% . 5%

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Mol	Chain	Length	Quality of chain
3	G	209	
4	F	246	
4	H	246	
5	I	2	
6	J	3	

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
5	NAG	I	1	X	-	-	-
7	NAG	C	2000	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13690 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called T-cell surface glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2181	1398	384	392	7			
1	C	274	Total	C	N	O	S	0	0	0
			2147	1378	374	388	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P15813
A	1	PRO	-	expression tag	UNP P15813
A	2	GLY	-	expression tag	UNP P15813
A	278	HIS	-	expression tag	UNP P15813
A	279	HIS	-	expression tag	UNP P15813
A	280	HIS	-	expression tag	UNP P15813
A	281	HIS	-	expression tag	UNP P15813
A	282	HIS	-	expression tag	UNP P15813
A	283	HIS	-	expression tag	UNP P15813
C	0	SER	-	expression tag	UNP P15813
C	1	PRO	-	expression tag	UNP P15813
C	2	GLY	-	expression tag	UNP P15813
C	278	HIS	-	expression tag	UNP P15813
C	279	HIS	-	expression tag	UNP P15813
C	280	HIS	-	expression tag	UNP P15813
C	281	HIS	-	expression tag	UNP P15813
C	282	HIS	-	expression tag	UNP P15813
C	283	HIS	-	expression tag	UNP P15813

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			805	514	138	151	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	99	Total	C	N	O	S	0	1	0
			830	527	140	160	3			

- Molecule 3 is a protein called NKT15 T cell receptor alpha-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	199	Total	C	N	O	S	0	1	0
			1562	967	265	321	9			
3	G	202	Total	C	N	O	S	0	1	0
			1566	973	261	323	9			

- Molecule 4 is a protein called NKT15 T cell receptor beta-chain.

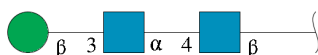
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	242	Total	C	N	O	S	0	1	0
			1940	1222	336	374	8			
4	H	245	Total	C	N	O	S	0	1	0
			1964	1236	339	380	9			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



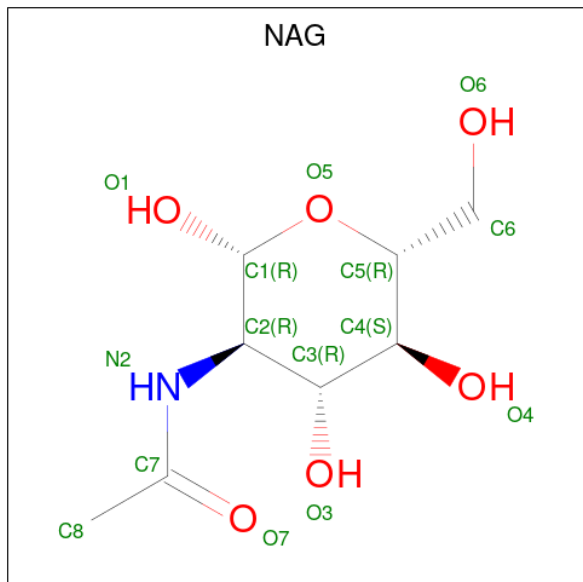
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O		0	0	0
			25	14	1	10				

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



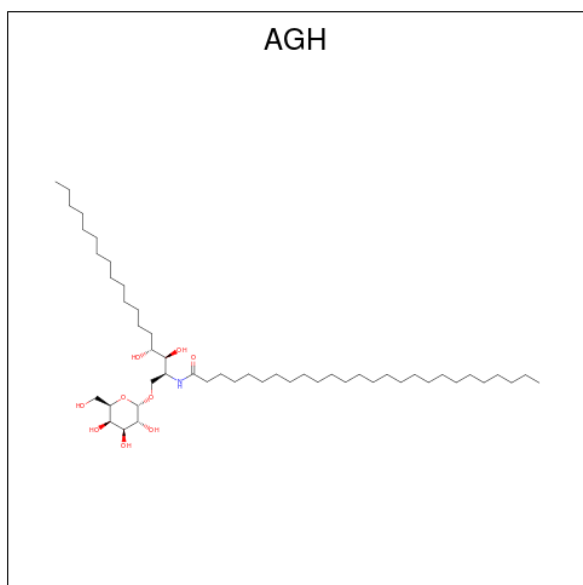
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is N-{(1S,2R,3S)-1-[(ALPHA-D-GALACTOPYRANOSYLOXY)METHYL]-2,3-DIHYDROXYHEPTADECYL}HEXACOSANAMIDE (CCD ID: AGH) (formula: $C_{50}H_{99}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			60	50	1	9		
8	C	1	Total	C	N	O	0	0
			60	50	1	9		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	Mg	0	0
			1	1		

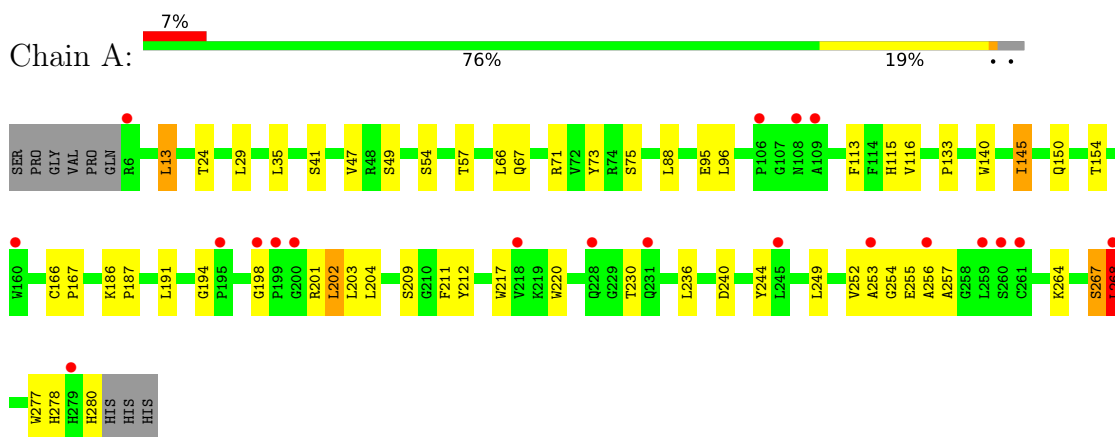
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	95	Total	O	0	0
			95	95		
10	B	42	Total	O	0	0
			42	42		
10	C	88	Total	O	0	0
			88	88		
10	D	35	Total	O	0	0
			35	35		
10	E	40	Total	O	0	0
			40	40		
10	F	52	Total	O	0	0
			52	52		
10	G	62	Total	O	0	0
			62	62		
10	H	68	Total	O	0	0
			68	68		

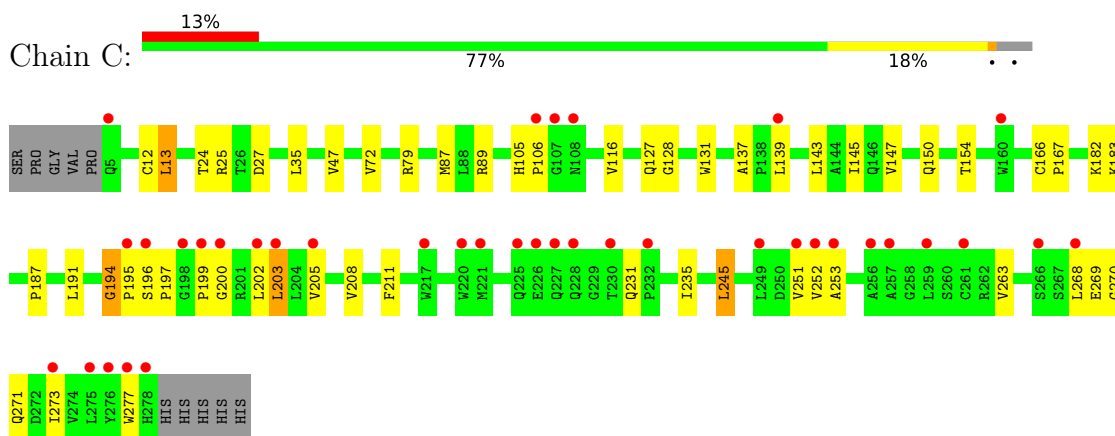
3 Residue-property plots

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.

