



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:42 PM BST

PDB ID : 3SCM  
Title : Crystal structure of autoreactive-Valpha14-Vbeta6 NKT TCR in complex with CD1d-isoglobotrihexosylceramide  
Authors : Clarke, A.J.; Rossjohn, J.  
Deposited on : 2011-06-08  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

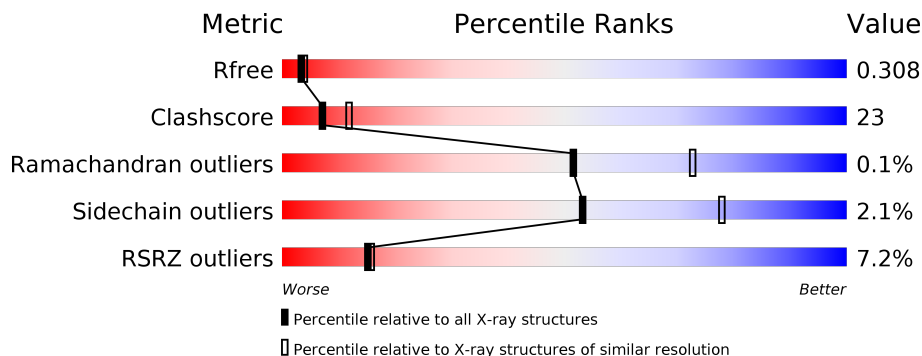
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	
2	B	99	
3	C	207	
4	D	245	
5	E	2	

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 6780 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2324	1480	404	426	14	6	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	SEE REMARK 999	UNP P11609
A	280	GLY	-	expression tag	UNP P11609
A	281	SER	-	expression tag	UNP P11609
A	282	LEU	-	expression tag	UNP P11609
A	283	HIS	-	expression tag	UNP P11609
A	284	HIS	-	expression tag	UNP P11609
A	285	ILE	-	expression tag	UNP P11609
A	286	LEU	-	expression tag	UNP P11609
A	287	ASP	-	expression tag	UNP P11609
A	288	ALA	-	expression tag	UNP P11609
A	289	GLN	-	expression tag	UNP P11609
A	290	LYS	-	expression tag	UNP P11609
A	291	MET	-	expression tag	UNP P11609
A	292	VAL	-	expression tag	UNP P11609
A	293	TRP	-	expression tag	UNP P11609
A	294	ASN	-	expression tag	UNP P11609
A	295	HIS	-	expression tag	UNP P11609
A	296	ARG	-	expression tag	UNP P11609
A	297	HIS	-	expression tag	UNP P11609
A	298	HIS	-	expression tag	UNP P11609
A	299	HIS	-	expression tag	UNP P11609
A	300	HIS	-	expression tag	UNP P11609
A	301	HIS	-	expression tag	UNP P11609
A	302	HIS	-	expression tag	UNP P11609

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	814	520	138	149	7	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	SEE REMARK 999	UNP P01887

- Molecule 3 is a protein called NKT TCR Valpha14 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	191	1478	915	254	302	7	3	0	0

- Molecule 4 is a protein called NKT TCR autoreactive-Vbeta6 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	239	1900	1202	326	365	7	5	0	0

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



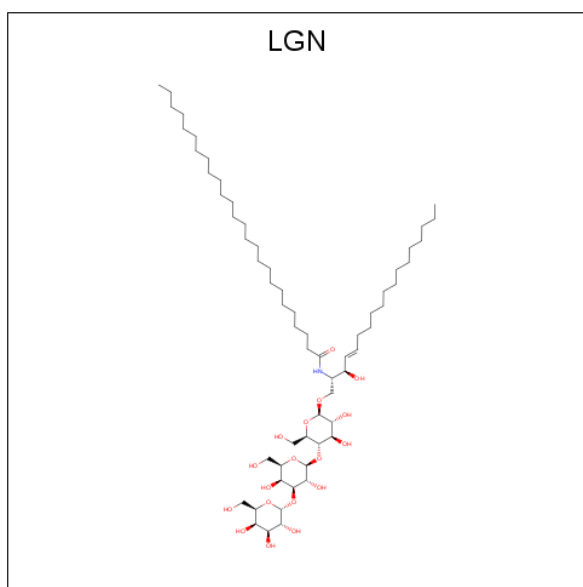
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	2	28	16	2	10		0	0	0

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



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

- Molecule 7 is N-[(2S,3R,4E)-1-1-[[alpha-D-galactopyranosyl-(1->3)-beta-D-galactopyranosyl-(1->4)-beta-D-glucopyranosyl]oxy]-3-hydroxyoctadec-4-en-2-yl]hexacosanamide (three-letter code: LGN) (formula: C<sub>62</sub>H<sub>117</sub>NO<sub>18</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	79	60	1	18	0	0

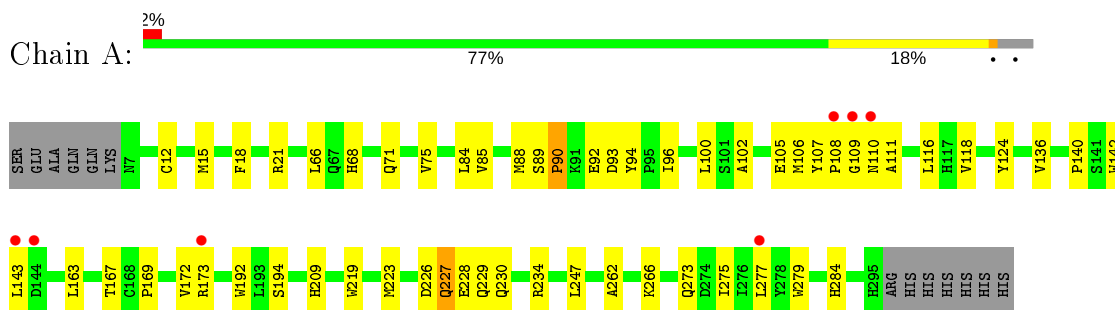
- Molecule 8 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
8	A	64	Total O 64 64	0	0
8	B	15	Total O 15 15	0	0
8	C	20	Total O 20 20	0	0
8	D	30	Total O 30 30	0	0

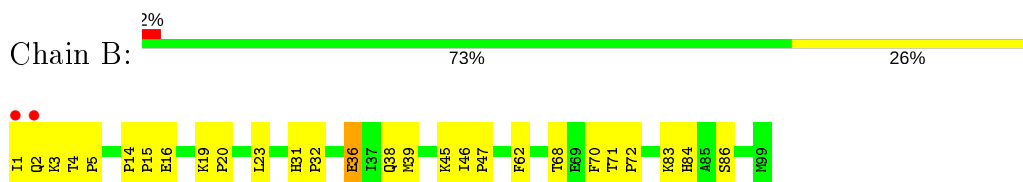
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

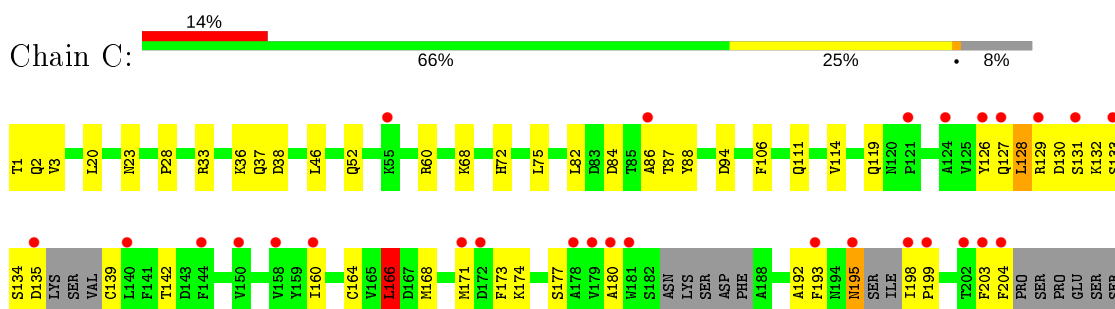
- Molecule 1: Antigen-presenting glycoprotein CD1d1



