



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 02:48 AM EDT

PDB ID : 4X6D  
Title : CD1a ternary complex with endogenous lipids and BK6 TCR  
Authors : Birkinshaw, R.W.; Rossjohn, J.  
Deposited on : 2014-12-08  
Resolution : 2.98 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.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

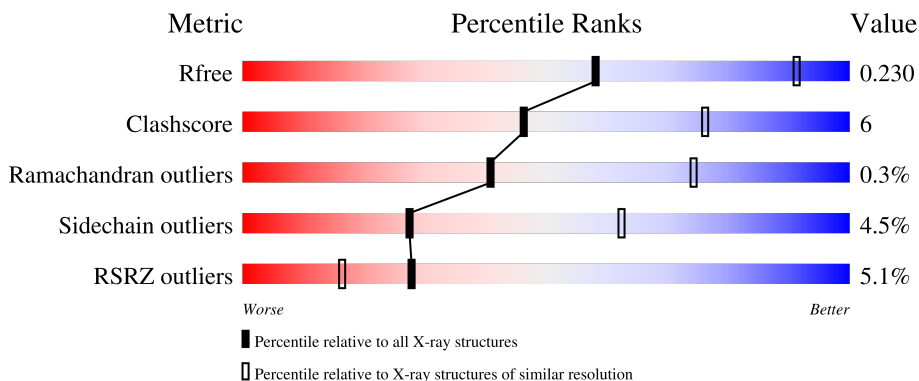
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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.



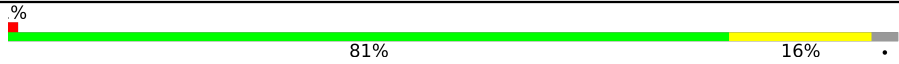

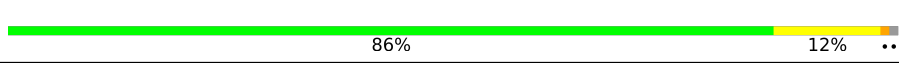

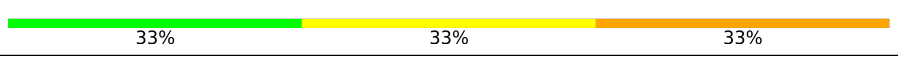
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div>
1	C	275	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div>
2	B	99	<div style="display: flex; align-items: center;"> <div style="width: 16%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div>
2	D	99	<div style="display: flex; align-items: center;"> <div style="width: 19%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div>
3	E	207	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	G	207	 <p>% 81% 16% •</p>
4	F	245	 <p>2% 84% 14% •</p>
4	H	245	 <p>86% 12% ••</p>
5	I	3	 <p>33% 67%</p>
5	J	3	 <p>33% 33% 33%</p>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12304 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 CD1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	Total	C	N	O	S	0	0	0
			2153	1379	375	391	8			
1	C	218	Total	C	N	O	S	0	0	0
			1787	1152	312	318	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ILE	THR	variant	UNP P06126
A	51	TRP	CYS	variant	UNP P06126
C	13	ILE	THR	variant	UNP P06126
C	51	TRP	CYS	variant	UNP P06126

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	86	Total	C	N	O	S	0	0	0
			719	463	119	135	2			
2	D	78	Total	C	N	O	S	0	0	0
			657	427	107	121	2			

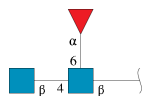
- Molecule 3 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	189	Total	C	N	O	S	0	0	0
			1474	924	238	302	10			
3	G	200	Total	C	N	O	S	0	0	0
			1560	975	253	322	10			

- Molecule 4 is a protein called TCR beta.

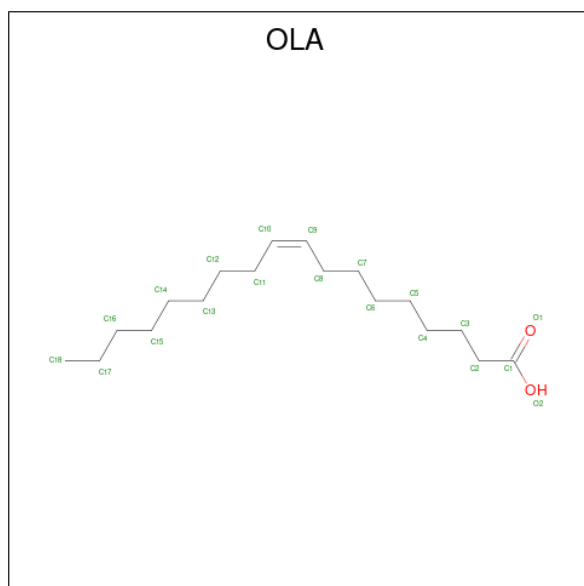
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	241	Total 1917	C 1216	N 333	O 358	S 10	0	0	0
4	H	242	Total 1922	C 1219	N 334	O 359	S 10	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



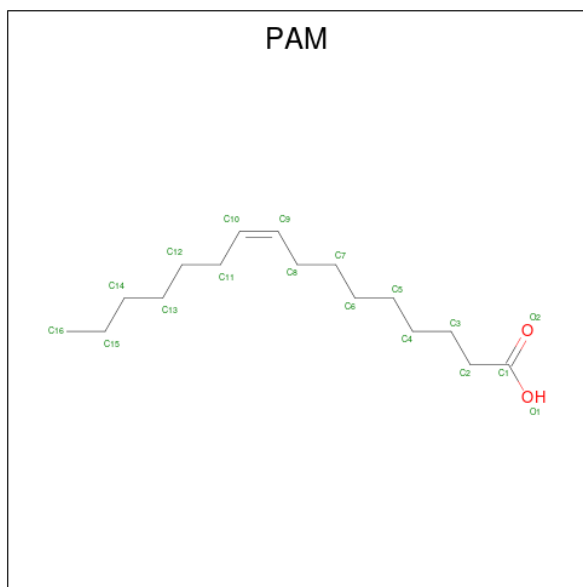
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	3	Total 38	C 22	N 2	O 14	0	0	0
5	J	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula:  $C_{18}H_{34}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	Total 20	C 18	O 2	0	0

- Molecule 7 is PALMITOLEIC ACID (three-letter code: PAM) (formula:  $C_{16}H_{30}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 18 16 2	0	0

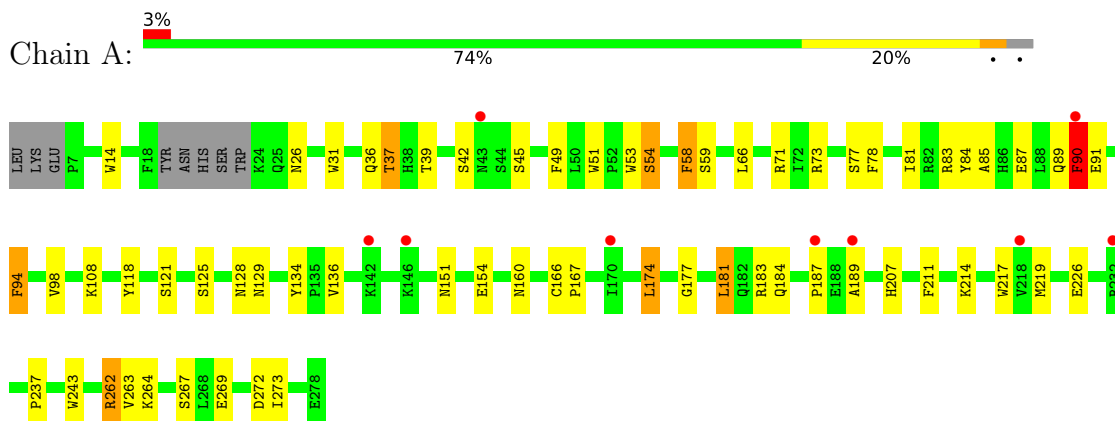
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total O 1 1	0	0