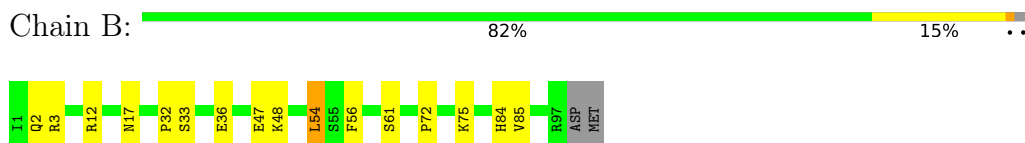
- Molecule 1: T-cell surface glycoprotein CD1d



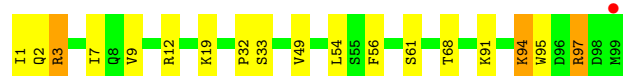
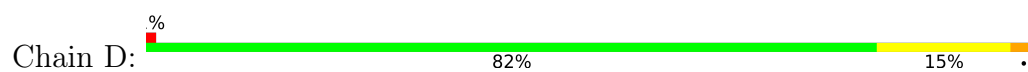
- Molecule 1: T-cell surface glycoprotein CD1d



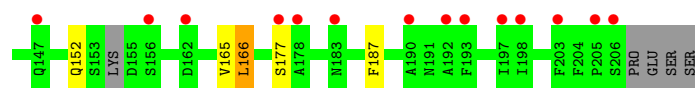
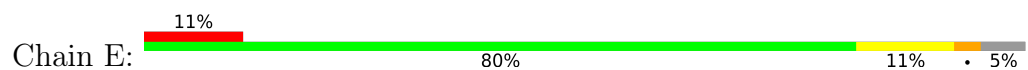
- Molecule 2: Beta-2-microglobulin



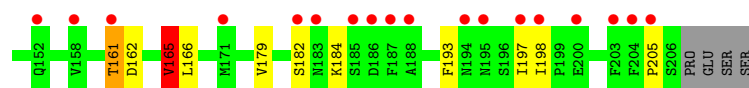
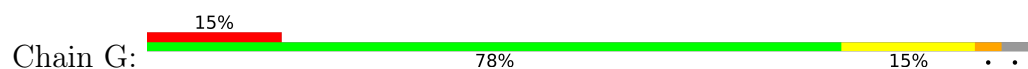
- Molecule 2: Beta-2-microglobulin



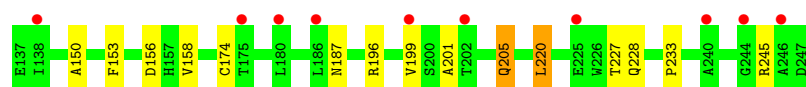
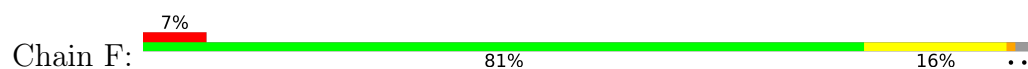
• Molecule 3: NKT15 T cell receptor alpha-chain



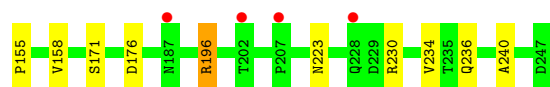
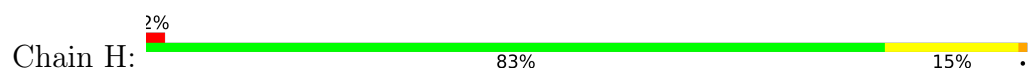
• Molecule 3: NKT15 T cell receptor alpha-chain



• Molecule 4: NKT15 T cell receptor beta-chain



• Molecule 4: NKT15 T cell receptor beta-chain

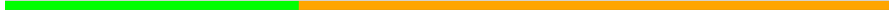


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MDG1
MDG2

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

Chain J:  33% 67%

MDG1
MDG2
MDG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.11Å 82.36Å 117.18Å 90.00° 101.26° 90.00°	Depositor
Resolution (Å)	47.28 – 2.50 47.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.5 (47.28-2.50) 90.5 (47.28-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.279 0.232 , 0.258	Depositor DCC
R_{free} test set	3288 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.057 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13690	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: BMA, NDG, AGH, MG, 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	0.50	0/2249	0.79	1/3066 (0.0%)
1	C	0.48	0/2213	0.81	2/3022 (0.1%)
2	B	0.46	0/828	0.73	0/1122
2	D	0.47	0/853	0.76	1/1156 (0.1%)
3	E	0.46	0/1590	0.73	0/2156
3	G	0.47	0/1598	0.74	2/2176 (0.1%)
4	F	0.46	0/1993	0.75	0/2712
4	H	0.46	0/2018	0.74	2/2747 (0.1%)
All	All	0.47	0/13342	0.76	8/18157 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	SER	N-CA-C	6.95	120.21	111.24
3	G	165	VAL	CB-CA-C	-5.56	103.28	110.84
1	C	194	GLY	CA-C-N	5.56	126.79	119.84
1	C	194	GLY	C-N-CA	5.56	126.79	119.84
3	G	131	SER	N-CA-C	5.24	116.68	111.07
2	D	3	ARG	N-CA-C	5.22	117.48	109.07
4	H	132	GLU	CA-C-N	5.17	125.16	119.89
4	H	132	GLU	C-N-CA	5.17	125.16	119.89