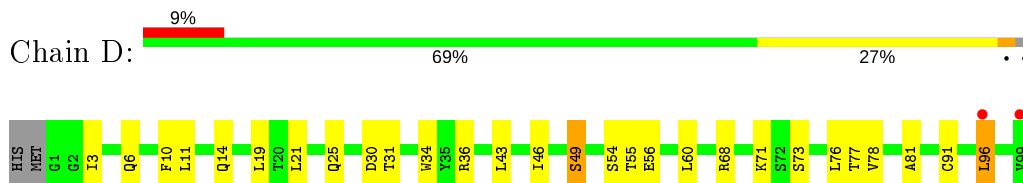
- Molecule 2: Beta-2-microglobulin

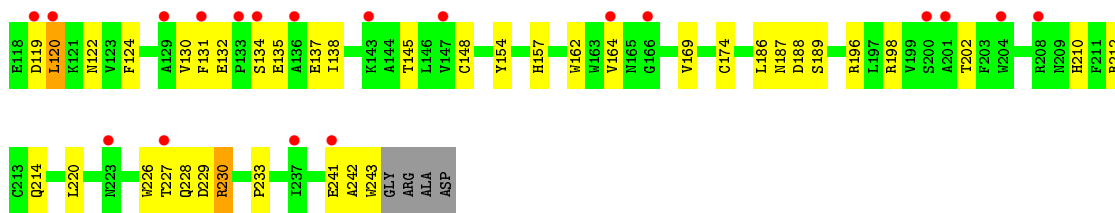


- Molecule 3: NKT TCR Valpha14 chain




- Molecule 4: NKT TCR autoreactive-Vbeta6 chain





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

Chain E:  100%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.52Å 94.52Å 289.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.86 – 2.50 60.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (89.86-2.50) 97.8 (60.69-2.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.273 , 0.318 0.265 , 0.308	Depositor DCC
$R_{free}$ test set	2301 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LGN, 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	0.66	2/2394 (0.1%)	0.55	2/3255 (0.1%)
2	B	0.35	0/840	0.52	0/1140
3	C	0.37	0/1501	0.59	2/2035 (0.1%)
4	D	0.44	0/1947	0.59	3/2640 (0.1%)
All	All	0.51	2/6682 (0.0%)	0.57	7/9070 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLU	CD-OE2	-20.95	1.02	1.25
1	A	12	CYS	CB-SG	-5.70	1.72	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GLU	OE1-CD-OE2	9.35	134.52	123.30
3	C	195	ASN	N-CA-C	-8.36	88.44	111.00
1	A	105	GLU	CG-CD-OE2	-6.31	105.68	118.30
4	D	3	ILE	O-C-N	6.07	132.41	122.70
3	C	166	LEU	CA-CB-CG	5.72	128.46	115.30
4	D	3	ILE	CA-C-N	-5.20	105.77	117.20
4	D	119	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2324	0	2220	52	3
2	B	814	0	788	60	0
3	C	1478	0	1420	105	0
4	D	1900	0	1831	109	0
5	E	28	0	25	0	0
6	A	28	0	26	0	0
7	A	79	0	109	0	0
8	A	64	0	0	1	0
8	B	15	0	0	0	0
8	C	20	0	0	0	0
8	D	30	0	0	2	0
All	All	6780	0	6419	295	3

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 23.