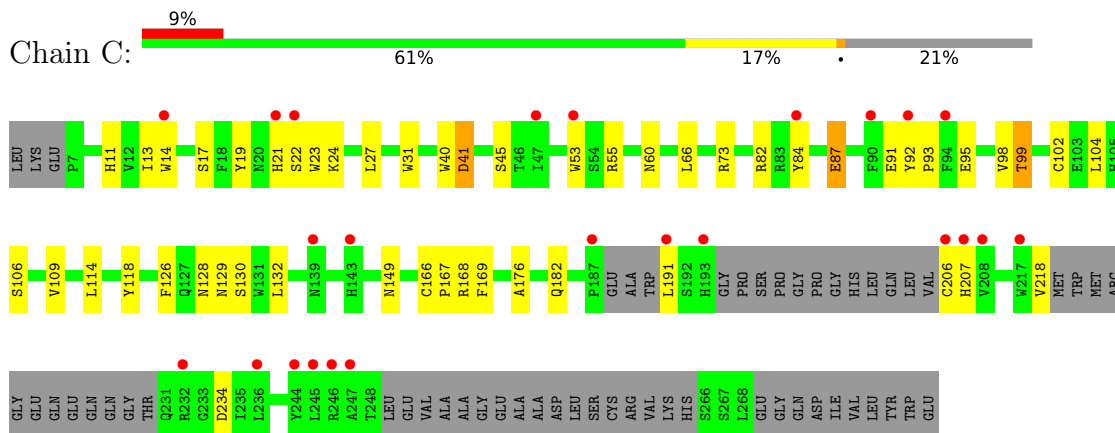
### 3 Residue-property plots [i](#)

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.

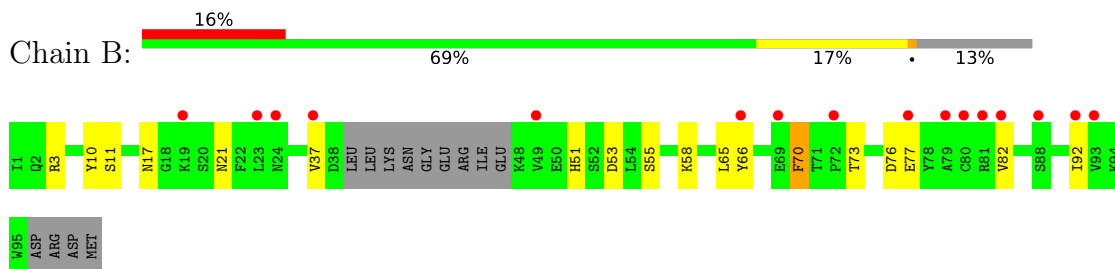
- Molecule 1: T-cell surface glycoprotein CD1a



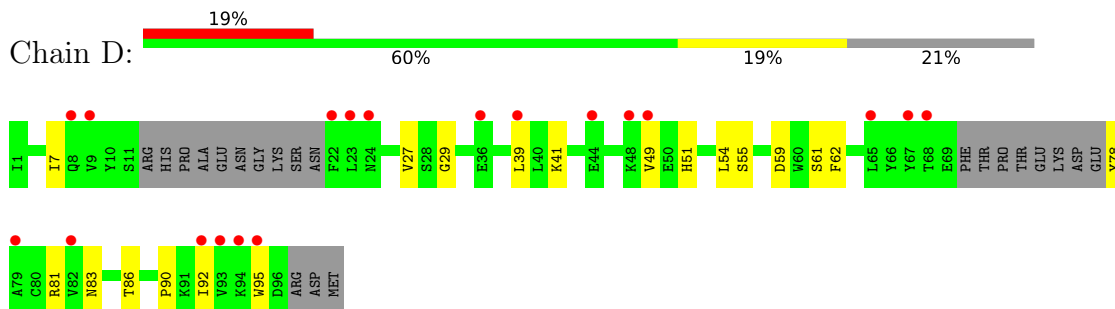
- Molecule 1: T-cell surface glycoprotein CD1a