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	2181	0	2091	42	0
1	C	2147	0	2040	26	0
2	B	805	0	768	8	0
2	D	830	0	779	10	0
3	E	1562	0	1481	20	0
3	G	1566	0	1465	25	0
4	F	1940	0	1833	27	0
4	H	1964	0	1859	20	0
5	I	25	0	22	0	0
6	J	39	0	33	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
8	A	60	0	99	2	0
8	C	60	0	99	4	0
9	H	1	0	0	0	0
10	A	95	0	0	2	0
10	B	42	0	0	0	0
10	C	88	0	0	2	0
10	D	35	0	0	1	0
10	E	40	0	0	2	0
10	F	52	0	0	1	0
10	G	62	0	0	1	0
10	H	68	0	0	6	0
All	All	13690	0	12595	163	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 6.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:SER:HB2	1:A:268:LEU:HB2	1.29	1.15
1:A:253:ALA:HB1	1:A:254:GLY:HA3	1.11	1.05
1:A:253:ALA:CB	1:A:254:GLY:HA3	1.90	1.01
4:F:98:ARG:HB3	4:F:99:ASP:HB2	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:LYS:H	2:D:94:LYS:HE2	1.35	0.91
1:A:253:ALA:HB1	1:A:254:GLY:CA	2.02	0.86
1:C:105:HIS:HB3	1:C:106:PRO:HD2	1.59	0.85
3:G:161:THR:HG22	3:G:179:VAL:H	1.40	0.84
4:H:230:ARG:HG2	10:H:422:HOH:O	1.83	0.79
1:A:255:GLU:HA	1:A:257:ALA:HB3	1.64	0.79
1:A:267:SER:CB	1:A:268:LEU:HB2	2.11	0.78
1:C:154:THR:HG23	8:C:3000:AGH:HAB2	1.64	0.77
4:F:42:GLU:HG2	10:F:341:HOH:O	1.85	0.77
1:C:202:LEU:HG	1:C:253:ALA:HA	1.67	0.75
1:A:253:ALA:CB	1:A:254:GLY:CA	2.62	0.74
3:G:49:MET:SD	10:G:432:HOH:O	2.46	0.73
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.73	0.70
3:G:130:ASP:HB2	3:G:133:SER:O	1.91	0.69
3:G:72:GLN:HE21	3:G:72:GLN:HA	1.57	0.69
4:H:3:ASP:HB2	10:H:255:HOH:O	1.93	0.68
1:A:267:SER:H	1:A:268:LEU:HB3	1.57	0.68
1:C:72:VAL:HB	10:C:558:HOH:O	1.93	0.68
3:E:60:ARG:NH2	3:E:84:ASP:OD1	2.25	0.68
1:A:267:SER:HB2	1:A:268:LEU:CB	2.18	0.64
1:A:166:CYS:HB3	1:A:167:PRO:HD3	1.80	0.64
4:H:25:GLN:HE22	4:H:29:HIS:HB2	1.60	0.64
3:G:35:TYR:CE2	3:G:91:VAL:HG11	2.33	0.63
1:A:47:VAL:HB	1:A:67:GLN:HE22	1.63	0.63
4:F:98:ARG:H	4:F:99:ASP:C	2.07	0.62
4:F:83:ARG:H	4:F:86:HIS:HD2	1.47	0.62
3:E:33:ARG:HB2	3:E:91:VAL:HG13	1.82	0.61
3:G:23:ASN:ND2	3:G:72:GLN:HE22	1.97	0.61
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.81	0.61
4:H:83:ARG:HG2	4:H:86:HIS:CE1	2.35	0.61
1:A:267:SER:N	1:A:268:LEU:HB3	2.15	0.61
2:B:33:SER:HB2	2:B:54:LEU:HD11	1.82	0.60
1:A:209:SER:HB2	1:A:244:TYR:HD1	1.66	0.60
1:A:71:ARG:HD2	10:A:286:HOH:O	2.02	0.60
4:F:83:ARG:H	4:F:86:HIS:CD2	2.20	0.59
2:B:47:GLU:HG3	3:E:71:LYS:HG3	1.85	0.59
3:E:76:HIS:HB2	10:E:327:HOH:O	2.03	0.59
1:C:251:VAL:HG12	1:C:252:VAL:N	2.16	0.59
1:A:154:THR:HG23	8:A:3000:AGH:HAB2	1.85	0.58
2:D:7:ILE:HD12	2:D:91:LYS:HD3	1.88	0.56
1:C:166:CYS:HB3	1:C:167:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:HIS:HB3	1:C:106:PRO:CD	2.35	0.55
1:C:187:PRO:HB3	1:C:211:PHE:HB3	1.87	0.55
1:A:133:PRO:HD3	1:A:145:ILE:HG12	1.89	0.54
1:A:186:LYS:HG2	1:A:267:SER:HB3	1.89	0.54
4:F:98:ARG:HB3	4:F:99:ASP:CB	2.28	0.54
3:E:98:THR:O	4:F:31:LYS:NZ	2.31	0.54
1:A:198:GLY:HA3	1:A:201:ARG:H	1.72	0.54
1:C:251:VAL:HG12	1:C:252:VAL:H	1.72	0.54
4:H:63:GLU:HG3	10:H:254:HOH:O	2.08	0.54
3:G:33:ARG:HB2	3:G:91:VAL:HG13	1.90	0.53
3:E:35:TYR:HE1	3:E:91:VAL:HG11	1.74	0.53
4:F:120:LEU:HD22	4:F:220:LEU:HD11	1.91	0.53
1:A:240:ASP:OD1	2:B:12:ARG:NH1	2.43	0.52
3:E:51:PHE:HB2	10:E:213:HOH:O	2.09	0.52
1:A:150:GLN:NE2	3:G:98:THR:H	2.06	0.52
3:G:35:TYR:HD1	3:G:45:SER:HA	1.74	0.51
1:C:13:LEU:HG	2:D:56:PHE:CZ	2.46	0.51
3:E:35:TYR:CE1	3:E:91:VAL:HG11	2.45	0.51
3:E:49:MET:HE3	3:E:66:LEU:HB2	1.93	0.51
1:A:95:GLU:HG3	2:B:32:PRO:HB3	1.92	0.51
2:D:1:ILE:CB	2:D:32:PRO:HD3	2.41	0.50
2:D:49:VAL:HG12	2:D:68:THR:HB	1.92	0.50
3:G:161:THR:HG23	3:G:162:ASP:O	2.10	0.50
2:D:33:SER:HB2	2:D:54:LEU:HD21	1.92	0.50
1:A:13:LEU:HG	2:B:56:PHE:CZ	2.47	0.50
1:A:202:LEU:HD22	1:A:204:LEU:HD23	1.94	0.50
1:A:95:GLU:HG2	10:A:304:HOH:O	2.11	0.49
1:C:25:ARG:NH1	1:C:27:ASP:OD1	2.42	0.49
3:G:40:GLY:HA2	10:H:425:HOH:O	2.11	0.49
1:A:113:PHE:HB2	1:A:115:HIS:CE1	2.47	0.49
4:F:220:LEU:HD22	4:F:233:PRO:HG2	1.93	0.49
3:E:23:ASN:OD1	3:E:72:GLN:NE2	2.46	0.49
4:F:21:LEU:HD22	4:F:112:THR:HG21	1.94	0.49
1:A:256:ALA:HA	1:A:257:ALA:HB3	1.93	0.49
1:C:147:VAL:HG11	3:E:99:LEU:HD13	1.94	0.49
4:H:130:VAL:HG23	4:H:240:ALA:HB3	1.94	0.49
1:C:196:SER:HB3	1:C:203:LEU:HD22	1.95	0.48
2:D:97:ARG:HB3	10:D:439:HOH:O	2.13	0.48
1:A:35:LEU:HD11	1:A:212:TYR:OH	2.14	0.48
3:G:182:SER:OG	3:G:184:LYS:HG2	2.13	0.47
1:A:191:LEU:HB2	1:A:280:HIS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:98:ARG:N	4:F:99:ASP:C	2.72	0.47
2:B:17:ASN:HA	2:B:72:PRO:O	2.15	0.47
4:F:132:GLU:HG2	4:F:245:ARG:HH21	1.79	0.47
4:F:201:ALA:O	4:F:205:GLN:HB2	2.14	0.47
1:C:87:MET:HE2	4:F:50:TYR:CD2	2.51	0.46
4:H:53:ASN:ND2	10:H:328:HOH:O	2.47	0.46
3:G:138:VAL:HG11	4:H:147:VAL:HG11	1.96	0.46
1:A:47:VAL:H	1:A:67:GLN:NE2	2.13	0.46
1:C:263:VAL:HB	1:C:273:ILE:HB	1.98	0.46
4:F:121:LYS:HE2	4:F:228:GLN:HE22	1.81	0.46
4:F:6:GLN:O	4:F:9:ARG:NH1	2.36	0.46
4:H:21:LEU:HD22	4:H:112:THR:HG21	1.97	0.46
1:A:220:TRP:HD1	1:A:230:THR:HG23	1.81	0.46
2:B:3:ARG:HH11	2:B:61:SER:HB3	1.81	0.46
1:A:49:SER:HB3	1:A:54:SER:HB2	1.98	0.45
1:A:73:TYR:CE2	8:A:3000:AGH:HA12	2.50	0.45
1:A:267:SER:CA	1:A:268:LEU:CB	2.94	0.45
1:C:194:GLY:O	1:C:203:LEU:HB2	2.17	0.45
3:G:27:SER:HA	3:G:28:PRO:C	2.41	0.45
3:G:141:PHE:HB2	3:G:193:PHE:CE1	2.52	0.45
1:C:47:VAL:HG11	8:C:3000:AGH:HAQ1	1.98	0.44
1:C:199:PRO:HA	1:C:200:GLY:HA2	1.77	0.44
3:G:128:LEU:HD12	4:H:133:PRO:HA	1.99	0.44
3:E:32:LEU:HB2	3:E:92:VAL:HG22	1.98	0.44
3:E:177:SER:OG	4:F:196:ARG:HD2	2.17	0.44
1:A:194:GLY:HA3	1:A:203:LEU:HD23	2.00	0.44
2:D:95:TRP:CZ3	2:D:97:ARG:HD2	2.53	0.44
4:H:25:GLN:HE22	4:H:29:HIS:CB	2.30	0.44
4:F:99:ASP:O	4:F:102:LEU:N	2.51	0.44
3:G:130:ASP:N	3:G:130:ASP:OD1	2.51	0.44
4:F:153:PHE:HE2	4:F:156:ASP:HA	1.83	0.43
3:G:60:ARG:NH2	3:G:84:ASP:OD1	2.51	0.43
6:J:1:NAG:H62	6:J:2:NDG:C1	2.48	0.43
4:F:6:GLN:HB2	4:F:110:PRO:HD2	2.01	0.43
1:A:88:LEU:HD13	1:A:140:TRP:CE3	2.54	0.43
1:C:131:TRP:HB3	1:C:145:ILE:HD12	2.00	0.43
4:F:127:GLU:O	4:F:150:ALA:HA	2.18	0.43
3:G:119:GLN:O	3:G:121:PRO:HD3	2.19	0.43
3:E:166:LEU:H	3:E:166:LEU:HD13	1.84	0.43
1:C:251:VAL:CG1	1:C:252:VAL:N	2.81	0.42
1:A:255:GLU:HA	1:A:256:ALA:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:3000:AGH:O2A	3:E:95:ARG:HG3	2.19	0.42
4:F:19:ILE:HD11	4:F:82:ALA:HB2	2.01	0.42
4:F:97:LEU:H	4:F:97:LEU:HD23	1.84	0.42
4:H:113:ARG:HH11	4:H:113:ARG:HB3	1.84	0.42
1:C:12:CYS:HB3	8:C:3000:AGH:HAN1	2.00	0.42
1:C:251:VAL:CG1	1:C:252:VAL:H	2.32	0.42
4:F:121:LYS:HE2	4:F:228:GLN:NE2	2.34	0.42
3:G:116:PRO:HG3	3:G:165:VAL:HG13	2.02	0.42
1:A:277:TRP:HA	1:A:278:HIS:HA	1.53	0.42
1:C:202:LEU:HB2	1:C:251:VAL:O	2.19	0.42
2:D:9:VAL:HG11	2:D:95:TRP:HB2	2.02	0.42
2:B:84:HIS:CE1	2:B:85:VAL:HG12	2.54	0.42
3:E:20:LEU:HD22	3:E:110:THR:HG21	2.02	0.42
1:C:150:GLN:OE1	3:E:97:SER:HB2	2.20	0.42
4:F:98:ARG:HD3	4:F:99:ASP:OD2	2.20	0.42
3:E:48:ILE:HD11	4:F:105:GLU:HG3	2.02	0.42
2:D:3:ARG:HH11	2:D:61:SER:HB3	1.85	0.41
4:H:32:MET:HE2	4:H:32:MET:HB3	1.90	0.41
1:C:235:ILE:HD12	10:C:434:HOH:O	2.20	0.41
1:A:150:GLN:HE22	3:G:98:THR:H	1.69	0.41
1:A:267:SER:CB	1:A:268:LEU:CB	2.91	0.41
3:E:130:ASP:HB2	3:E:131:SER:H	1.68	0.41
4:H:12:VAL:HB	4:H:155:PRO:HG3	2.02	0.41
4:H:176:ASP:OD1	4:H:196:ARG:NH1	2.49	0.41
1:C:208:VAL:HB	1:C:245:LEU:HD23	2.03	0.41
3:G:23:ASN:CG	3:G:72:GLN:HE22	2.29	0.40
3:G:87:SER:HB2	3:G:111:GLN:HE22	1.86	0.40
4:H:113:ARG:HB3	4:H:113:ARG:NH1	2.36	0.40
3:G:125:VAL:O	3:G:205:PRO:HD3	2.21	0.40
4:H:234:VAL:O	4:H:236:GLN:HG2	2.21	0.40
3:E:166:LEU:HB3	4:F:174:CYS:HB2	2.03	0.40
4:H:44:HIS:HB3	4:H:60:LEU:HB2	2.03	0.40
1:A:191:LEU:O	1:A:280:HIS:HB2	2.22	0.40
3:G:161:THR:CG2	3:G:179:VAL:H	2.20	0.40
4:H:30:ASP:HB3	4:H:50:TYR:O	2.20	0.40
4:H:80:GLU:HG2	10:H:318:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/284 (96%)	263 (96%)	9 (3%)	1 (0%)	30	49
1	C	272/284 (96%)	244 (90%)	21 (8%)	7 (3%)	4	7
2	B	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
2	D	98/99 (99%)	93 (95%)	4 (4%)	1 (1%)	12	24
3	E	192/209 (92%)	184 (96%)	7 (4%)	1 (0%)	24	43
3	G	199/209 (95%)	190 (96%)	9 (4%)	0	100	100
4	F	239/246 (97%)	230 (96%)	8 (3%)	1 (0%)	30	49
4	H	244/246 (99%)	234 (96%)	10 (4%)	0	100	100
All	All	1612/1676 (96%)	1532 (95%)	69 (4%)	11 (1%)	18	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	LEU
1	C	271	GLN
3	E	187	PHE
1	C	137	ALA
1	C	195	PRO
1	C	277	TRP
2	D	2	GLN
4	F	39	PRO
1	C	128	GLY
1	C	197	PRO
1	C	270	GLY