All (295) 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)
3:C:203:PHE:O	3:C:204:PHE:CD2	1.86	1.29
4:D:210:HIS:NE2	4:D:241:GLU:CG	1.90	1.25
4:D:19:LEU:CB	4:D:78:VAL:HB	1.67	1.24
2:B:38:GLN:NE2	2:B:45:LYS:HE2	1.53	1.23
3:C:164:CYS:SG	4:D:174:CYS:SG	1.23	1.21
2:B:2:GLN:HB3	2:B:31:HIS:CB	1.73	1.18
4:D:186:LEU:O	4:D:186:LEU:HD12	1.42	1.17
3:C:128:LEU:H	3:C:128:LEU:CD1	1.59	1.16
3:C:203:PHE:CE2	3:C:204:PHE:O	2.03	1.12
4:D:210:HIS:NE2	4:D:241:GLU:HG2	1.49	1.11
3:C:128:LEU:HA	3:C:129:ARG:HB2	1.31	1.11
4:D:226:TRP:CH2	4:D:230:ARG:O	2.04	1.10
3:C:52:GLN:HA	3:C:68:LYS:HG3	1.15	1.10
2:B:2:GLN:HG2	2:B:31:HIS:CD2	1.86	1.10
3:C:128:LEU:H	3:C:128:LEU:HD13	1.10	1.10
2:B:38:GLN:HE22	2:B:45:LYS:CE	1.65	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:GLN:CG	2:B:31:HIS:CD2	2.37	1.07
2:B:2:GLN:HB3	2:B:31:HIS:HB3	1.10	1.07
2:B:2:GLN:CB	2:B:31:HIS:CD2	2.38	1.07
3:C:128:LEU:HD22	3:C:128:LEU:O	1.55	1.06
2:B:38:GLN:HE22	2:B:45:LYS:HE2	0.89	1.05
4:D:19:LEU:HB2	4:D:78:VAL:CB	1.87	1.05
4:D:227:THR:HG22	4:D:227:THR:O	1.53	1.04
2:B:23:LEU:HB2	2:B:70:PHE:CD2	1.94	1.03
3:C:128:LEU:HD23	4:D:131:PHE:CD2	1.93	1.03
2:B:2:GLN:HB2	2:B:31:HIS:HD2	1.18	1.03
3:C:126:TYR:CD1	4:D:137:GLU:HB2	1.94	1.02
2:B:2:GLN:HB2	2:B:31:HIS:CD2	1.94	1.02
2:B:2:GLN:CB	2:B:31:HIS:HB3	1.89	1.02
3:C:126:TYR:CE1	4:D:137:GLU:HB2	1.95	1.01
4:D:14:GLN:OE1	4:D:120:LEU:HD23	1.61	1.01
3:C:129:ARG:N	3:C:130:ASP:HB2	1.79	0.97
1:A:275:ILE:HG22	1:A:277:LEU:CD1	1.94	0.97
2:B:23:LEU:HB2	2:B:70:PHE:CE2	2.01	0.96
4:D:226:TRP:HH2	4:D:230:ARG:O	1.42	0.96
2:B:1:ILE:CB	2:B:86:SER:HB3	1.96	0.95
2:B:2:GLN:CB	2:B:31:HIS:HD2	1.77	0.94
3:C:129:ARG:N	3:C:130:ASP:CB	2.30	0.94
1:A:227:GLN:HE21	1:A:229:GLN:HE22	1.08	0.93
2:B:2:GLN:HG2	2:B:31:HIS:CG	2.04	0.93
3:C:130:ASP:H	4:D:131:PHE:HD2	1.14	0.92
3:C:128:LEU:C	3:C:128:LEU:HD22	1.90	0.92
4:D:11:LEU:HD21	4:D:19:LEU:HD12	1.50	0.92
3:C:131:SER:OG	4:D:132:GLU:OE1	1.87	0.91
4:D:19:LEU:HB2	4:D:78:VAL:HB	0.91	0.91
4:D:21:LEU:CD1	4:D:34:TRP:CH2	2.53	0.90
1:A:279:TRP:O	1:A:284:HIS:ND1	2.05	0.89
1:A:89:SER:OG	1:A:90:PRO:HD3	1.70	0.89
3:C:128:LEU:N	3:C:128:LEU:CD1	2.30	0.89
1:A:275:ILE:CG2	1:A:277:LEU:CD1	2.52	0.88
3:C:128:LEU:HD13	3:C:128:LEU:O	1.73	0.88
3:C:126:TYR:CE1	4:D:137:GLU:CB	2.56	0.88
3:C:168:MET:O	3:C:171:MET:O	1.91	0.86
3:C:130:ASP:N	4:D:131:PHE:HD2	1.72	0.86
2:B:1:ILE:CB	2:B:86:SER:N	2.38	0.86
3:C:129:ARG:H	3:C:130:ASP:HB2	1.39	0.86
4:D:226:TRP:CZ3	4:D:230:ARG:O	2.30	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:OE1	8:A:358:HOH:O	1.94	0.84
2:B:46:ILE:HG23	2:B:47:PRO:HD2	1.57	0.84
2:B:2:GLN:N	2:B:31:HIS:O	2.10	0.84
2:B:2:GLN:CB	2:B:31:HIS:CB	2.54	0.82
3:C:129:ARG:CA	3:C:130:ASP:HB3	2.10	0.82
3:C:129:ARG:HA	3:C:130:ASP:HB3	1.61	0.82
2:B:38:GLN:HE21	2:B:45:LYS:HG2	1.42	0.82
3:C:203:PHE:O	3:C:204:PHE:CG	2.32	0.82
1:A:140:PRO:HD2	1:A:143:LEU:HD11	1.62	0.81
3:C:37:GLN:O	3:C:86:ALA:HB1	1.80	0.81
3:C:128:LEU:CD2	3:C:128:LEU:O	2.29	0.80
3:C:198:ILE:HG23	3:C:199:PRO:HD2	1.64	0.80
3:C:129:ARG:H	3:C:130:ASP:CB	1.90	0.80
2:B:3:LYS:O	2:B:86:SER:CB	2.30	0.80
4:D:186:LEU:O	4:D:186:LEU:CD1	2.27	0.79
3:C:52:GLN:CA	3:C:68:LYS:HG3	2.05	0.79
3:C:126:TYR:HE1	4:D:137:GLU:HA	1.47	0.79
4:D:145:THR:HG22	4:D:198:ARG:HB2	1.62	0.79
2:B:2:GLN:CB	2:B:31:HIS:CG	2.66	0.79
3:C:198:ILE:HG22	3:C:199:PRO:N	1.97	0.78
2:B:46:ILE:HD13	2:B:68:THR:HG21	1.64	0.78
4:D:21:LEU:HD13	4:D:34:TRP:CH2	2.19	0.77
3:C:130:ASP:HA	4:D:131:PHE:CD2	2.19	0.77
4:D:227:THR:CG2	4:D:227:THR:O	2.30	0.77
1:A:109:GLY:O	1:A:110:ASN:HB2	1.85	0.76
3:C:160:ILE:HD13	3:C:193:PHE:HB3	1.68	0.76
1:A:169:PRO:O	1:A:173:ARG:HG3	1.85	0.75
3:C:129:ARG:CA	3:C:130:ASP:CB	2.64	0.75
3:C:38:ASP:HA	3:C:86:ALA:HB2	1.67	0.75
2:B:1:ILE:CB	2:B:86:SER:CB	2.65	0.74
1:A:227:GLN:NE2	1:A:229:GLN:HE22	1.83	0.74
3:C:126:TYR:CE1	4:D:137:GLU:CA	2.71	0.74
3:C:128:LEU:N	3:C:128:LEU:HD13	1.85	0.73
2:B:2:GLN:CG	2:B:31:HIS:HD2	1.97	0.73
3:C:203:PHE:CG	3:C:204:PHE:N	2.56	0.73
3:C:38:ASP:HA	3:C:86:ALA:CB	2.18	0.72
1:A:275:ILE:CG2	1:A:277:LEU:HD11	2.19	0.72
2:B:1:ILE:CB	2:B:86:SER:CA	2.68	0.72
4:D:130:VAL:HG11	4:D:242:ALA:HB2	1.73	0.71
3:C:131:SER:O	4:D:130:VAL:O	2.09	0.71
2:B:2:GLN:HB3	2:B:31:HIS:C	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:SER:HB2	4:D:54:SER:O	1.90	0.70
3:C:126:TYR:CE1	4:D:137:GLU:HA	2.27	0.70
3:C:126:TYR:HE1	4:D:137:GLU:CA	2.04	0.69
4:D:187:ASN:O	4:D:188:ASP:CG	2.30	0.69
3:C:198:ILE:CG2	3:C:199:PRO:N	2.56	0.69
3:C:128:LEU:CA	3:C:129:ARG:HB2	2.16	0.69
3:C:52:GLN:HA	3:C:68:LYS:CG	2.09	0.69
4:D:145:THR:HG22	4:D:198:ARG:CB	2.22	0.69
1:A:140:PRO:HD2	1:A:143:LEU:CD1	2.23	0.69
4:D:6:GLN:NE2	4:D:91:CYS:H	1.91	0.69
2:B:2:GLN:CG	2:B:31:HIS:CG	2.72	0.68
3:C:33:ARG:NH1	4:D:100:ARG:O	2.23	0.68
4:D:21:LEU:CD1	4:D:34:TRP:CZ2	2.76	0.68
3:C:130:ASP:OD1	3:C:134:SER:O	2.12	0.67
3:C:23:ASN:OD1	3:C:72:HIS:HD2	1.78	0.67
3:C:128:LEU:CD1	3:C:128:LEU:O	2.42	0.67
2:B:38:GLN:NE2	2:B:45:LYS:HG2	2.09	0.67
2:B:38:GLN:NE2	2:B:45:LYS:CE	2.37	0.67
3:C:130:ASP:CA	4:D:131:PHE:HD2	2.08	0.67
3:C:37:GLN:C	3:C:86:ALA:HB1	2.15	0.67
2:B:2:GLN:HB3	2:B:31:HIS:CG	2.30	0.66
4:D:154:TYR:CE1	4:D:188:ASP:HA	2.30	0.66
3:C:164:CYS:CB	4:D:174:CYS:SG	2.76	0.66
1:A:275:ILE:HG22	1:A:277:LEU:HD12	1.74	0.66
3:C:128:LEU:HB3	8:D:272:HOH:O	1.94	0.66
3:C:130:ASP:HA	4:D:131:PHE:CE2	2.31	0.66
2:B:46:ILE:CG2	2:B:47:PRO:HD2	2.26	0.65
4:D:130:VAL:CG1	4:D:242:ALA:HB2	2.27	0.65
2:B:3:LYS:O	2:B:86:SER:HB3	1.96	0.65
4:D:11:LEU:CD2	4:D:19:LEU:HD12	2.26	0.65
3:C:128:LEU:H	3:C:128:LEU:HD12	1.56	0.65
4:D:186:LEU:C	4:D:186:LEU:HD12	2.17	0.64
4:D:188:ASP:C	4:D:188:ASP:OD1	2.35	0.64
4:D:21:LEU:HD11	4:D:34:TRP:CH2	2.33	0.64
2:B:2:GLN:CG	2:B:31:HIS:HB3	2.28	0.64
3:C:132:LYS:O	3:C:133:SER:HB3	1.98	0.64
1:A:140:PRO:CD	1:A:143:LEU:HD11	2.29	0.63
4:D:19:LEU:CB	4:D:78:VAL:CB	2.61	0.63
3:C:128:LEU:HA	3:C:129:ARG:CB	2.15	0.62
3:C:177:SER:OG	4:D:196:ARG:CD	2.47	0.62
2:B:2:GLN:HB3	2:B:31:HIS:CA	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:ASP:CA	4:D:131:PHE:CD2	2.83	0.62
4:D:19:LEU:N	4:D:78:VAL:O	2.31	0.62
3:C:203:PHE:CD2	3:C:204:PHE:N	2.68	0.62
1:A:142:TRP:CZ3	1:A:143:LEU:HD23	2.35	0.61
4:D:120:LEU:HD11	4:D:220:LEU:HD21	1.82	0.61
3:C:129:ARG:N	3:C:130:ASP:HB3	2.10	0.61
4:D:19:LEU:O	4:D:77:THR:HA	2.01	0.61
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.66	0.60