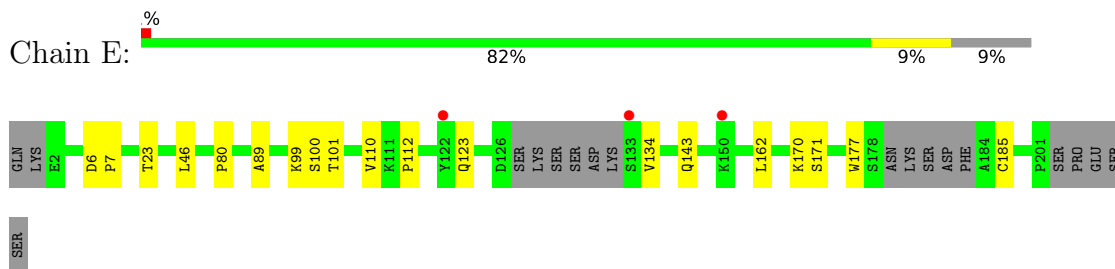
- Molecule 2: Beta-2-microglobulin



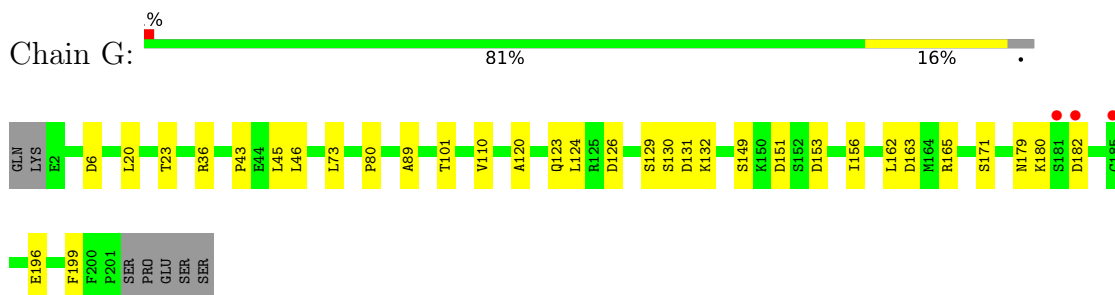
- Molecule 2: Beta-2-microglobulin



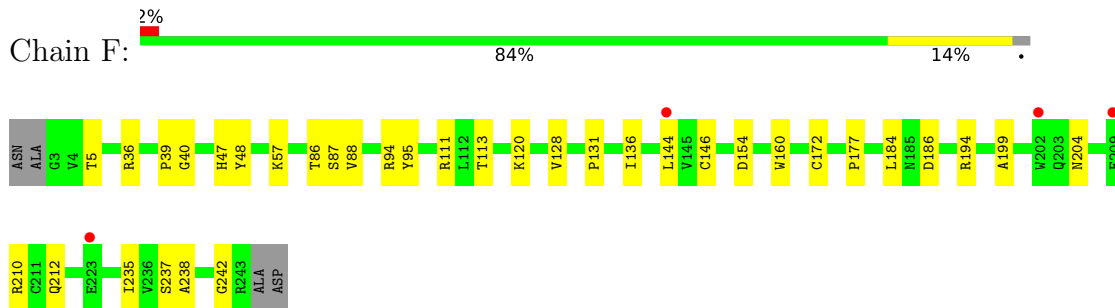
- Molecule 3: TCR alpha



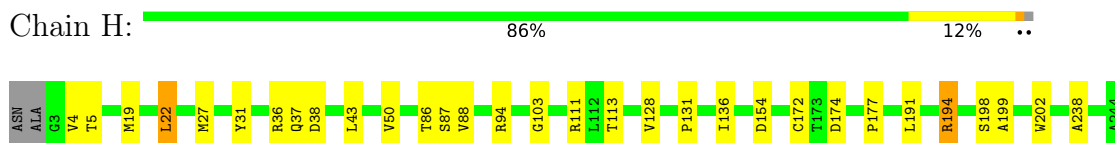
- Molecule 3: TCR alpha



- Molecule 4: TCR beta



- Molecule 4: TCR beta





ASP

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%

MAG1  
MAG2  
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 33% 33%

MAG1  
MAG2  
FUC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.13Å 126.32Å 226.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.98 48.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.98) 100.0 (48.00-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.96Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, $R_{free}$	0.177 , 0.229 0.179 , 0.230	Depositor DCC
$R_{free}$ test set	2663 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.8	Xtrriage
Anisotropy	0.406	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: PAM, OLA, NAG, FUC

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	0.38	0/2221	0.53	0/3021
1	C	0.32	0/1844	0.50	0/2503
2	B	0.32	0/741	0.46	0/1005
2	D	0.32	0/674	0.45	0/911
3	E	0.45	0/1507	0.59	0/2045
3	G	0.45	0/1596	0.59	0/2165
4	F	0.44	0/1970	0.58	0/2678
4	H	0.45	0/1975	0.61	1/2685 (0.0%)
All	All	0.41	0/12528	0.56	1/17013 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	22	LEU	CA-CB-CG	6.26	129.70	115.30