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	233/249 (94%)	218 (94%)	15 (6%)	16	33
1	C	226/249 (91%)	208 (92%)	18 (8%)	11	24
2	B	90/94 (96%)	85 (94%)	5 (6%)	19	39
2	D	93/94 (99%)	89 (96%)	4 (4%)	26	51
3	E	182/191 (95%)	170 (93%)	12 (7%)	15	32
3	G	180/191 (94%)	168 (93%)	12 (7%)	15	31
4	F	212/217 (98%)	199 (94%)	13 (6%)	17	35
4	H	215/217 (99%)	199 (93%)	16 (7%)	13	27
All	All	1431/1502 (95%)	1336 (93%)	95 (7%)	15	32

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	24	THR
1	A	29	LEU
1	A	41	SER
1	A	57	THR
1	A	66	LEU
1	A	75	SER
1	A	96	LEU
1	A	116	VAL
1	A	145	ILE
1	A	202	LEU
1	A	236	LEU
1	A	249	LEU
1	A	252	VAL
1	A	268	LEU
2	B	2	GLN
2	B	36	GLU
2	B	48	LYS
2	B	54	LEU
2	B	75	LYS
1	C	13	LEU
1	C	24	THR
1	C	35	LEU
1	C	79	ARG

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Mol	Chain	Res	Type
1	C	89	ARG
1	C	116	VAL
1	C	127	GLN
1	C	139	LEU
1	C	143	LEU
1	C	182	LYS
1	C	183	LYS
1	C	191	LEU
1	C	203	LEU
1	C	205	VAL
1	C	231	GLN
1	C	245	LEU
1	C	268	LEU
1	C	269	GLU
2	D	12	ARG
2	D	19	LYS
2	D	94	LYS
2	D	97	ARG
3	E	6	SER
3	E	16	LYS
3	E	32	LEU
3	E	72	GLN
3	E	91	VAL
3	E	95	ARG
3	E	99	LEU
3	E	128	LEU
3	E	130	ASP
3	E	152	GLN
3	E	165	VAL
3	E	166	LEU
4	F	11	LEU
4	F	45	LEU
4	F	52	VAL
4	F	59	ASP
4	F	71	ARG
4	F	121	LYS
4	F	135	GLU
4	F	158	VAL
4	F	187	ASN
4	F	199	VAL
4	F	205	GLN
4	F	220	LEU

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Mol	Chain	Res	Type
4	F	227	THR
3	G	1	ASN
3	G	32	LEU
3	G	33	ARG
3	G	72	GLN
3	G	91	VAL
3	G	128	LEU
3	G	130	ASP
3	G	161	THR
3	G	165	VAL
3	G	166	LEU
3	G	197	ILE
3	G	198	ILE
4	H	9	ARG
4	H	11	LEU
4	H	17	LYS
4	H	20	THR
4	H	25	GLN
4	H	36	GLN
4	H	45	LEU
4	H	52	VAL
4	H	63	GLU
4	H	70	ILE
4	H	73	GLU
4	H	102	LEU
4	H	158	VAL
4	H	171	SER
4	H	196	ARG
4	H	223	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	62	GLN
1	A	67	GLN
1	A	105	HIS
1	A	111	ASN
1	A	142	ASN
1	A	150	GLN
1	A	168	GLN
2	B	89	GLN

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Mol	Chain	Res	Type
1	C	14	GLN
1	C	115	HIS
1	C	127	GLN
1	C	231	GLN
2	D	2	GLN
2	D	89	GLN
3	E	21	GLN
3	E	72	GLN
3	E	127	GLN
3	E	152	GLN
3	E	183	ASN
3	E	194	ASN
3	E	195	ASN
4	F	44	HIS
4	F	53	ASN
4	F	86	HIS
4	F	89	GLN
4	F	187	ASN
4	F	228	GLN
3	G	1	ASN
3	G	2	GLN
3	G	21	GLN
3	G	23	ASN
3	G	54	ASN
3	G	72	GLN
3	G	111	GLN
3	G	127	GLN
3	G	195	ASN
4	H	25	GLN
4	H	44	HIS
4	H	53	ASN
4	H	223	ASN

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

5 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
5	NAG	I	1	1,5	14,14,15	0.56	0	17,19,21	1.15	1 (5%)
5	BMA	I	2	5	11,11,12	0.53	0	15,15,17	0.71	0
6	NAG	J	1	1,6	14,14,15	0.49	0	17,19,21	1.39	4 (23%)
6	NDG	J	2	6	14,14,15	0.80	1 (7%)	17,19,21	1.18	2 (11%)
6	BMA	J	3	6	11,11,12	0.67	0	15,15,17	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	BMA	I	2	5	-	2/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NDG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	2	NDG	C1-C2	2.04	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	NDG	C4-C3-C2	3.44	116.07	111.02
6	J	1	NAG	C1-O5-C5	3.05	116.28	112.19
5	I	1	NAG	C1-O5-C5	2.84	115.99	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1	NAG	O4-C4-C3	-2.61	104.23	110.38
6	J	1	NAG	O4-C4-C5	2.37	115.17	109.32
6	J	1	NAG	O5-C1-C2	-2.16	107.96	111.29
6	J	2	NDG	O5-C5-C4	-2.09	105.75	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	I	1	NAG	C1

All (8) torsion outliers are listed below:

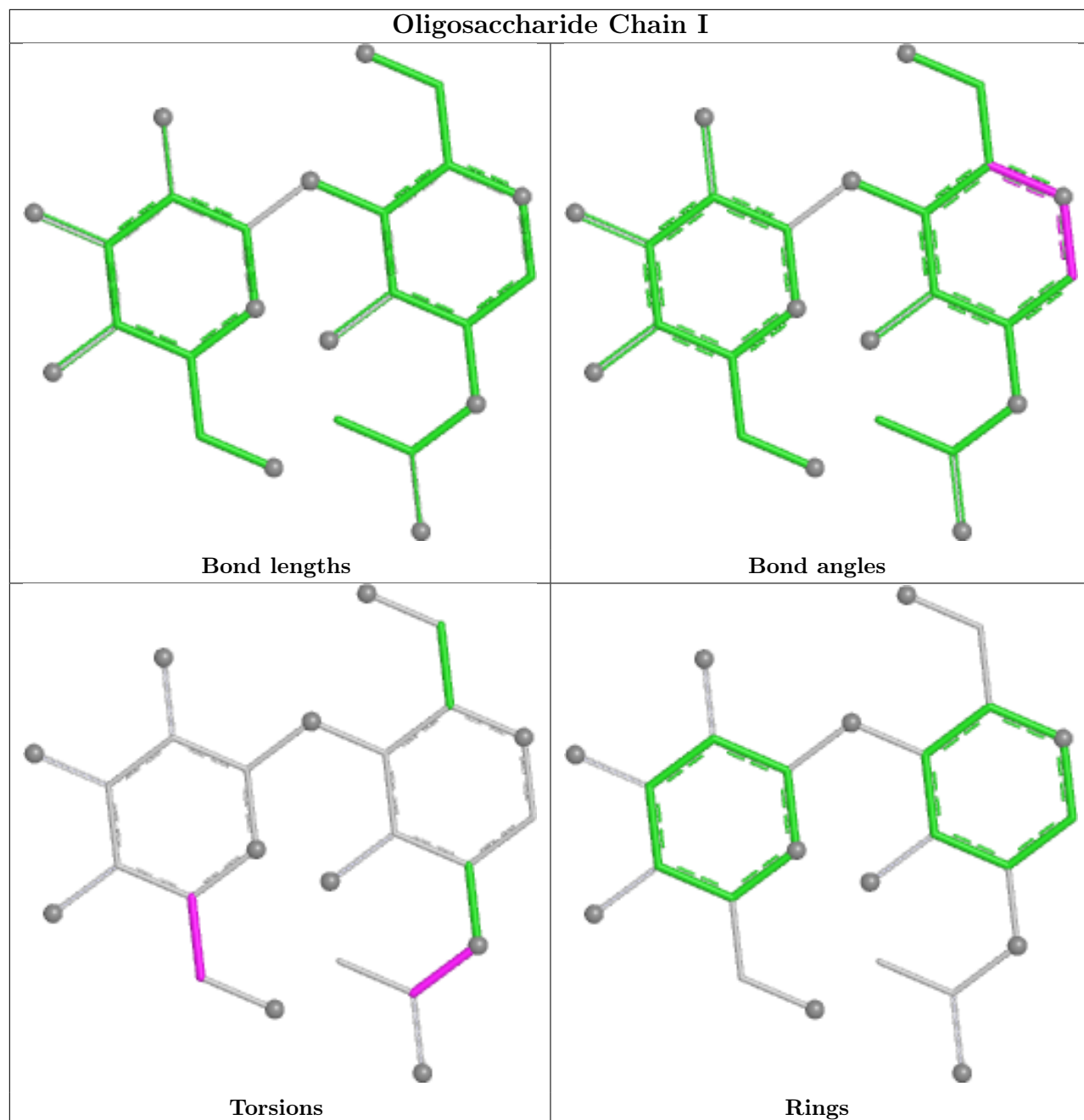
Mol	Chain	Res	Type	Atoms
5	I	2	BMA	O5-C5-C6-O6
5	I	2	BMA	C4-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
6	J	2	NDG	O5-C5-C6-O6
6	J	2	NDG	C4-C5-C6-O6
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2

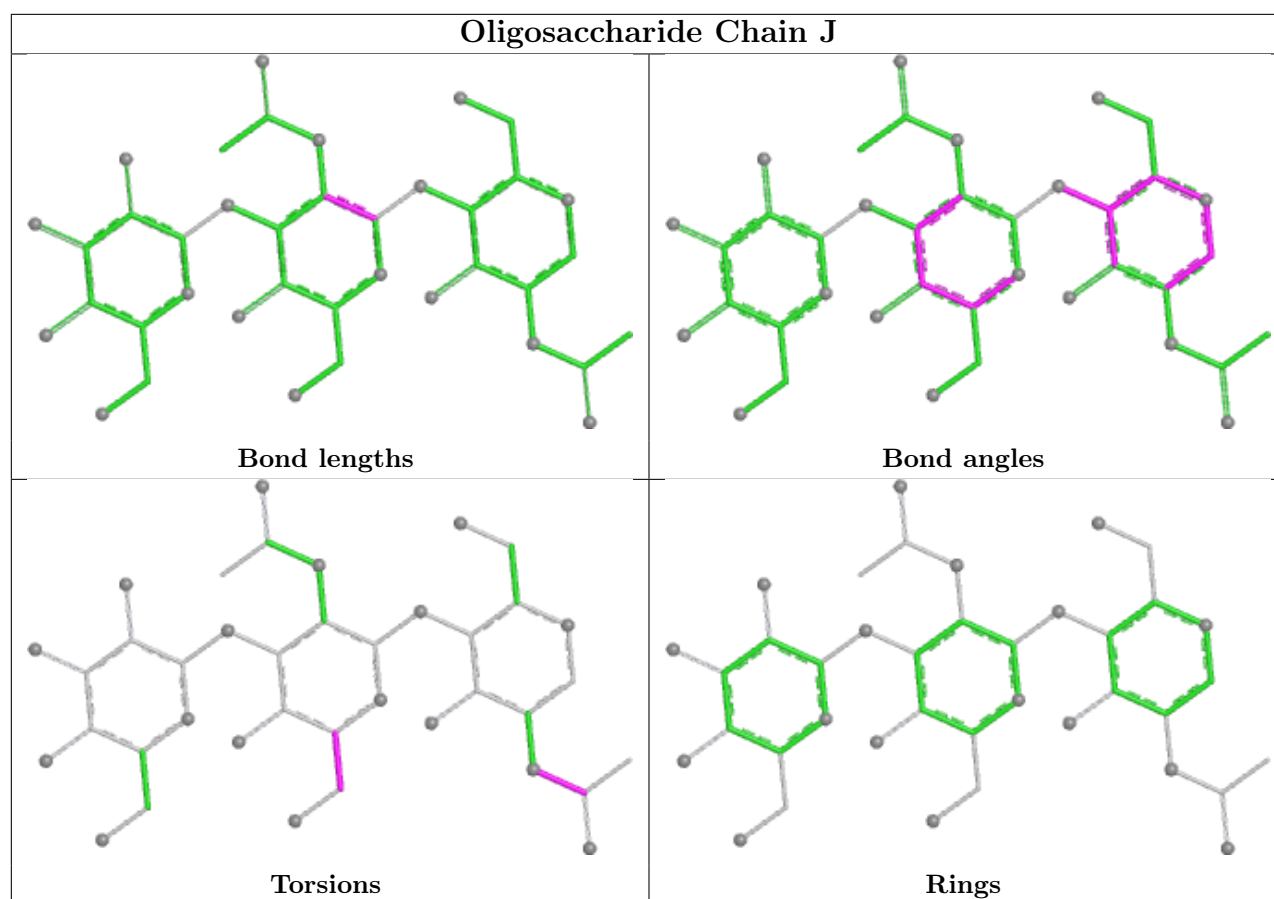
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
6	J	2	NDG	1	0

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





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
7	NAG	A	2000	1	14,14,15	0.54	0	17,19,21	2.72	5 (29%)
8	AGH	C	3000	-	60,60,60	0.42	0	66,69,69	0.77	1 (1%)
7	NAG	C	2000	1	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
8	AGH	A	3000	-	60,60,60	0.49	1 (1%)	66,69,69	0.75	1 (1%)

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
7	NAG	A	2000	1	-	4/6/23/26	0/1/1/1
8	AGH	C	3000	-	-	23/58/78/78	0/1/1/1
7	NAG	C	2000	1	1/1/5/7	4/6/23/26	0/1/1/1
8	AGH	A	3000	-	-	19/58/78/78	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	3000	AGH	O1A-C1A	2.70	1.44	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2000	NAG	C1-O5-C5	8.22	123.20	112.19
7	A	2000	NAG	C2-N2-C7	3.98	128.23	122.90
7	A	2000	NAG	C4-C3-C2	-3.76	105.51	111.02
7	C	2000	NAG	C1-O5-C5	3.70	117.14	112.19
8	C	3000	AGH	C1-C2-N2	-3.16	105.16	109.66
7	A	2000	NAG	C1-C2-N2	2.82	114.88	110.43
8	A	3000	AGH	C1-C2-N2	-2.46	106.15	109.66
7	A	2000	NAG	C8-C7-N2	2.46	120.20	116.12
7	C	2000	NAG	O7-C7-C8	-2.10	118.31	122.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	2000	NAG	C1

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2000	NAG	C1-C2-N2-C7
7	A	2000	NAG	C8-C7-N2-C2
7	A	2000	NAG	O7-C7-N2-C2
7	C	2000	NAG	C8-C7-N2-C2
7	C	2000	NAG	O7-C7-N2-C2
8	C	3000	AGH	C14-C15-C16-C17
8	C	3000	AGH	CAJ-CAK-CAL-CAM
8	A	3000	AGH	C11-C12-C13-C14