4:D:186:LEU:HD11	4:D:189:SER:HA	1.82	0.60
1:A:18:PHE:HB2	1:A:96:ILE:HB	1.84	0.60
1:A:275:ILE:HG22	1:A:277:LEU:HD13	1.84	0.60
4:D:117:VAL:O	4:D:117:VAL:HG23	2.01	0.60
4:D:164:VAL:HG22	4:D:169:VAL:CG1	2.32	0.60
4:D:229:ASP:HB3	4:D:230:ARG:HE	1.66	0.60
3:C:198:ILE:HG23	3:C:199:PRO:CD	2.32	0.60
3:C:38:ASP:OD1	3:C:86:ALA:HB2	2.02	0.60
4:D:117:VAL:O	4:D:117:VAL:CG2	2.50	0.60
3:C:130:ASP:OD1	3:C:130:ASP:O	2.21	0.59
1:A:107:TYR:HB2	1:A:111:ALA:HB3	1.85	0.59
3:C:130:ASP:OD2	3:C:135:ASP:HA	2.03	0.59
3:C:198:ILE:CG2	3:C:199:PRO:CD	2.81	0.59
4:D:210:HIS:NE2	4:D:241:GLU:HG3	2.06	0.58
1:A:226:ASP:OD1	1:A:227:GLN:N	2.37	0.58
3:C:86:ALA:O	3:C:88:TYR:CE1	2.57	0.58
3:C:20:LEU:HD12	3:C:75:LEU:HD23	1.87	0.57
2:B:71:THR:O	2:B:71:THR:HG23	2.03	0.57
3:C:1:THR:HG23	3:C:3:VAL:H	1.69	0.57
3:C:126:TYR:O	3:C:139:CYS:HB2	2.04	0.57
2:B:2:GLN:H	2:B:32:PRO:HD3	1.68	0.57
1:A:142:TRP:CH2	1:A:143:LEU:HD23	2.39	0.57
4:D:30:ASP:OD2	4:D:71:LYS:HE3	2.05	0.57
3:C:192:ALA:O	3:C:193:PHE:CG	2.58	0.56
3:C:139:CYS:N	3:C:180:ALA:O	2.38	0.56
1:A:140:PRO:HG2	1:A:143:LEU:HD11	1.87	0.55
1:A:140:PRO:HG2	1:A:143:LEU:CD1	2.37	0.55
4:D:145:THR:HG22	4:D:198:ARG:CG	2.37	0.55
1:A:107:TYR:HB3	1:A:108:PRO:HD2	1.88	0.55
4:D:120:LEU:CD1	4:D:220:LEU:HD21	2.37	0.54
3:C:129:ARG:H	3:C:130:ASP:HB3	1.69	0.54
3:C:106:PHE:CE2	4:D:43:LEU:HD22	2.43	0.54
2:B:2:GLN:H	2:B:32:PRO:CD	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:LEU:HD23	4:D:131:PHE:CE2	2.42	0.53
2:B:2:GLN:CB	2:B:31:HIS:C	2.76	0.53
4:D:164:VAL:HG22	4:D:169:VAL:HG11	1.91	0.53
3:C:36:LYS:HB2	3:C:46:LEU:HD21	1.91	0.53
4:D:19:LEU:O	4:D:78:VAL:N	2.41	0.52
3:C:198:ILE:CG2	3:C:199:PRO:HD2	2.36	0.52
1:A:140:PRO:CG	1:A:143:LEU:HD11	2.39	0.52
1:A:140:PRO:HG2	1:A:143:LEU:HG	1.91	0.52
3:C:203:PHE:CZ	3:C:204:PHE:O	2.57	0.52
4:D:187:ASN:O	4:D:188:ASP:CB	2.57	0.52
1:A:223:MET:SD	1:A:228:GLU:HG2	2.50	0.52
1:A:102:ALA:HB2	1:A:116:LEU:HG	1.92	0.52
3:C:128:LEU:CG	3:C:128:LEU:O	2.58	0.52
4:D:154:TYR:CZ	4:D:188:ASP:HA	2.45	0.52
4:D:186:LEU:HD11	4:D:189:SER:CA	2.39	0.52
3:C:60:ARG:NH2	3:C:84:ASP:OD1	2.41	0.52
4:D:10:PHE:HB3	4:D:157:HIS:ND1	2.25	0.51
1:A:163:LEU:HA	1:A:167:THR:HB	1.93	0.51
4:D:212:ARG:NH1	4:D:214:GLN:OE1	2.44	0.51
2:B:71:THR:CG2	2:B:71:THR:O	2.59	0.51
2:B:19:LYS:O	2:B:72:PRO:HD2	2.11	0.51
3:C:127:GLN:O	4:D:134:SER:HB2	2.10	0.51
4:D:134:SER:OG	8:D:270:HOH:O	2.19	0.51
2:B:84:HIS:HD2	2:B:86:SER:OG	1.94	0.50
4:D:55:THR:O	4:D:55:THR:OG1	2.30	0.50
1:A:21:ARG:NH1	4:D:56:GLU:OE2	2.45	0.50
1:A:109:GLY:O	1:A:110:ASN:CB	2.57	0.50
2:B:39:MET:CB	2:B:46:ILE:HD12	2.41	0.50
4:D:21:LEU:HD12	4:D:34:TRP:CZ2	2.46	0.50
4:D:227:THR:O	4:D:228:GLN:NE2	2.45	0.50
1:A:140:PRO:HG2	1:A:143:LEU:CG	2.42	0.49
4:D:145:THR:CG2	4:D:198:ARG:HG3	2.41	0.49
4:D:96:LEU:HD12	4:D:96:LEU:O	2.12	0.49
1:A:142:TRP:CH2	1:A:143:LEU:CD2	2.96	0.49
4:D:19:LEU:CD2	4:D:81:ALA:HB2	2.42	0.49
1:A:84:LEU:O	1:A:88:MET:HG2	2.13	0.49
3:C:173:PHE:O	3:C:174:LYS:HG3	2.13	0.49
1:A:192:TRP:CE3	2:B:14:PRO:HG3	2.48	0.49
2:B:2:GLN:HB3	2:B:31:HIS:O	2.13	0.49
2:B:2:GLN:CA	2:B:31:HIS:O	2.61	0.48
3:C:38:ASP:HA	3:C:86:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:LEU:CB	2:B:70:PHE:CD2	2.83	0.48
3:C:192:ALA:C	3:C:193:PHE:CD2	2.86	0.48
1:A:219:TRP:HB3	1:A:266:LYS:HB2	1.95	0.47
2:B:23:LEU:CB	2:B:70:PHE:CE2	2.86	0.47
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.50	0.47
1:A:275:ILE:CG2	1:A:277:LEU:HD12	2.37	0.47
2:B:38:GLN:NE2	2:B:45:LYS:CG	2.78	0.47
4:D:154:TYR:CZ	4:D:188:ASP:HB2	2.49	0.47
3:C:177:SER:OG	4:D:196:ARG:HD2	2.16	0.46
4:D:230:ARG:HA	4:D:230:ARG:HD3	1.58	0.46
2:B:2:GLN:CB	2:B:31:HIS:O	2.64	0.46
4:D:145:THR:CG2	4:D:198:ARG:CG	2.94	0.46
4:D:122:ASN:O	4:D:124:PHE:CD2	2.68	0.46
4:D:130:VAL:HG11	4:D:242:ALA:CB	2.45	0.46
1:A:275:ILE:HG21	1:A:277:LEU:HD11	1.95	0.45
3:C:126:TYR:CZ	4:D:137:GLU:HG3	2.51	0.45
4:D:36:ARG:HB2	4:D:46:ILE:HD11	1.99	0.45
1:A:106:MET:SD	1:A:172:VAL:HG21	2.56	0.45
1:A:262:ALA:HA	1:A:277:LEU:O	2.16	0.45
3:C:28:PRO:HG2	3:C:94:ASP:O	2.16	0.45
4:D:60:LEU:HG	4:D:60:LEU:O	2.16	0.45
4:D:229:ASP:CB	4:D:230:ARG:HE	2.28	0.45
4:D:19:LEU:HB3	4:D:78:VAL:HB	1.82	0.45
2:B:2:GLN:CG	2:B:31:HIS:CB	2.91	0.45
4:D:186:LEU:CD1	4:D:189:SER:HB3	2.46	0.45
3:C:131:SER:HA	3:C:132:LYS:HA	1.60	0.45
3:C:1:THR:OG1	3:C:2:GLN:N	2.50	0.45
3:C:126:TYR:HB3	4:D:134:SER:HB3	1.99	0.45
3:C:166:LEU:HB3	4:D:174:CYS:HB2	1.98	0.45
2:B:39:MET:HB2	2:B:46:ILE:HD12	1.99	0.44
3:C:198:ILE:HA	3:C:199:PRO:HD3	1.77	0.44
2:B:14:PRO:HA	2:B:15:PRO:HD3	1.89	0.44
3:C:130:ASP:CG	3:C:134:SER:O	2.55	0.44
4:D:11:LEU:HD21	4:D:19:LEU:CD1	2.35	0.44
4:D:164:VAL:HG23	4:D:164:VAL:O	2.18	0.44
2:B:16:GLU:O	2:B:72:PRO:HG2	2.18	0.44
3:C:128:LEU:N	3:C:128:LEU:HD12	2.18	0.44
4:D:220:LEU:HD22	4:D:233:PRO:HG2	2.00	0.44
1:A:92:GLU:HG3	1:A:142:TRP:CZ2	2.53	0.44
4:D:21:LEU:O	4:D:21:LEU:HD12	2.18	0.44
3:C:87:THR:OG1	3:C:111:GLN:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:LEU:HD23	4:D:81:ALA:HB2	1.99	0.43
1:A:140:PRO:CD	1:A:143:LEU:CD1	2.90	0.43
2:B:36:GLU:HB3	2:B:83:LYS:HB2	2.01	0.43
3:C:192:ALA:O	3:C:193:PHE:CD2	2.71	0.43
1:A:230:GLN:HA	1:A:230:GLN:OE1	2.19	0.43
1:A:194:SER:OG	1:A:209:HIS:HE1	2.02	0.43
4:D:135:GLU:HA	4:D:138:ILE:HD13	2.01	0.43
1:A:234:ARG:HD3	1:A:247:LEU:HD21	2.01	0.43
1:A:68:HIS:HA	1:A:71:GLN:OE1	2.19	0.42
4:D:145:THR:HG23	4:D:198:ARG:HG3	1.99	0.42
4:D:148:CYS:HB2	4:D:162:TRP:CH2	2.54	0.42
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.87	0.42
3:C:192:ALA:C	3:C:193:PHE:CG	2.93	0.42
4:D:34:TRP:CD1	4:D:76:LEU:HB2	2.54	0.42
1:A:85:VAL:HG11	1:A:94:TYR:CE1	2.55	0.42
3:C:23:ASN:OD1	3:C:72:HIS:CD2	2.66	0.41
3:C:82:LEU:HA	3:C:114:VAL:HG11	2.01	0.41
4:D:148:CYS:HB2	4:D:162:TRP:CZ2	2.55	0.41
3:C:128:LEU:HB2	3:C:129:ARG:C	2.40	0.41
4:D:186:LEU:O	4:D:186:LEU:CG	2.68	0.41
4:D:68:ARG:HD2	4:D:73:SER:O	2.21	0.41
1:A:219:TRP:CE3	1:A:266:LYS:HG3	2.56	0.41
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.85	0.41
3:C:52:GLN:CD	3:C:68:LYS:HB2	2.40	0.41
1:A:15:MET:HG2	2:B:62:PHE:CE2	2.52	0.41
1:A:100:LEU:HG	1:A:118:VAL:HG22	2.02	0.41
2:B:4:THR:HA	2:B:5:PRO:HD3	1.97	0.41
4:D:122:ASN:N	4:D:122:ASN:HD22	2.17	0.40
4:D:122:ASN:N	4:D:122:ASN:ND2	2.69	0.40
3:C:203:PHE:O	3:C:204:PHE:CE2	2.59	0.40
4:D:21:LEU:HD11	4:D:34:TRP:CZ2	2.56	0.40
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.87	0.40
3:C:126:TYR:HE2	3:C:142:THR:CG2	2.34	0.40