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	2153	0	2038	50	0
1	C	1787	0	1693	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	719	0	683	10	0
2	D	657	0	636	8	0
3	E	1474	0	1383	8	0
3	G	1560	0	1467	19	0
4	F	1917	0	1840	20	0
4	H	1922	0	1845	19	0
5	I	38	0	34	4	0
5	J	38	0	31	2	0
6	A	20	0	33	0	0
7	C	18	0	29	3	0
8	H	1	0	0	0	0
All	All	12304	0	11712	152	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 (152) 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:84:TYR:HD1	1:A:87:GLU:OE2	1.41	1.02
1:A:84:TYR:CD1	1:A:87:GLU:OE2	2.18	0.96
1:C:168:ARG:HD2	5:J:1:NAG:C8	2.06	0.84
1:A:51:TRP:O	1:A:54:SER:HB2	1.79	0.83
3:G:149:SER:HB2	3:G:156:ILE:HD12	1.60	0.83
1:A:84:TYR:HA	1:A:87:GLU:OE2	1.81	0.81
1:A:90:PHE:HD1	1:A:90:PHE:H	1.33	0.76
3:G:45:LEU:HD22	4:H:103:GLY:HA3	1.67	0.76
1:C:92:TYR:HB2	1:C:93:PRO:HD3	1.71	0.73
3:G:151:ASP:OD2	3:G:180:LYS:NZ	2.22	0.72
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.74	0.69
4:F:86:THR:HG23	4:F:113:THR:HA	1.77	0.67
4:F:120:LYS:NZ	4:F:186:ASP:OD2	2.29	0.65
2:D:29:GLY:HA2	2:D:61:SER:HB3	1.80	0.64
1:A:89:GLN:HA	1:A:89:GLN:OE1	1.97	0.63
4:H:86:THR:HG23	4:H:113:THR:HA	1.80	0.63
1:A:219:MET:HG2	1:A:226:GLU:HG3	1.82	0.62
1:A:81:ILE:O	1:A:85:ALA:N	2.34	0.61
1:A:94:PHE:HD2	1:A:118:TYR:HE1	1.47	0.60
3:G:163:ASP:OD2	3:G:165:ARG:NH1	2.35	0.60
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.84	0.60
1:A:37:THR:O	1:A:54:SER:OG	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:TYR:HD1	1:C:87:GLU:HG3	1.69	0.57
1:A:217:TRP:HB3	1:A:264:LYS:HB2	1.85	0.57
1:C:24:LYS:HE3	1:C:82:ARG:HE	1.69	0.57
2:D:54:LEU:HD11	2:D:62:PHE:HB3	1.87	0.56
1:A:217:TRP:HZ3	1:A:262:ARG:HG2	1.71	0.56
4:H:31:TYR:CE1	4:H:50:VAL:HG12	2.41	0.55
3:E:134:VAL:HG22	3:E:177:TRP:HB3	1.89	0.54
1:A:237:PRO:HG2	2:B:65:LEU:HD13	1.89	0.54
1:A:90:PHE:CD2	1:A:94:PHE:HE2	2.26	0.54
1:A:237:PRO:O	2:B:10:TYR:OH	2.25	0.54
4:F:94:ARG:HD2	4:F:95:TYR:O	2.08	0.53
1:C:114:LEU:HB3	1:C:126:PHE:HB3	1.90	0.53
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.44	0.53
3:G:36:ARG:HB2	3:G:46:LEU:HD22	1.92	0.52
1:A:84:TYR:CD1	1:A:87:GLU:CD	2.82	0.52
3:E:112:PRO:HB2	3:E:170:LYS:HD3	1.91	0.52
3:G:196:GLU:N	3:G:196:GLU:OE1	2.41	0.52
1:A:53:TRP:CE3	1:A:177:GLY:HA3	2.45	0.52
3:E:80:PRO:HA	3:E:110:VAL:HB	1.92	0.52
1:A:14:TRP:HB2	1:A:98:VAL:HB	1.92	0.52
1:C:168:ARG:CD	5:J:1:NAG:C8	2.78	0.51
5:I:1:NAG:O3	5:I:2:NAG:O6	2.26	0.51
1:A:90:PHE:CD1	1:A:90:PHE:N	2.72	0.51
4:F:210:ARG:NH1	4:F:212:GLN:HB2	2.25	0.51
4:H:111:ARG:NH2	4:H:154:ASP:OD2	2.44	0.50
1:A:37:THR:HG22	1:A:51:TRP:HD1	1.77	0.50
1:A:184:GLN:HB3	1:A:267:SER:HB3	1.92	0.50
1:C:169:PHE:CD2	7:C:304:PAM:H10	2.47	0.50
2:D:83:ASN:HD22	2:D:90:PRO:HG3	1.76	0.50
4:F:120:LYS:HZ1	3:G:151:ASP:HA	1.76	0.50
1:A:90:PHE:HD2	1:A:94:PHE:HE2	1.60	0.49
4:F:204:ASN:O	4:F:242:GLY:HA3	2.12	0.49
1:C:55:ARG:NH2	1:C:60:ASN:OD1	2.44	0.49
4:F:87:SER:OG	4:F:88:VAL:N	2.46	0.49
4:H:36:ARG:HH21	4:H:87:SER:HB2	1.77	0.49
1:A:90:PHE:CD2	1:A:94:PHE:CE2	3.01	0.48
4:H:37:GLN:HB2	4:H:43:LEU:HD23	1.95	0.48
4:H:154:ASP:OD1	4:H:177:PRO:HG3	2.13	0.48
1:A:125:SER:HB2	1:A:134:TYR:CE1	2.49	0.48
4:H:128:VAL:HG23	4:H:238:ALA:HB3	1.96	0.47
3:E:6:ASP:OD1	3:E:7:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:212:GLN:HG3	4:F:235:ILE:HG23	1.96	0.47
1:A:90:PHE:HD1	1:A:90:PHE:N	2.03	0.47
4:F:39:PRO:HA	4:F:40:GLY:HA2	1.58	0.47
4:H:87:SER:OG	4:H:88:VAL:N	2.47	0.47
1:C:17:SER:HA	1:C:95:GLU:HG2	1.95	0.47
3:G:162:LEU:HB3	4:H:172:CYS:HB2	1.97	0.46
4:H:31:TYR:HE1	4:H:50:VAL:HG12	1.80	0.46
2:B:51:HIS:HB3	2:B:66:TYR:CE2	2.50	0.46
3:E:162:LEU:HB3	4:F:172:CYS:HB2	1.98	0.46
4:F:154:ASP:OD1	4:F:177:PRO:HG3	2.15	0.46
1:A:58:PHE:HE2	1:A:66:LEU:HD11	1.81	0.46
1:C:53:TRP:HB2	1:C:176:ALA:HB1	1.98	0.46
1:C:191:LEU:HA	1:C:206:CYS:N	2.31	0.46
1:C:14:TRP:CH2	7:C:304:PAM:H22	2.51	0.46
1:C:31:TRP:CZ2	2:D:55:SER:HB2	2.50	0.46
3:G:129:SER:C	3:G:131:ASP:H	2.19	0.46
1:C:11:HIS:HB2	1:C:99:THR:HG22	1.98	0.46
2:D:39:LEU:HB2	2:D:49:VAL:HG21	1.97	0.45
1:A:90:PHE:HD2	1:A:94:PHE:CE2	2.35	0.45
3:G:126:ASP:HB2	3:G:132:LYS:HB2	1.98	0.45
1:A:26:ASN:HB2	1:A:78:PHE:CE2	2.52	0.45
1:A:58:PHE:N	1:A:58:PHE:CD1	2.82	0.45
1:A:89:GLN:O	1:A:90:PHE:C	2.54	0.45
4:H:131:PRO:HD2	4:H:202:TRP:CZ2	2.51	0.45
1:C:91:GLU:OE2	1:C:118:TYR:OH	2.34	0.45
1:A:58:PHE:CE2	1:A:66:LEU:HD11	2.52	0.45
3:E:123:GLN:HG3	3:E:185:CYS:SG	2.57	0.45
1:A:263:VAL:HB	1:A:273:ILE:HB	1.99	0.45
1:C:128:ASN:HB3	1:C:129:ASN:H	1.62	0.45
2:B:17:ASN:OD1	2:B:73:THR:HA	2.17	0.44
1:C:166:CYS:HB3	1:C:167:PRO:HD3	1.98	0.44
7:C:304:PAM:H111	7:C:304:PAM:H81	1.72	0.44
1:A:166:CYS:HB3	1:A:167:PRO:HD3	1.99	0.44
4:H:174:ASP:HB2	4:H:191:LEU:HD12	1.99	0.44
4:H:194:ARG:N	4:H:194:ARG:HD3	2.32	0.44
4:F:184:LEU:HB3	3:G:153:ASP:OD2	2.18	0.44
1:A:264:LYS:NZ	1:A:272:ASP:OD2	2.45	0.44
4:F:131:PRO:HD3	4:F:144:LEU:HG	2.00	0.44
2:B:11:SER:HB2	2:B:21:ASN:HD21	1.82	0.44
1:C:191:LEU:N	1:C:207:HIS:HD2	2.16	0.44
3:G:120:ALA:HB2	3:G:199:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD13	1:A:174:LEU:HA	1.80	0.43
4:F:36:ARG:HH21	4:F:87:SER:HB2	1.83	0.43
3:G:43:PRO:HG2	4:H:43:LEU:HD11	1.99	0.43
1:A:128:ASN:HB3	1:A:129:ASN:H	1.46	0.43
1:C:104:LEU:HD12	1:C:109:VAL:HA	1.99	0.43
4:H:136:ILE:HG23	4:H:199:ALA:HB1	2.00	0.43
1:C:130:SER:HB2	1:C:149:ASN:ND2	2.34	0.43
4:H:4:VAL:HG23	4:H:27:MET:CE	2.49	0.43
1:A:36:GLN:OE1	2:B:53:ASP:HB2	2.18	0.43
1:C:13:ILE:HG22	1:C:99:THR:HG23	2.00	0.43
1:A:181:LEU:H	1:A:181:LEU:HG	1.46	0.43
1:A:189:ALA:HA	1:A:207:HIS:O	2.19	0.42
2:D:41:LYS:HD3	2:D:78:TYR:OH	2.18	0.42
1:A:214:LYS:HD2	1:A:243:TRP:CE2	2.54	0.42
1:C:40:TRP:CG	1:C:41:ASP:N	2.87	0.42
1:A:77:SER:O	1:A:81:ILE:HG13	2.19	0.42
4:F:128:VAL:HG23	4:F:238:ALA:HB3	2.00	0.42
3:G:20:LEU:HD12	3:G:73:LEU:HD23	2.01	0.42
4:H:19:MET:HE2	4:H:19:MET:HB3	1.67	0.42
3:G:129:SER:O	3:G:131:ASP:N	2.53	0.42
5:I:1:NAG:HO3	5:I:2:NAG:HO6	1.57	0.42
1:A:49:PHE:HD1	1:A:54:SER:HB3	1.85	0.42
3:G:89:ALA:HA	3:G:101:THR:O	2.20	0.42
1:A:31:TRP:CZ2	2:B:55:SER:HB2	2.55	0.41
4:H:37:GLN:HB2	4:H:43:LEU:CD2	2.50	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.77	0.41
2:D:59:ASP:OD1	2:D:59:ASP:N	2.43	0.41
1:A:108:LYS:HE2	1:A:108:LYS:HB3	1.91	0.41
1:C:14:TRP:HB2	1:C:98:VAL:HB	2.02	0.41
1:C:132:LEU:HD13	1:C:132:LEU:HA	1.88	0.41
5:I:1:NAG:O3	5:I:2:NAG:O5	2.38	0.41
1:A:151:ASN:ND2	1:A:154:GLU:HG2	2.35	0.41
3:G:80:PRO:HA	3:G:110:VAL:HB	2.03	0.41
4:F:111:ARG:NH2	4:F:154:ASP:HB3	2.36	0.41
1:A:51:TRP:HB3	1:A:53:TRP:NE1	2.36	0.41
5:I:1:NAG:O4	5:I:2:NAG:H83	2.19	0.41
4:F:136:ILE:HG23	4:F:199:ALA:HB1	2.03	0.41
4:F:146:CYS:HB2	4:F:160:TRP:CZ2	2.56	0.41
3:G:123:GLN:C	3:G:124:LEU:HD12	2.41	0.41
2:D:81:ARG:HG3	2:D:92:ILE:HG13	2.04	0.40
4:F:47:HIS:HD2	4:F:57:LYS:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:HB2	1:A:78:PHE:HE2	1.85	0.40
1:A:45:SER:HB3	1:A:71:ARG:HD3	2.02	0.40
1:A:94:PHE:CD2	1:A:118:TYR:HE1	2.35	0.40
3:E:99:LYS:HE3	4:F:48:TYR:CE1	2.57	0.40
2:B:58:LYS:HB3	2:B:58:LYS:HE2	1.90	0.40
3:E:89:ALA:HA	3:E:101:THR:O	2.22	0.40
3:G:126:ASP:HB3	3:G:129:SER:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/275 (96%)	244 (93%)	17 (6%)	2 (1%)	19	55
1	C	208/275 (76%)	184 (88%)	23 (11%)	1 (0%)	29	66
2	B	82/99 (83%)	77 (94%)	5 (6%)	0	100	100
2	D	72/99 (73%)	68 (94%)	4 (6%)	0	100	100
3	E	183/207 (88%)	179 (98%)	4 (2%)	0	100	100
3	G	198/207 (96%)	192 (97%)	5 (2%)	1 (0%)	29	66
4	F	239/245 (98%)	232 (97%)	7 (3%)	0	100	100
4	H	240/245 (98%)	232 (97%)	8 (3%)	0	100	100
All	All	1485/1652 (90%)	1408 (95%)	73 (5%)	4 (0%)	41	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	90	PHE
3	G	130	SER