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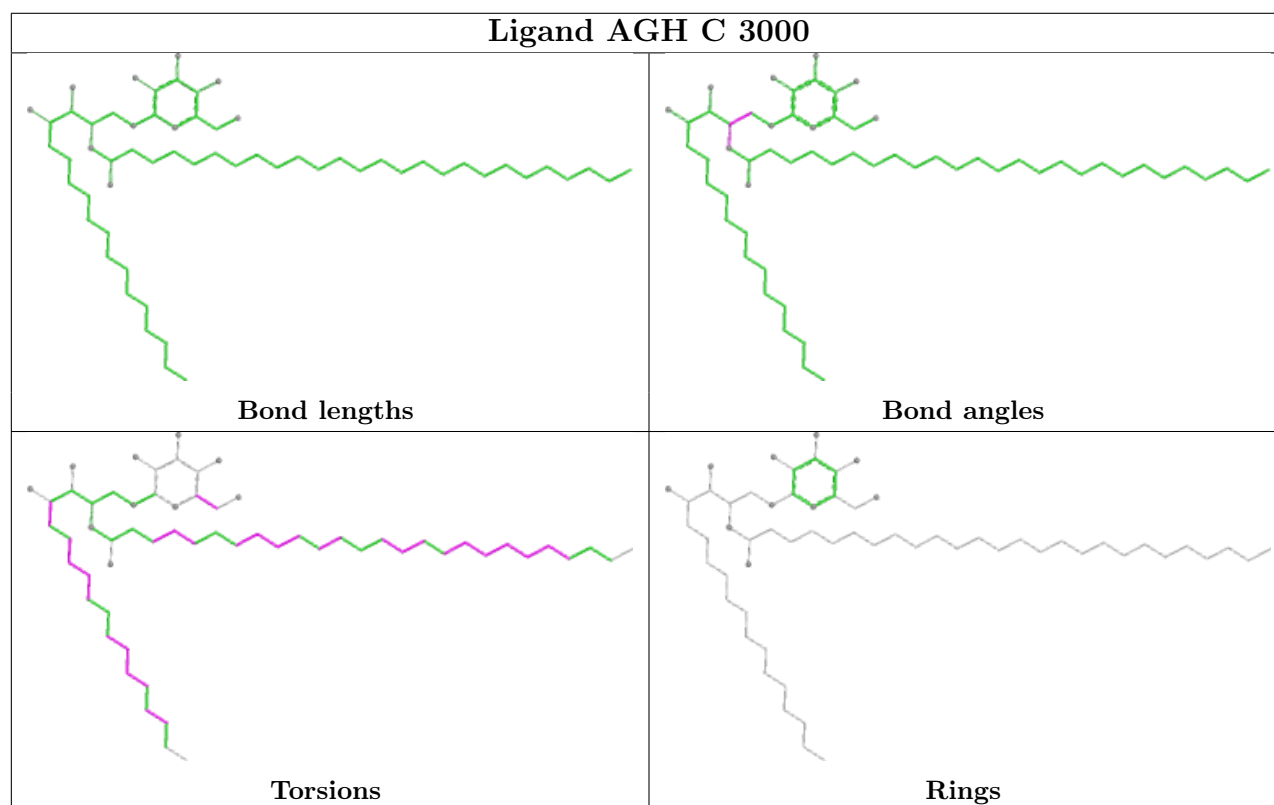
Mol	Chain	Res	Type	Atoms
8	C	3000	AGH	C7-C8-C9-C10
8	A	3000	AGH	CAF-CAG-CAH-CAI
8	A	3000	AGH	CAJ-CAK-CAL-CAM
8	C	3000	AGH	C10-C11-C12-C13
8	A	3000	AGH	C14-C15-C16-C17
8	A	3000	AGH	CAH-CAI-CAJ-CAK
8	C	3000	AGH	O4-C4-C5-C6
8	C	3000	AGH	CAF-CAG-CAH-CAI
8	A	3000	AGH	CAQ-CAR-CAS-CAT
8	C	3000	AGH	CAM-CAN-CAO-CAP
8	C	3000	AGH	CAH-CAI-CAJ-CAK
8	A	3000	AGH	CAG-CAH-CAI-CAJ
8	A	3000	AGH	CAP-CAQ-CAR-CAS
8	C	3000	AGH	CAS-CAT-CAU-CAV
8	C	3000	AGH	C6-C7-C8-C9
8	C	3000	AGH	C12-C13-C14-C15
8	C	3000	AGH	CAB-CAC-CAD-CAE
8	C	3000	AGH	CAG-CAH-CAI-CAJ
8	C	3000	AGH	CAN-CAO-CAP-CAQ
8	A	3000	AGH	CAW-CAX-CAY-CAZ
8	A	3000	AGH	C10-C11-C12-C13
8	C	3000	AGH	CAQ-CAR-CAS-CAT
7	C	2000	NAG	O5-C5-C6-O6
8	C	3000	AGH	CAP-CAQ-CAR-CAS
8	A	3000	AGH	C9-C10-C11-C12
8	A	3000	AGH	C11-C10-C9-C8
7	A	2000	NAG	C4-C5-C6-O6
8	A	3000	AGH	CAV-CAW-CAX-CAY
8	C	3000	AGH	CAU-CAV-CAW-CAX
8	C	3000	AGH	C5-C6-C7-C8
8	A	3000	AGH	CAR-CAS-CAT-CAU
8	C	3000	AGH	CAR-CAS-CAT-CAU
8	A	3000	AGH	CAM-CAN-CAO-CAP
8	A	3000	AGH	CAL-CAM-CAN-CAO
8	C	3000	AGH	CAC-CAD-CAE-CAF
8	A	3000	AGH	C13-C14-C15-C16
8	C	3000	AGH	CAT-CAU-CAV-CAW
8	A	3000	AGH	C6-C7-C8-C9
7	C	2000	NAG	C3-C2-N2-C7
8	A	3000	AGH	CAA-CAB-CAC-CAD
8	C	3000	AGH	C4A-C5M-C6A-O5A
8	C	3000	AGH	C11-C12-C13-C14