All (3) 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)
1:A:93:ASP:OD2	1:A:273:GLN:NE2[6_424]	1.50	0.70
1:A:93:ASP:OD2	1:A:273:GLN:CD[6_424]	1.80	0.40
1:A:93:ASP:OD2	1:A:273:GLN:OE1[6_424]	2.00	0.20

## 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	287/302 (95%)	280 (98%)	6 (2%)	1 (0%)	41	61
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	183/207 (88%)	174 (95%)	9 (5%)	0	100	100
4	D	237/245 (97%)	226 (95%)	11 (5%)	0	100	100
All	All	804/853 (94%)	774 (96%)	29 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/264 (96%)	250 (99%)	2 (1%)	81	93
2	B	92/93 (99%)	91 (99%)	1 (1%)	73	89
3	C	170/186 (91%)	167 (98%)	3 (2%)	59	81
4	D	207/211 (98%)	198 (96%)	9 (4%)	29	53
All	All	721/754 (96%)	706 (98%)	15 (2%)	53	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	227	GLN
2	B	36	GLU
3	C	128	LEU
3	C	166	LEU
3	C	195	ASN
4	D	25	GLN
4	D	31	THR
4	D	49	SER
4	D	96	LEU
4	D	113	ARG
4	D	120	LEU
4	D	202	THR
4	D	230	ARG
4	D	243	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	134	GLN
1	A	154	GLN
1	A	186	GLN
1	A	209	HIS
1	A	229	GLN
1	A	248	GLN
2	B	2	GLN
2	B	29	GLN
2	B	31	HIS
2	B	38	GLN
2	B	84	HIS
3	C	72	HIS
3	C	119	GLN
4	D	6	GLN
4	D	84	ASN
4	D	122	ASN
4	D	228	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	1	1,5	14,14,15	0.63	0	17,19,21	1.33	2 (11%)
5	NAG	E	2	5	14,14,15	0.72	0	17,19,21	1.45	2 (11%)

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	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	C1-O5-C5	-3.88	106.94	112.19
5	E	1	NAG	O4-C4-C3	-3.72	101.76	110.35
5	E	1	NAG	C4-C3-C2	2.86	115.20	111.02
5	E	2	NAG	C4-C3-C2	2.45	114.61	111.02

There are no chirality outliers.