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Mol	Chain	Res	Type
1	C	41	ASP

### 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	231/240 (96%)	213 (92%)	18 (8%)	12	40
1	C	195/240 (81%)	181 (93%)	14 (7%)	14	43
2	B	82/94 (87%)	77 (94%)	5 (6%)	18	51
2	D	75/94 (80%)	70 (93%)	5 (7%)	16	47
3	E	169/187 (90%)	164 (97%)	5 (3%)	41	73
3	G	180/187 (96%)	175 (97%)	5 (3%)	43	75
4	F	207/209 (99%)	204 (99%)	3 (1%)	67	86
4	H	207/209 (99%)	201 (97%)	6 (3%)	42	74
All	All	1346/1460 (92%)	1285 (96%)	61 (4%)	27	62

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	39	THR
1	A	42	SER
1	A	54	SER
1	A	59	SER
1	A	73	ARG
1	A	83	ARG
1	A	90	PHE
1	A	91	GLU
1	A	94	PHE
1	A	121	SER
1	A	136	VAL
1	A	160	ASN
1	A	174	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	181	LEU
1	A	183	ARG
1	A	262	ARG
1	A	269	GLU
2	B	3	ARG
2	B	70	PHE
2	B	76	ASP
2	B	77	GLU
2	B	92	ILE
1	C	19	TYR
1	C	21	HIS
1	C	22	SER
1	C	23	TRP
1	C	27	LEU
1	C	45	SER
1	C	73	ARG
1	C	87	GLU
1	C	99	THR
1	C	102	CYS
1	C	106	SER
1	C	182	GLN
1	C	218	VAL
1	C	234	ASP
2	D	7	ILE
2	D	27	VAL
2	D	51	HIS
2	D	86	THR
2	D	95	TRP
3	E	23	THR
3	E	46	LEU
3	E	100	SER
3	E	143	GLN
3	E	171	SER
4	F	5	THR
4	F	194	ARG
4	F	237	SER
3	G	6	ASP
3	G	23	THR
3	G	171	SER
3	G	179	ASN
3	G	182	ASP
4	H	5	THR

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Mol	Chain	Res	Type
4	H	22	LEU
4	H	38	ASP
4	H	94	ARG
4	H	194	ARG
4	H	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS

### 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](#)

6 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	5,1	14,14,15	1.16	1 (7%)	17,19,21	2.37	6 (35%)
5	NAG	I	2	5	14,14,15	0.63	0	17,19,21	1.14	1 (5%)
5	FUC	I	3	5	10,10,11	0.48	0	14,14,16	1.90	2 (14%)
5	NAG	J	1	5,1	14,14,15	1.02	1 (7%)	17,19,21	1.27	1 (5%)
5	NAG	J	2	5	14,14,15	0.34	0	17,19,21	0.34	0
5	FUC	J	3	5	10,10,11	0.40	0	14,14,16	1.33	2 (14%)

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	5,1	-	5/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	FUC	I	3	5	-	-	0/1/1/1
5	NAG	J	1	5,1	-	6/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	FUC	J	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	NAG	C1-C2	3.40	1.57	1.52
5	I	1	NAG	C1-C2	3.22	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C1-O5-C5	6.62	121.17	112.19
5	I	3	FUC	C1-C2-C3	5.08	115.91	109.67
5	I	1	NAG	C4-C3-C2	4.13	117.07	111.02
5	J	3	FUC	C1-C2-C3	3.24	113.65	109.67
5	I	1	NAG	C6-C5-C4	-3.23	105.45	113.00
5	I	1	NAG	O5-C5-C6	-3.15	102.27	107.20
5	J	1	NAG	C4-C3-C2	2.79	115.11	111.02
5	I	3	FUC	O5-C5-C4	2.64	114.25	109.52
5	I	1	NAG	O6-C6-C5	-2.41	103.03	111.29
5	I	2	NAG	O5-C1-C2	-2.37	107.54	111.29
5	J	3	FUC	O5-C5-C4	-2.36	105.28	109.52
5	I	1	NAG	O3-C3-C4	-2.07	105.56	110.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2

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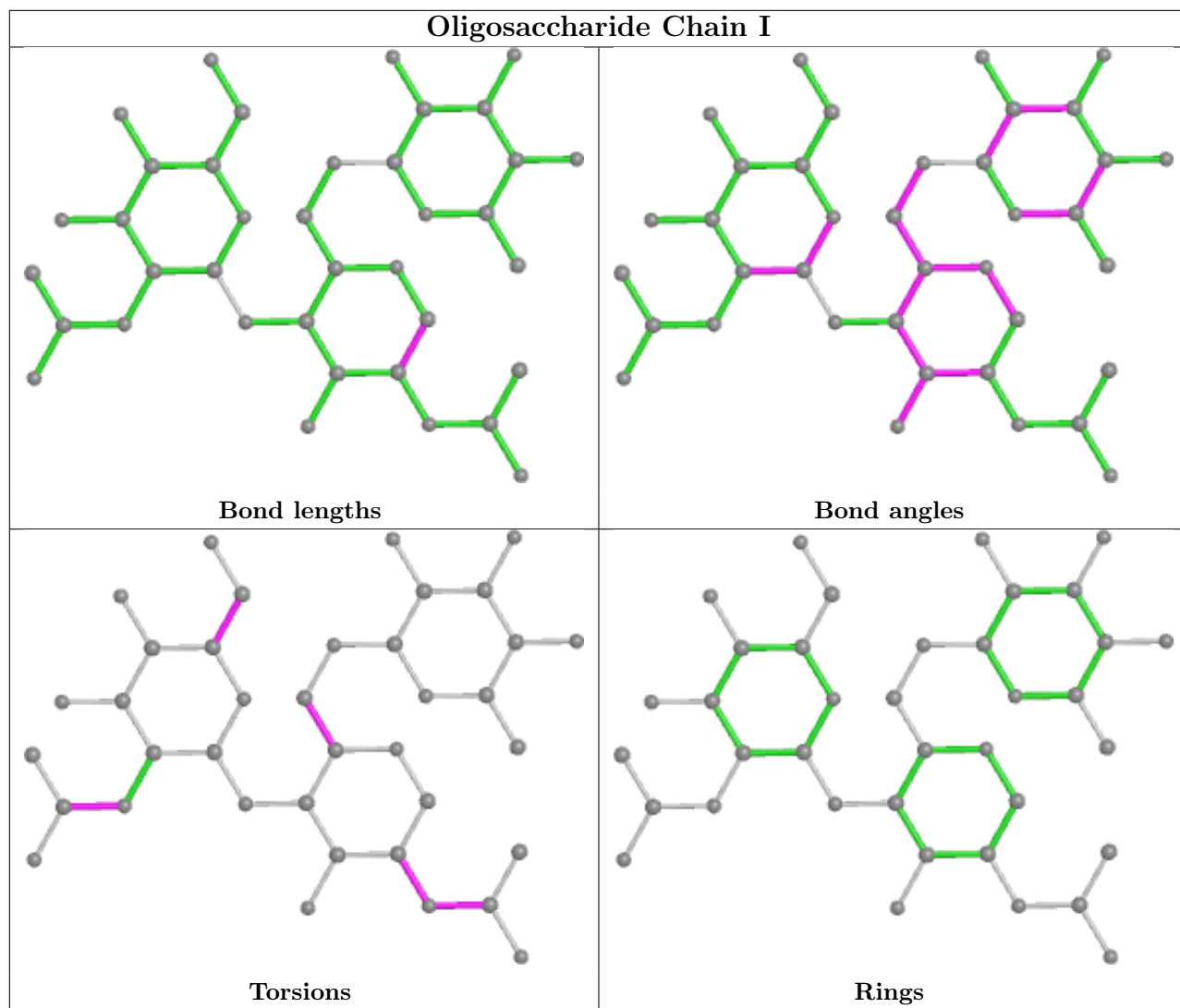
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	I	1	NAG	C1-C2-N2-C7
5	J	1	NAG	C1-C2-N2-C7
5	I	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C3-C2-N2-C7