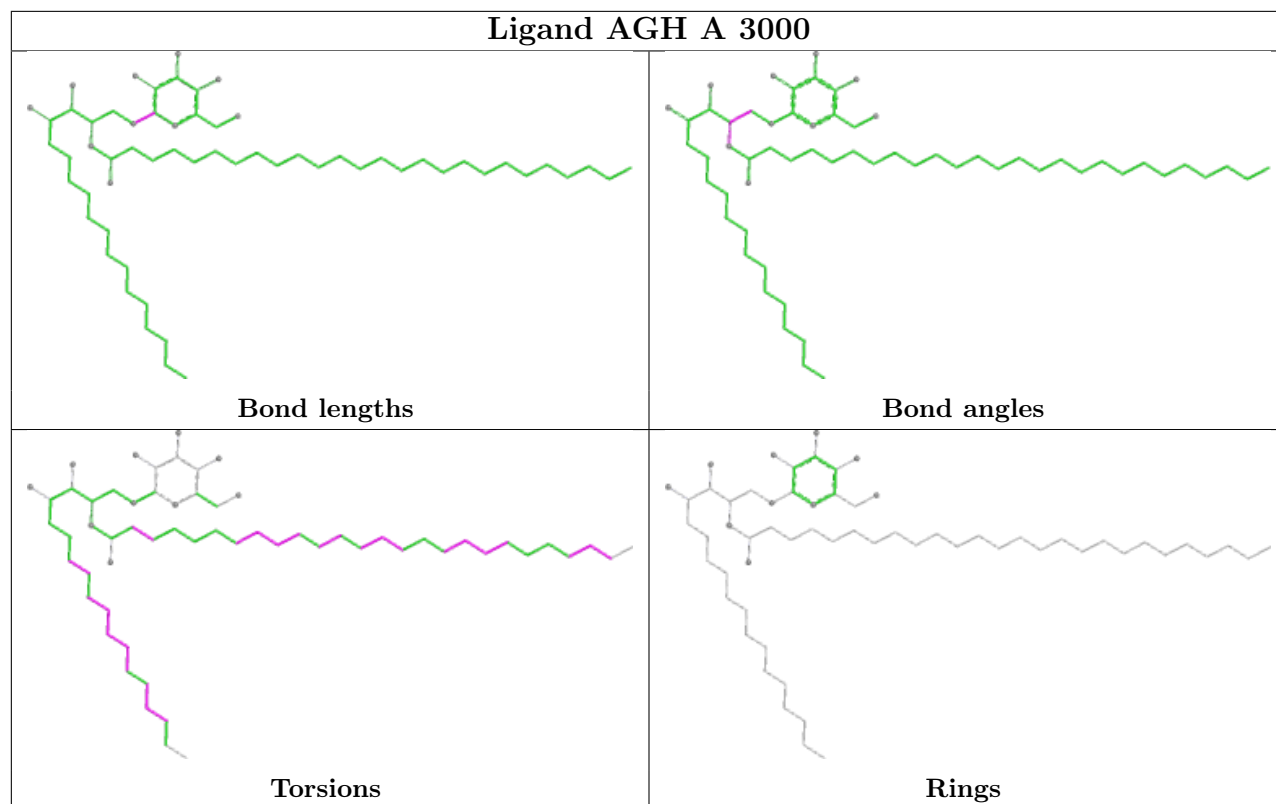
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3000	AGH	4	0
8	A	3000	AGH	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	275/284 (96%)	0.58	20 (7%) 21 19	22, 39, 59, 68	0
1	C	274/284 (96%)	0.98	38 (13%) 6 5	29, 43, 69, 74	0
2	B	97/99 (97%)	0.15	0 100 100	23, 31, 40, 43	0
2	D	99/99 (100%)	0.29	1 (1%) 79 76	18, 35, 44, 55	1 (1%)
3	E	199/209 (95%)	0.77	24 (12%) 8 7	16, 37, 70, 70	1 (0%)
3	G	202/209 (96%)	0.85	32 (15%) 5 4	16, 36, 70, 73	1 (0%)
4	F	242/246 (98%)	0.86	17 (7%) 22 20	21, 47, 56, 61	1 (0%)
4	H	245/246 (99%)	0.63	5 (2%) 65 61	15, 43, 54, 55	2 (0%)
All	All	1633/1676 (97%)	0.71	137 (8%) 17 15	15, 41, 64, 74	6 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	GLN	4.9
3	G	197	ILE	4.6
3	G	205	PRO	4.3
3	G	133	SER	4.2
1	C	199	PRO	4.1
3	G	183	ASN	4.0
1	C	251	VAL	4.0
1	C	198	GLY	4.0
1	A	253	ALA	3.9
3	E	206	SER	3.9
3	E	131	SER	3.7
1	C	202	LEU	3.6
4	F	102	LEU	3.6
3	E	138	VAL	3.6
3	E	134	SER	3.5
1	C	256	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	G	194	ASN	3.5
3	E	51	PHE	3.5
4	H	187	ASN	3.4
1	C	252	VAL	3.4
3	G	185	SER	3.4
4	F	186	LEU	3.4
1	C	277	TRP	3.3
3	G	203	PHE	3.3
4	F	97	LEU	3.2
1	C	203	LEU	3.2
3	G	135	ASP	3.2
3	E	183	ASN	3.2
2	D	99	MET	3.1
3	E	136	LYS	3.0
1	C	276	TYR	3.0
3	G	171	MET	3.0
1	A	260	SER	3.0
3	G	131	SER	3.0
3	G	134	SER	3.0
1	C	225	GLN	2.9
4	H	202	THR	2.9
1	C	259	LEU	2.9
1	C	200	GLY	2.9
3	G	195	ASN	2.8
3	E	128	LEU	2.8
1	C	278	HIS	2.8
3	G	137	SER	2.8
3	E	119	GLN	2.8
1	A	109	ALA	2.8
1	A	228	GLN	2.8
3	G	132	LYS	2.7
1	C	226	GLU	2.7
1	A	218	VAL	2.7
1	C	253	ALA	2.7
1	A	199	PRO	2.7
3	G	115[A]	TRP	2.7
1	C	275	LEU	2.6
3	E	124	ALA	2.6
3	E	178	ALA	2.6
1	C	227	GLN	2.6
1	C	108	ASN	2.5
1	C	257	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	156	SER	2.5
4	F	175	THR	2.5
1	A	106	PRO	2.5
1	A	200	GLY	2.5
3	G	198	ILE	2.5
4	F	225	GLU	2.5
1	C	217	TRP	2.5
3	G	149	ASN	2.5
4	F	199	VAL	2.5
3	G	182	SER	2.5
4	F	138	ILE	2.5
1	C	205	VAL	2.5
1	C	232	PRO	2.4
1	C	139	LEU	2.4
3	G	140	LEU	2.4
4	H	139	SER	2.4
4	F	244	GLY	2.4
3	E	197	ILE	2.4
3	G	128	LEU	2.4
3	G	141	PHE	2.4
3	G	187	PHE	2.4
1	A	195	PRO	2.4
3	G	130	ASP	2.4
3	G	200	GLU	2.4
1	C	195	PRO	2.3
3	E	205	PRO	2.3
4	F	99	ASP	2.3
1	C	230	THR	2.3
3	E	147	GLN	2.3
3	G	186	ASP	2.3
1	A	261	CYS	2.3
1	A	268	LEU	2.3
1	C	261	CYS	2.3
1	A	108	ASN	2.3
3	E	192	ALA	2.3
1	C	273	ILE	2.3
3	G	119	GLN	2.2
1	C	221	MET	2.2
1	C	249	LEU	2.2
3	E	120	ASN	2.2
3	G	161	THR	2.2
1	A	198	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	160	TRP	2.2
4	F	53	ASN	2.2
1	A	231	GLN	2.2
3	G	152	GLN	2.2
1	C	268	LEU	2.2
1	A	6	ARG	2.2
1	C	220	TRP	2.2
3	E	203	PHE	2.2
3	G	204	PHE	2.2
1	A	259	LEU	2.2
4	F	180	LEU	2.2
1	C	266	SER	2.2
1	C	160	TRP	2.2
1	C	5	GLN	2.1
4	F	136	ALA	2.1
3	G	126	TYR	2.1
3	E	162	ASP	2.1
3	G	158	VAL	2.1
3	E	190	ALA	2.1
3	E	193	PHE	2.1
4	F	240	ALA	2.1
1	C	107	GLY	2.1
3	E	177	SER	2.1
4	H	207	PRO	2.1
3	G	188	ALA	2.1
3	E	129	ARG	2.1
4	F	202	THR	2.1
3	E	198	ILE	2.1
1	C	196	SER	2.1
4	F	131	PHE	2.0
1	A	256	ALA	2.0
1	A	245	LEU	2.0
1	C	106	PRO	2.0
1	A	279	HIS	2.0
4	H	228	GLN	2.0
4	F	246	ALA	2.0
4	F	119	ASP	2.0

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

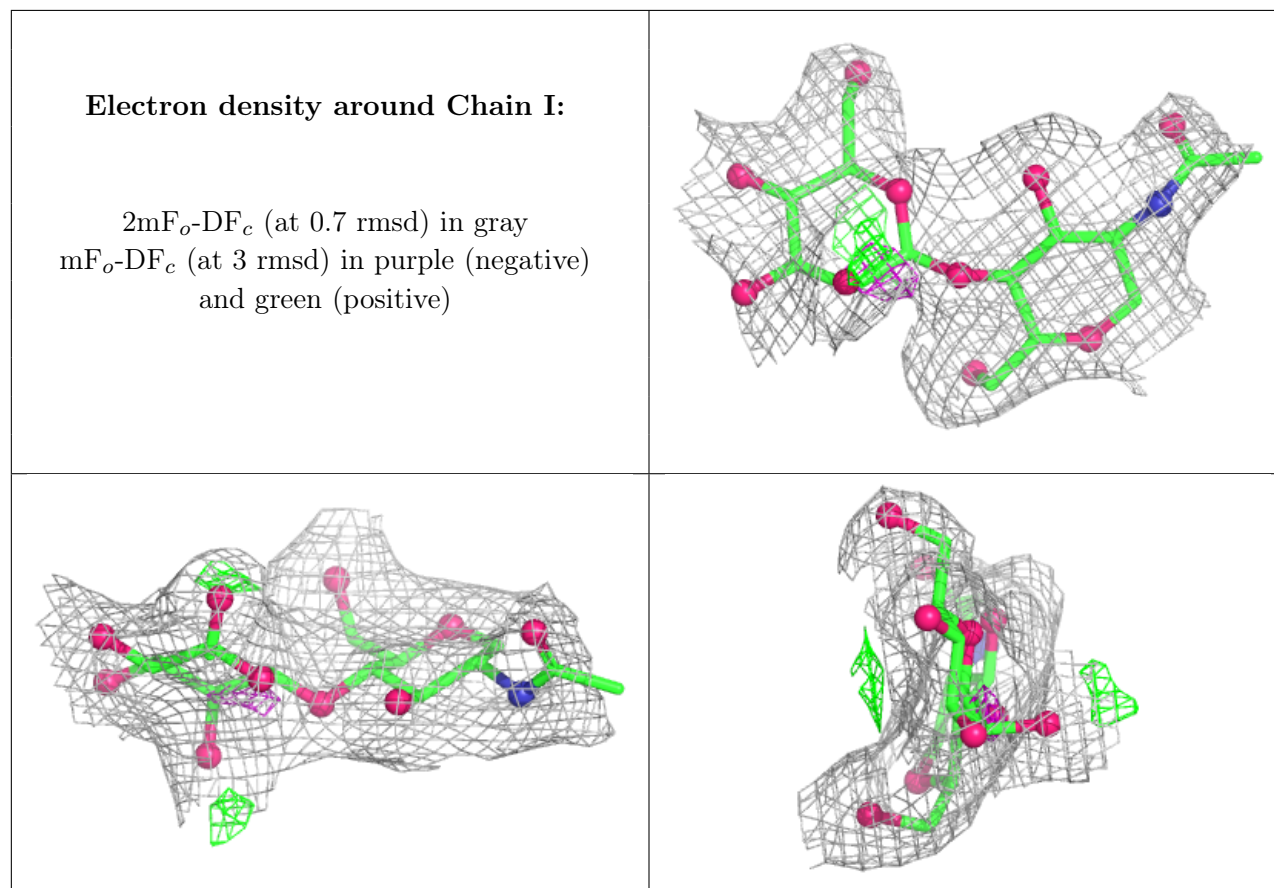
There are no non-standard protein/DNA/RNA residues in this entry.