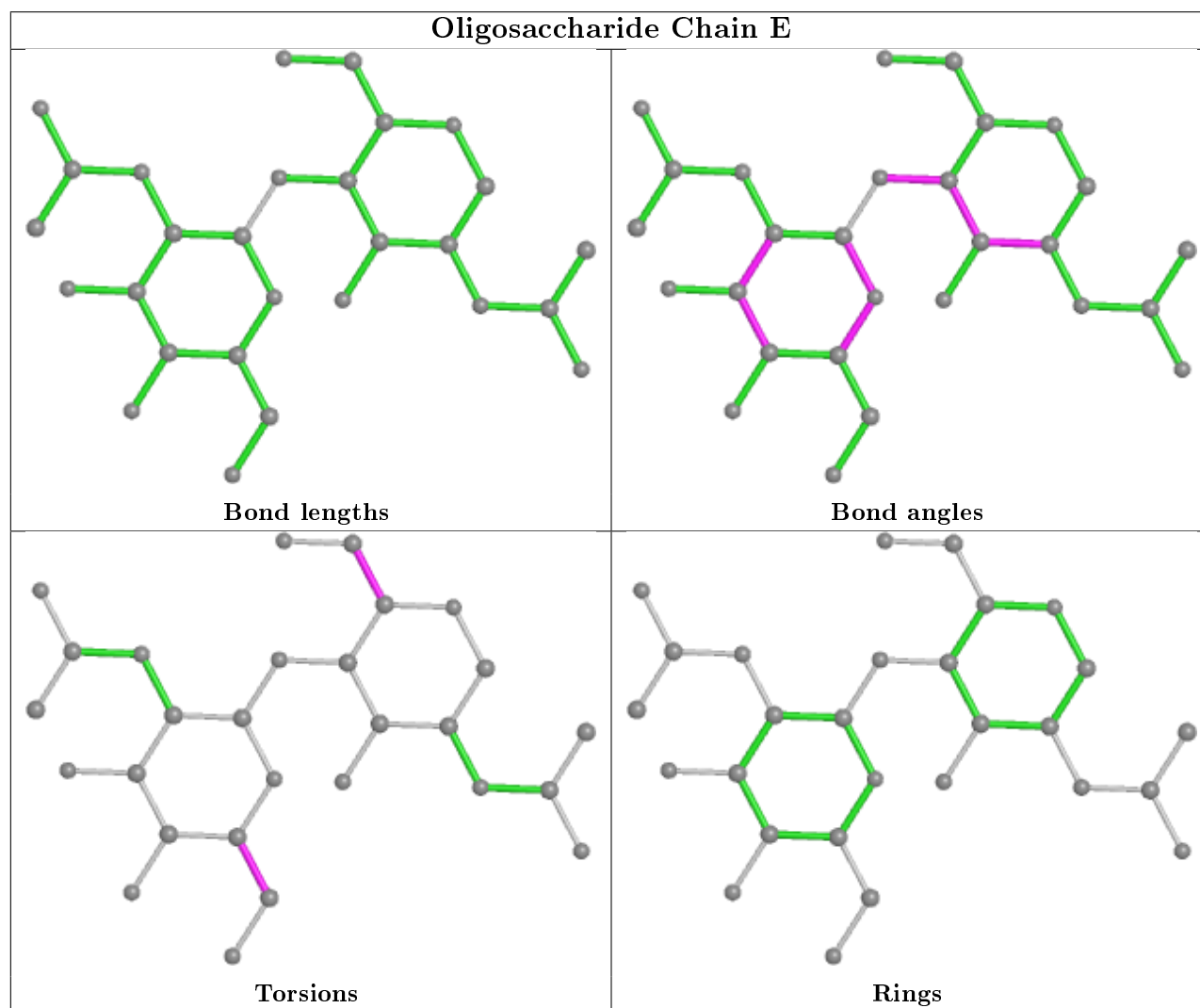
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	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](#)

3 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
7	LGN	A	307	-	80,81,83	1.60	11 (13%)	99,101,103	0.96	8 (8%)
6	NAG	A	303	1	14,14,15	0.42	0	17,19,21	2.13	3 (17%)
6	NAG	A	304	1	14,14,15	0.45	0	17,19,21	1.14	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LGN	A	307	-	-	28/65/125/127	0/3/3/3
6	NAG	A	303	1	-	2/6/23/26	0/1/1/1
6	NAG	A	304	1	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	307	LGN	CAP-CAO	-5.98	1.39	1.50
7	A	307	LGN	O5-C1	-4.38	1.30	1.41
7	A	307	LGN	OCK-CCL	-4.29	1.33	1.44
7	A	307	LGN	O5-C5	-4.20	1.34	1.44
7	A	307	LGN	C3-C4	3.93	1.62	1.52
7	A	307	LGN	OBY-CBX	3.89	1.51	1.41
7	A	307	LGN	OBY-CCF	3.81	1.53	1.44
7	A	307	LGN	OAQ-CAP	-2.77	1.38	1.43
7	A	307	LGN	CCO-CCL	-2.15	1.48	1.53
7	A	307	LGN	O4-C4	-2.13	1.38	1.43
7	A	307	LGN	C4-C5	2.07	1.58	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	303	NAG	C1-O5-C5	7.02	121.71	112.19
7	A	307	LGN	CCH-O4-C4	-3.42	109.51	117.96
7	A	307	LGN	CBX-OCR-CCQ	-3.40	109.54	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	304	NAG	C1-O5-C5	3.33	116.71	112.19
7	A	307	LGN	OAQ-CAP-CAR	3.00	115.88	107.93
6	A	303	NAG	C4-C3-C2	-2.68	107.09	111.02
6	A	303	NAG	O5-C5-C6	2.42	111.00	107.20
7	A	307	LGN	OAQ-CAP-CAO	2.41	117.31	110.85
7	A	307	LGN	CBU-O1-C1	-2.15	109.54	113.74
7	A	307	LGN	C1-O5-C5	-2.13	109.50	113.69
7	A	307	LGN	CBX-OBY-CCF	-2.13	109.50	113.69
7	A	307	LGN	CCH-OCK-CCL	-2.13	109.51	113.69