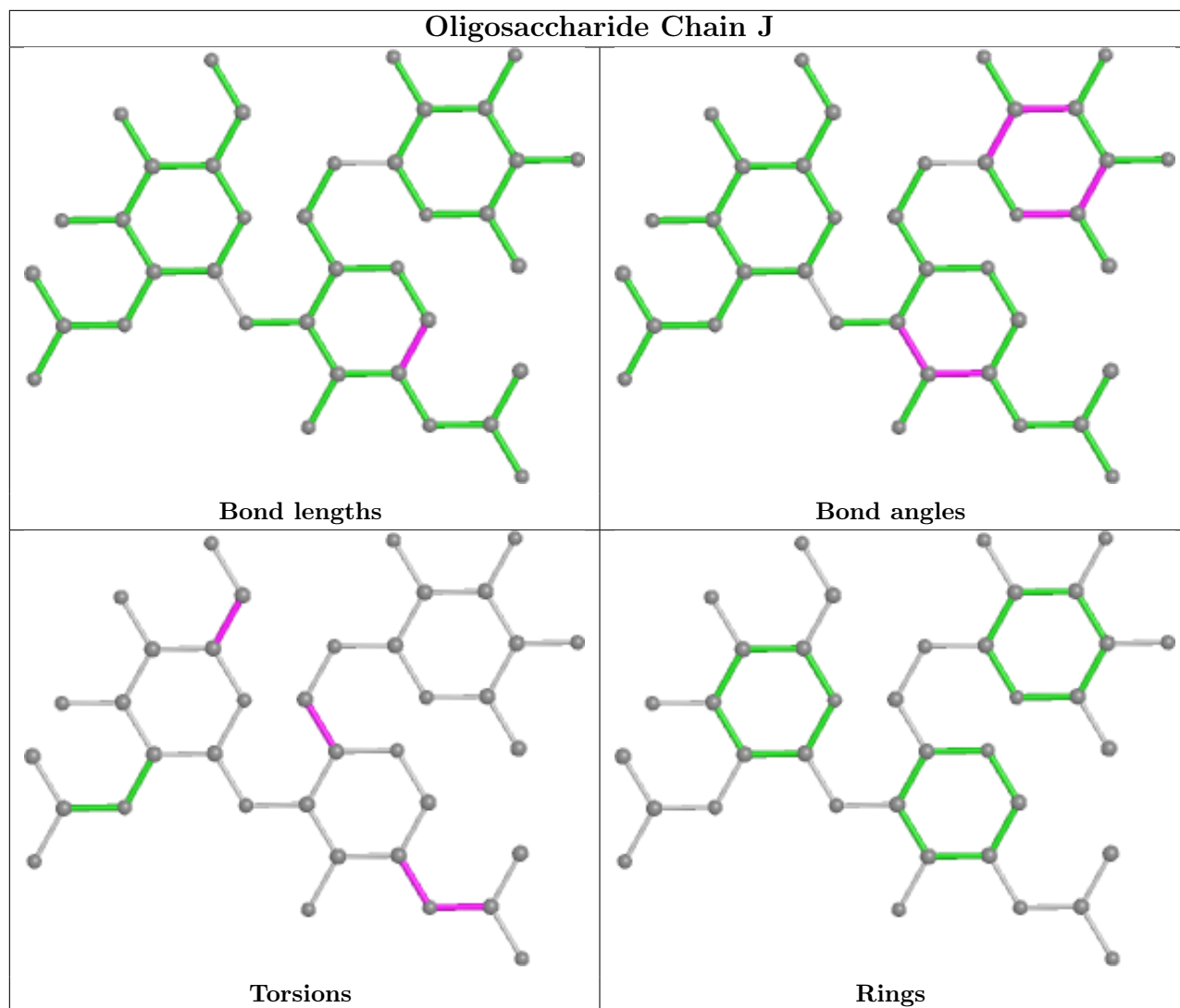
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	2	0
5	I	1	NAG	4	0
5	I	2	NAG	4	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](#)

2 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	PAM	C	304	-	17,17,17	0.84	1 (5%)	17,17,17	1.04	1 (5%)
6	OLA	A	304	-	19,19,19	0.80	1 (5%)	19,19,19	0.89	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
7	PAM	C	304	-	-	6/15/15/15	-
6	OLA	A	304	-	-	11/17/17/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	304	PAM	C10-C9	2.74	1.47	1.31
6	A	304	OLA	C10-C9	2.69	1.47	1.31

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	304	PAM	C3-C2-C1	-2.13	109.11	114.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	304	OLA	C1-C2-C3-C4
7	C	304	PAM	C1-C2-C3-C4
6	A	304	OLA	C5-C6-C7-C8
6	A	304	OLA	C11-C10-C9-C8
6	A	304	OLA	C14-C15-C16-C17
6	A	304	OLA	C3-C4-C5-C6
6	A	304	OLA	C4-C5-C6-C7
7	C	304	PAM	C5-C6-C7-C8
6	A	304	OLA	C13-C14-C15-C16
7	C	304	PAM	O2-C1-C2-C3
7	C	304	PAM	C12-C13-C14-C15
7	C	304	PAM	O1-C1-C2-C3
6	A	304	OLA	O1-C1-C2-C3
7	C	304	PAM	C10-C11-C12-C13
6	A	304	OLA	O2-C1-C2-C3
6	A	304	OLA	C7-C8-C9-C10
6	A	304	OLA	C15-C16-C17-C18