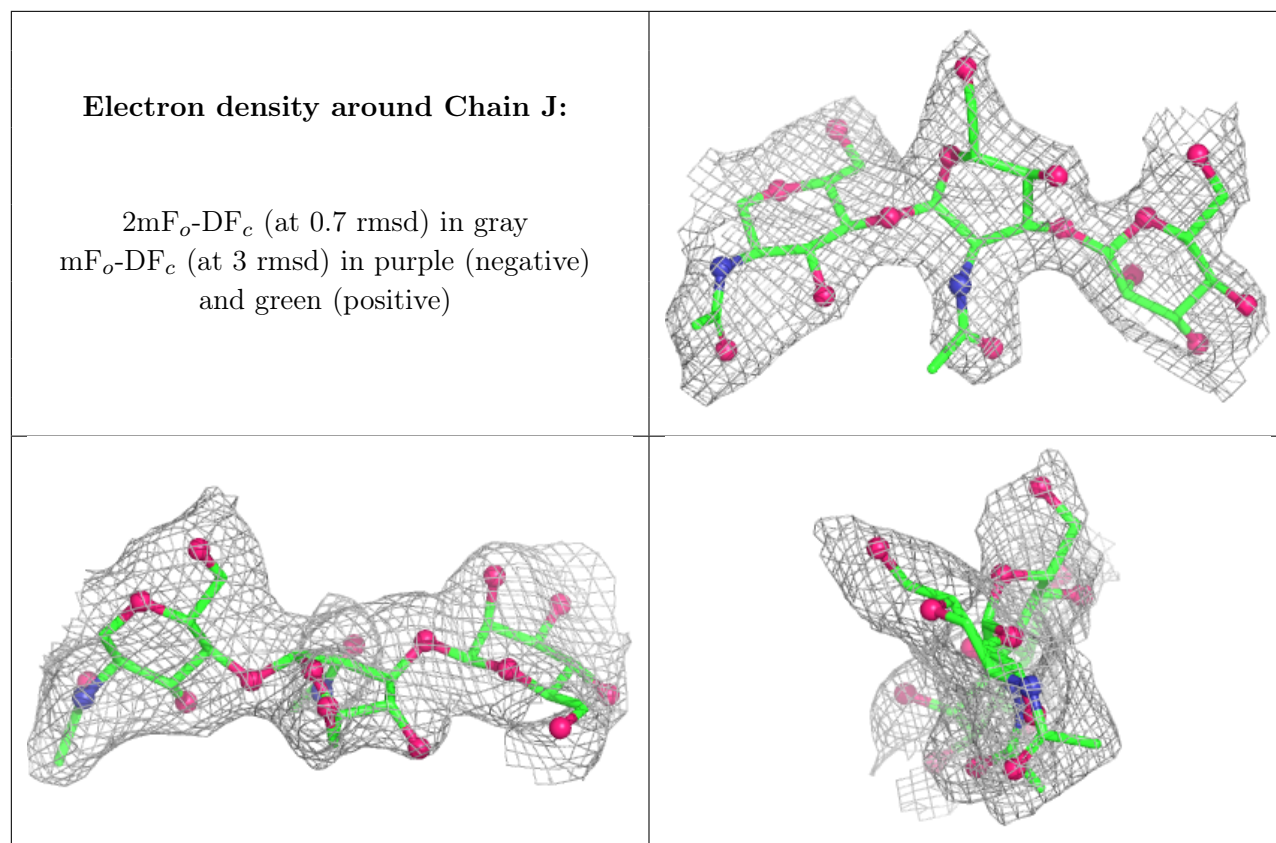
6.3 Carbohydrates [i](#)

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
5	BMA	I	2	11/12	0.53	0.16	55,56,56,57	0
6	BMA	J	3	11/12	0.71	0.12	65,65,65,65	0
6	NDG	J	2	14/15	0.75	0.14	60,63,63,64	0
5	NAG	I	1	14/15	0.84	0.13	45,50,52,53	0
6	NAG	J	1	14/15	0.90	0.11	46,49,53,57	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

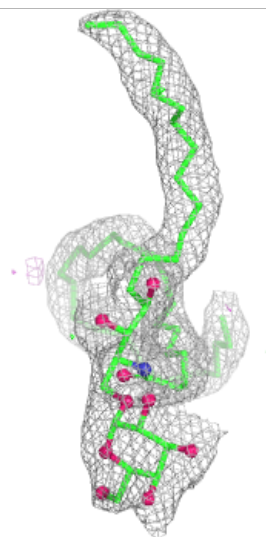
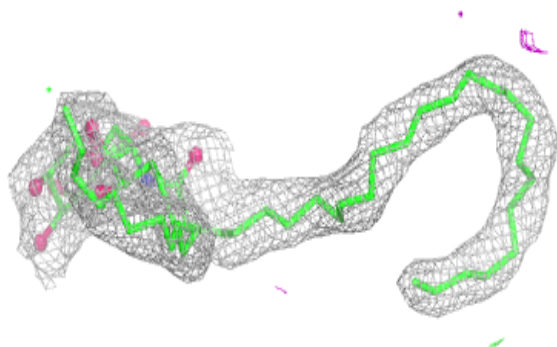
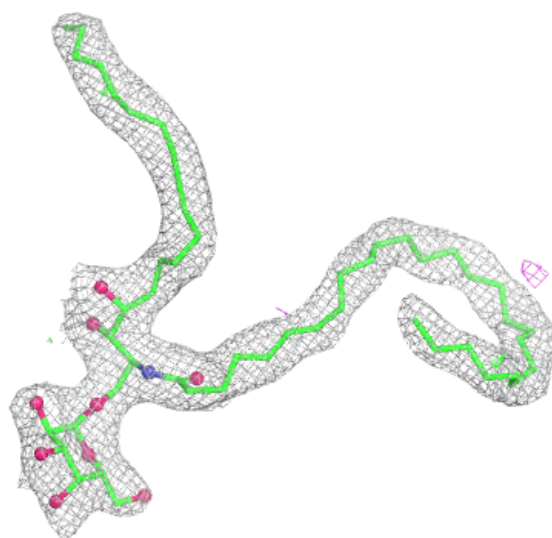
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	2000	14/15	0.82	0.11	38,40,41,41	0
7	NAG	C	2000	14/15	0.85	0.10	43,44,45,46	0
9	MG	H	1000	1/1	0.87	0.21	27,27,27,27	1
8	AGH	C	3000	60/60	0.93	0.10	26,31,34,35	0
8	AGH	A	3000	60/60	0.94	0.10	22,26,37,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

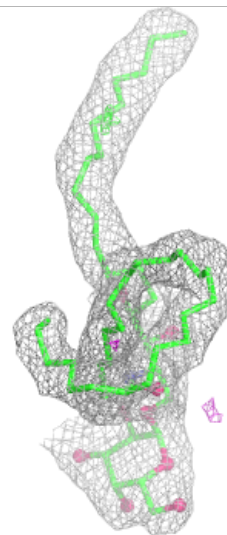
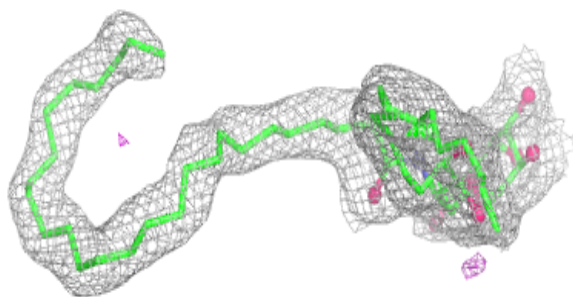
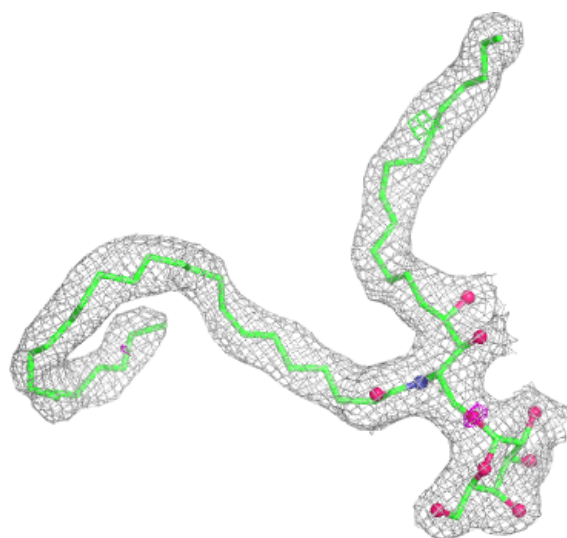
Electron density around AGH C 3000:

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



Electron density around AGH A 3000:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.