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	307	LGN	C2-C1-O1-CBU
7	A	307	LGN	O5-C1-O1-CBU
7	A	307	LGN	CAN-CAO-CAP-CAR
7	A	307	LGN	CAO-CAP-CAR-NAS
7	A	307	LGN	CAO-CAP-CAR-CBU
7	A	307	LGN	OBY-CCF-CDA-ODA
6	A	303	NAG	O5-C5-C6-O6
7	A	307	LGN	CCD-CCF-CDA-ODA
6	A	304	NAG	C8-C7-N2-C2
6	A	304	NAG	O7-C7-N2-C2
6	A	303	NAG	C4-C5-C6-O6
7	A	307	LGN	O5-C5-C6-O6
7	A	307	LGN	C4-C5-C6-O6
7	A	307	LGN	CAE-CAF-CAG-CAH
7	A	307	LGN	CBB-CBC-CBD-CBE
7	A	307	LGN	CAF-CAG-CAH-CAI
7	A	307	LGN	CAB-CAC-CAD-CAE
7	A	307	LGN	CAJ-CAK-CAL-CAM
7	A	307	LGN	CAC-CAD-CAE-CAF
7	A	307	LGN	CBE-CBF-CBG-CBH
7	A	307	LGN	CBA-CBB-CBC-CBD
7	A	307	LGN	CBO-CBP-CBQ-CBR
7	A	307	LGN	CAN-CAO-CAP-OAQ
7	A	307	LGN	OAQ-CAP-CAR-NAS
7	A	307	LGN	CAD-CAE-CAF-CAG
7	A	307	LGN	CAX-CAY-CAZ-CBA
7	A	307	LGN	CBC-CBD-CBE-CBF
7	A	307	LGN	CBM-CBN-CBO-CBP

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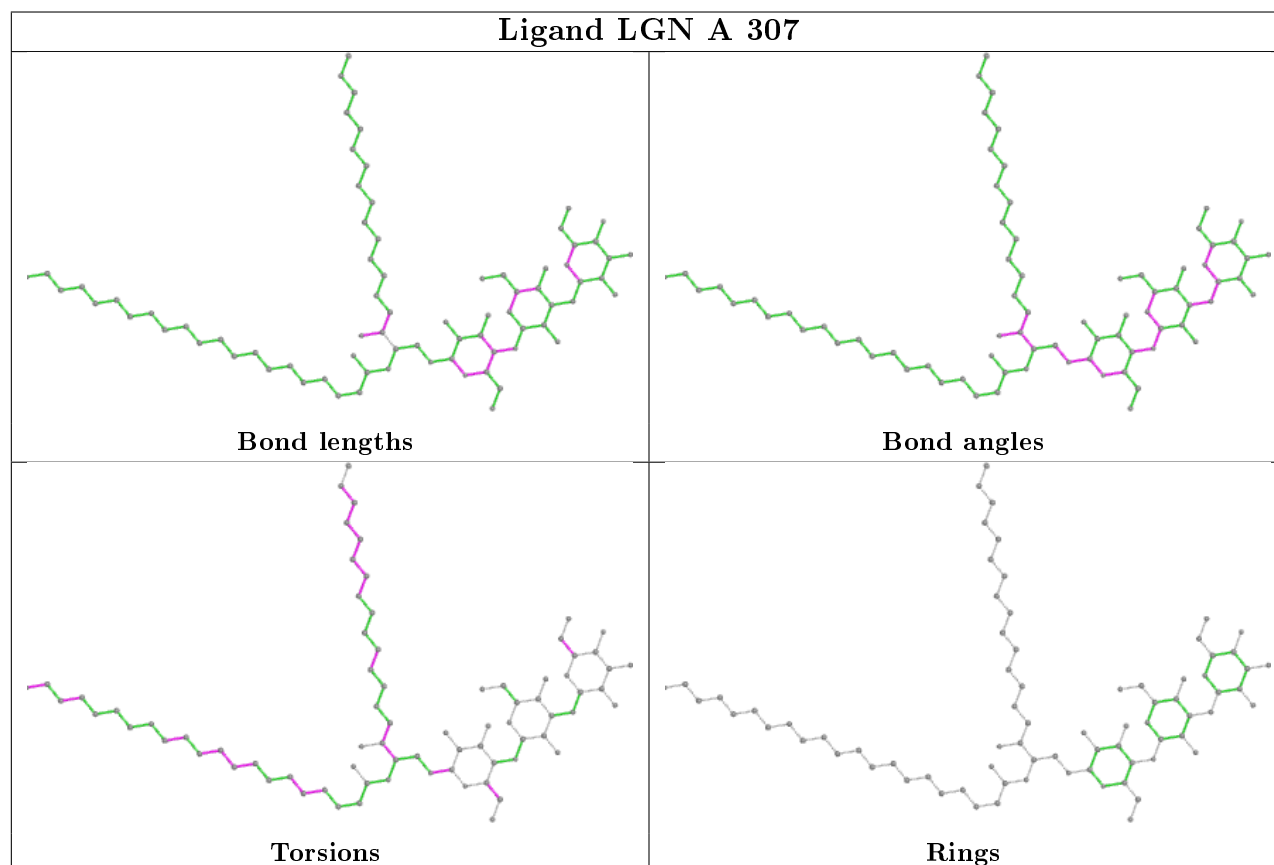
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Mol	Chain	Res	Type	Atoms
7	A	307	LGN	CBK-CBL-CBM-CBN
7	A	307	LGN	CAA-CAB-CAC-CAD
7	A	307	LGN	CBN-CBO-CBP-CBQ
7	A	307	LGN	CAW-CAX-CAY-CAZ

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 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	289/302 (95%)	0.33	7 (2%) 59 62	35, 46, 58, 64	5 (1%)
2	B	99/99 (100%)	0.40	2 (2%) 65 68	37, 48, 60, 62	1 (1%)
3	C	191/207 (92%)	0.90	28 (14%) 2 2	35, 55, 105, 120	5 (2%)
4	D	239/245 (97%)	0.72	22 (9%) 9 9	37, 68, 85, 89	5 (2%)
All	All	818/853 (95%)	0.59	59 (7%) 15 16	35, 51, 95, 120	16 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	7.9
2	B	2	GLN	5.6
3	C	126	TYR	5.5
3	C	193	PHE	5.4
3	C	129	ARG	4.7
4	D	133	PRO	4.4
3	C	178	ALA	4.2
3	C	86	ALA	4.0
3	C	150	VAL	3.9
3	C	140	LEU	3.9
3	C	203	PHE	3.8
3	C	202	THR	3.7
1	A	277	LEU	3.7
3	C	199	PRO	3.6
3	C	171	MET	3.5
4	D	143	LYS	3.4
3	C	158	VAL	3.4
4	D	200	SER	3.3
3	C	160	ILE	3.3
4	D	208	ARG	3.2
4	D	120	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	198	ILE	3.1
3	C	131	SER	3.1
1	A	143	LEU	2.8
1	A	109	GLY	2.8
4	D	129	ALA	2.8
1	A	144	ASP	2.8
1	A	110	ASN	2.7
3	C	127	GLN	2.7
4	D	134	SER	2.7
4	D	117	VAL	2.7
1	A	108	PRO	2.7
3	C	204	PHE	2.6
4	D	147	VAL	2.6
4	D	164	VAL	2.6
3	C	124	ALA	2.5
4	D	131	PHE	2.5
4	D	223	ASN	2.5
4	D	119	ASP	2.5
4	D	166	GLY	2.5
3	C	121	PRO	2.5
3	C	179	VAL	2.5
3	C	195	ASN	2.5
4	D	136	ALA	2.4
3	C	135	ASP	2.4
3	C	144	PHE	2.4
4	D	99	VAL	2.3
3	C	133	SER	2.3
4	D	201	ALA	2.2
3	C	172	ASP	2.2
4	D	241	GLU	2.2
3	C	55	LYS	2.2
3	C	180	ALA	2.2
4	D	204	TRP	2.1
4	D	227	THR	2.1
4	D	237	ILE	2.1
3	C	181	TRP	2.1
4	D	96	LEU	2.1
1	A	173	ARG	2.0