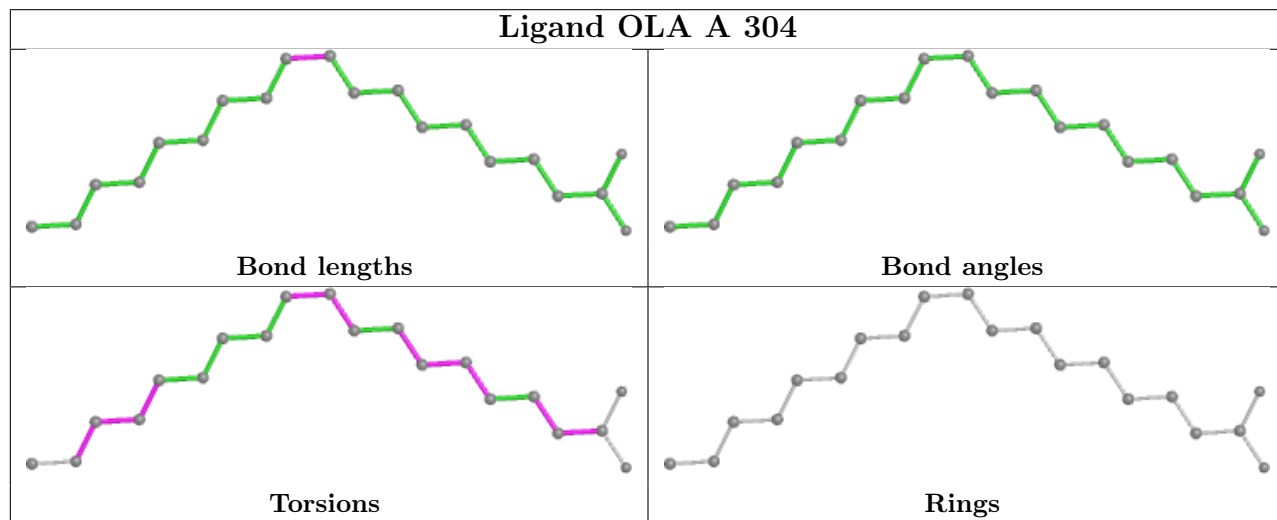
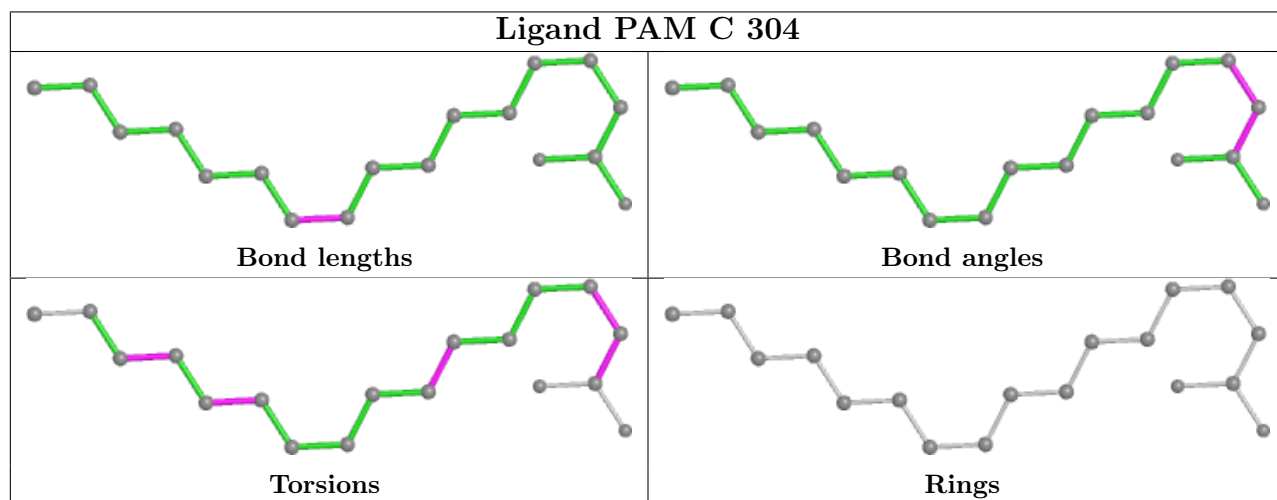
There are no ring outliers.



1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	304	PAM	3	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, 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	267/275 (97%)	0.29	9 (3%) 45 27	57, 100, 152, 204	0
1	C	218/275 (79%)	0.51	24 (11%) 5 3	57, 121, 186, 222	0
2	B	86/99 (86%)	1.00	16 (18%) 1 0	86, 136, 178, 200	0
2	D	78/99 (78%)	1.04	19 (24%) 0 0	87, 140, 177, 198	0
3	E	189/207 (91%)	0.12	3 (1%) 72 52	43, 73, 137, 178	0
3	G	200/207 (96%)	0.12	3 (1%) 73 54	46, 75, 141, 176	0
4	F	241/245 (98%)	0.06	4 (1%) 70 50	44, 76, 123, 150	0
4	H	242/245 (98%)	0.02	0 100 100	42, 74, 120, 154	0
All	All	1521/1652 (92%)	0.28	78 (5%) 28 16	42, 91, 161, 222	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	92	TYR	5.4
1	C	208	VAL	5.3
2	D	82	VAL	5.2
1	C	244	TYR	5.1
2	D	23	LEU	4.4
2	B	80	CYS	4.1
1	C	247	ALA	4.1
2	B	82	VAL	4.0
1	C	246	ARG	3.9
1	C	21	HIS	3.9
2	B	37	VAL	3.8
2	D	49	VAL	3.8
1	C	90	PHE	3.7
2	D	65	LEU	3.7
2	D	68	THR	3.6
2	B	79	ALA	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	92	ILE	3.4
2	D	94	LYS	3.4
2	D	24	ASN	3.3
2	D	44	GLU	3.2
3	G	182	ASP	3.2
2	D	95	TRP	3.1
2	B	23	LEU	3.1
1	C	193	HIS	3.0
1	C	191	LEU	2.9
2	B	93	VAL	2.9
1	C	217	TRP	2.9
2	D	48	LYS	2.9
3	G	185	CYS	2.8
1	C	47	ILE	2.8
1	C	84	TYR	2.8
1	A	189	ALA	2.8
3	G	181	SER	2.8
2	D	9	VAL	2.7
2	D	22	PHE	2.7
2	D	93	VAL	2.6
1	A	142	LYS	2.6
1	A	232	ARG	2.6
2	B	69	GLU	2.6
2	B	81	ARG	2.6
1	A	90	PHE	2.5
4	F	202	TRP	2.5
3	E	150	LYS	2.5
1	C	187	PRO	2.5
1	C	245	LEU	2.5
1	A	43	ASN	2.4
1	C	139	ASN	2.4
2	B	66	TYR	2.4
1	C	53	TRP	2.4
1	C	236	LEU	2.4
4	F	144	LEU	2.4
2	B	77	GLU	2.3
1	C	232	ARG	2.3
2	D	8	GLN	2.3
2	D	79	ALA	2.3
1	C	14	TRP	2.3
3	E	122	TYR	2.3
1	C	22	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	92	ILE	2.2
2	D	36	GLU	2.2
2	B	88	SER	2.2
4	F	223	GLU	2.2
2	B	72	PRO	2.2
1	C	143	HIS	2.2
2	B	49	VAL	2.2
1	A	187	PRO	2.1
1	C	207	HIS	2.1
2	B	19	LYS	2.1
2	B	24	ASN	2.1
1	A	218	VAL	2.1
2	D	39	LEU	2.1
2	D	67	TYR	2.0
1	C	206	CYS	2.0
1	A	146	LYS	2.0
3	E	133	SER	2.0
4	F	209	PHE	2.0
1	A	170	ILE	2.0
1	C	94	PHE	2.0