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

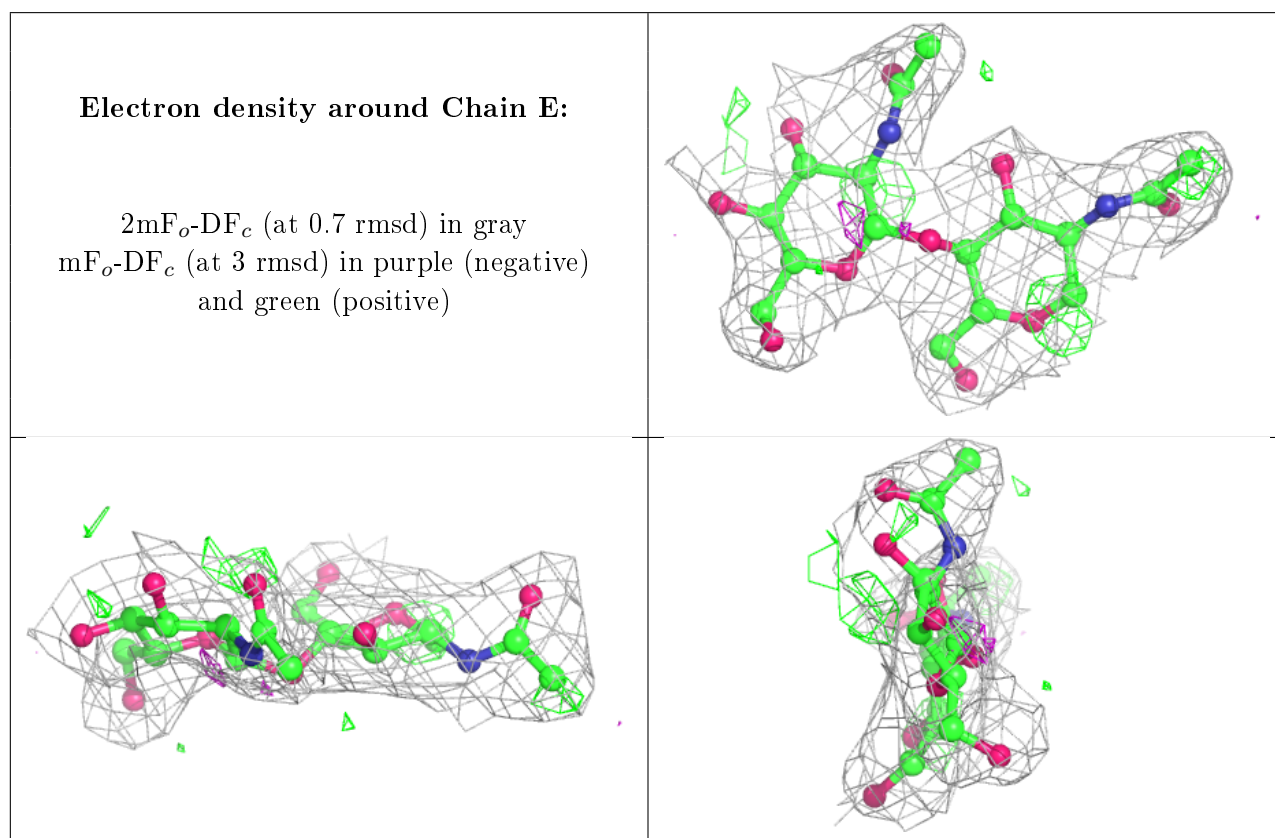
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	E	2	14/15	0.79	0.17	61,63,64,64	0
5	NAG	E	1	14/15	0.91	0.16	48,50,54,57	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

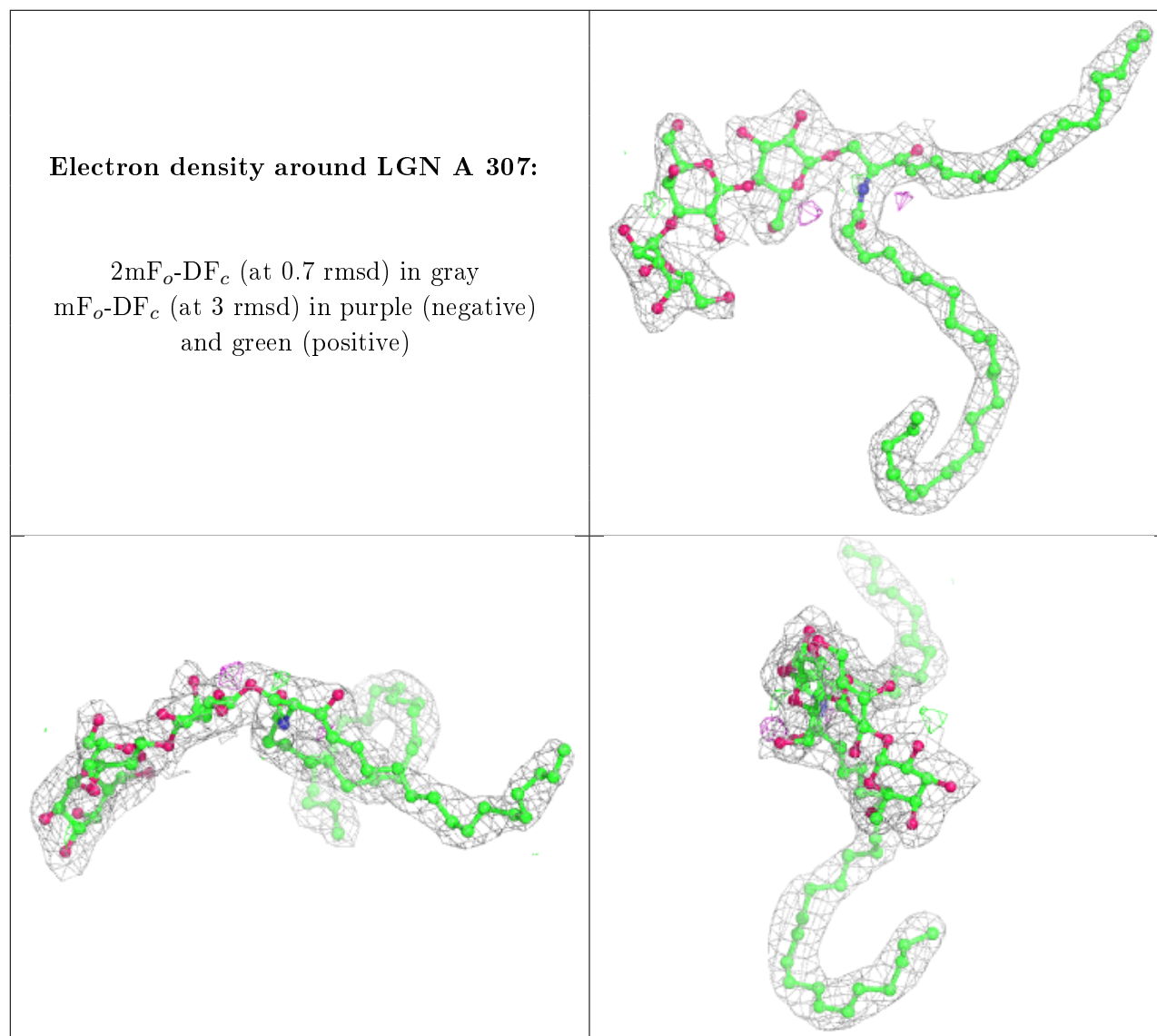
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	A	303	14/15	0.87	0.15	57,60,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	304	14/15	0.90	0.14	55,57,58,58	0
7	LGN	A	307	79/81	0.93	0.19	39,44,52,53	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.