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

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

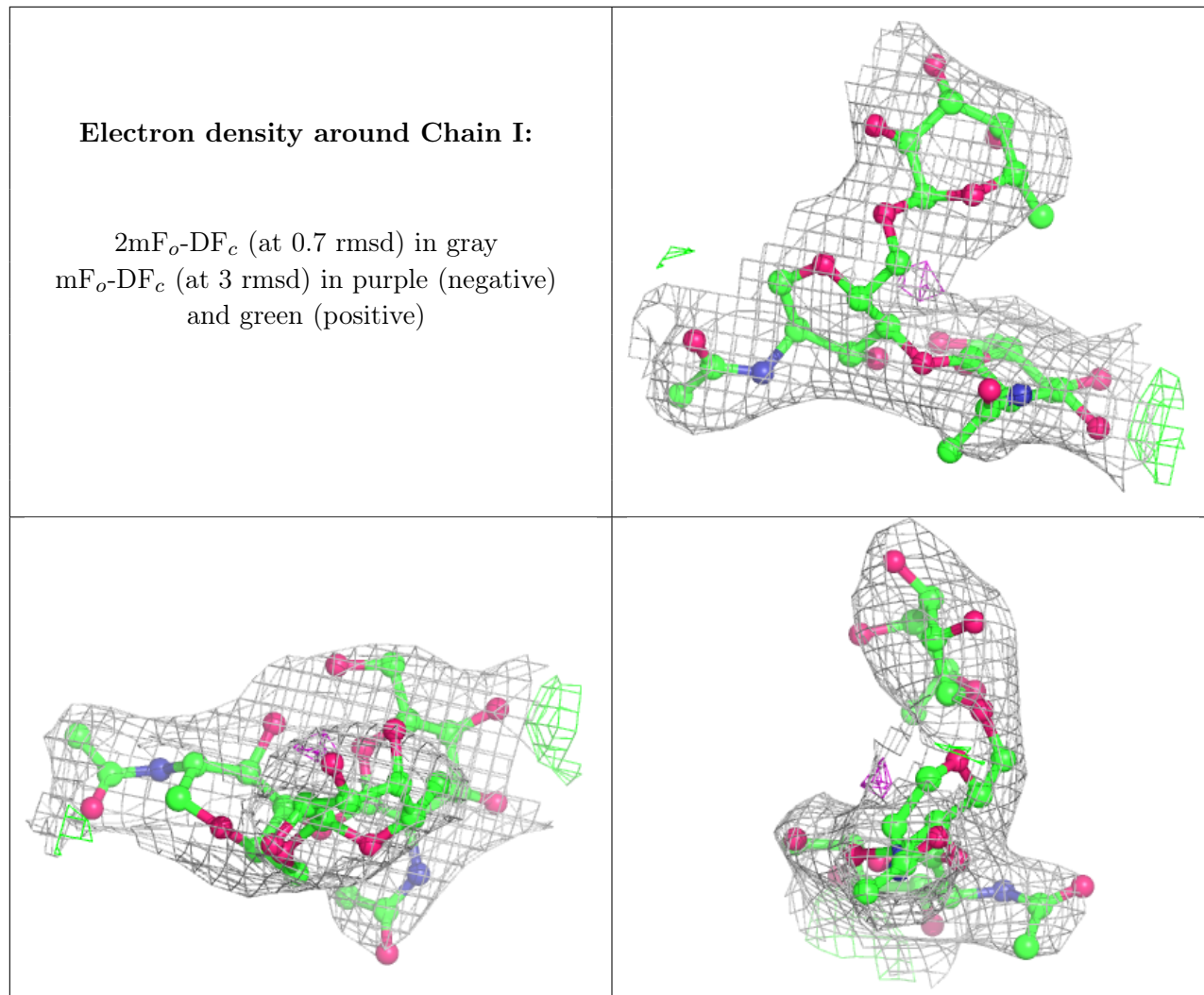
## 6.3 Carbohydrates [i](#)

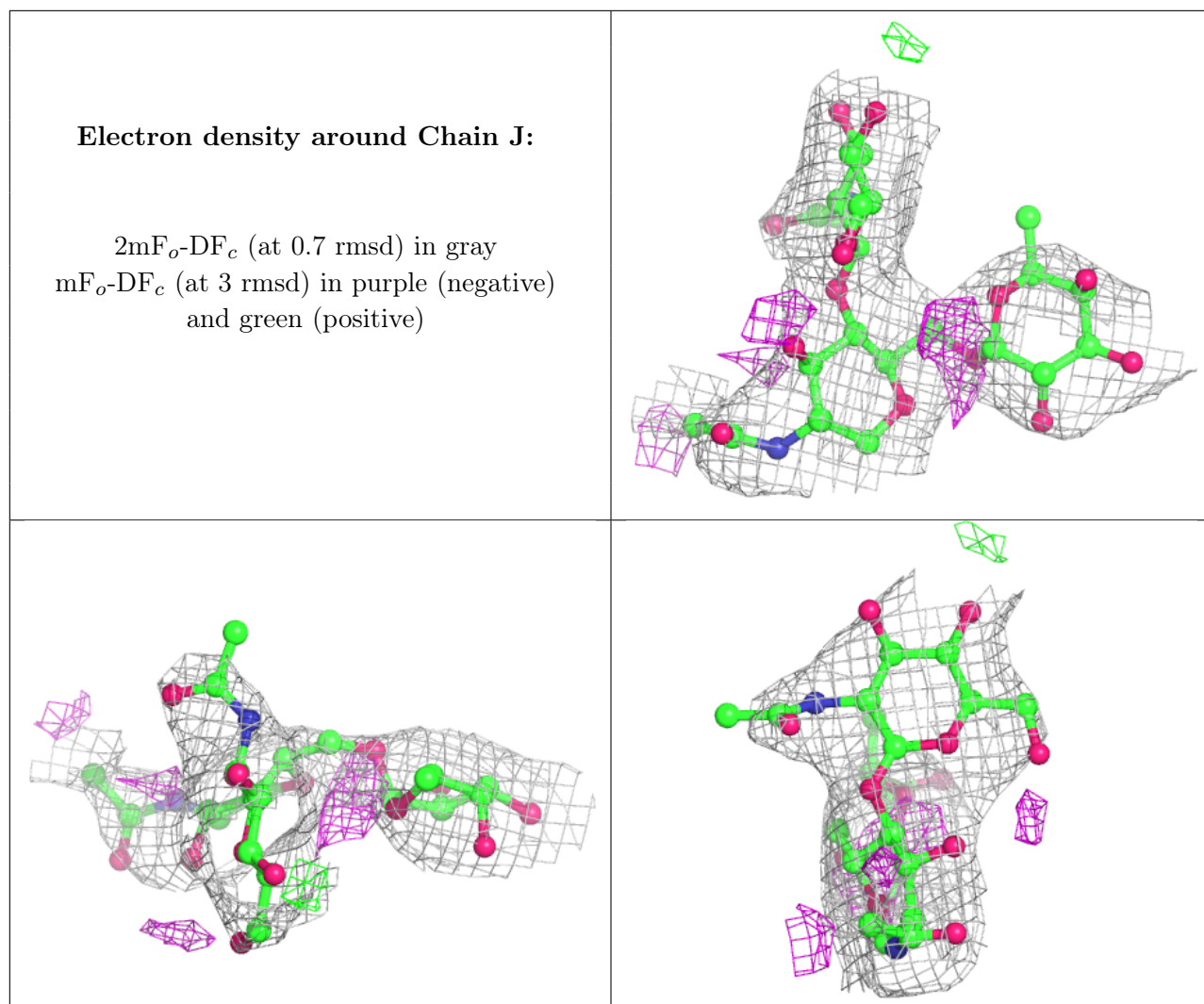
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	J	2	14/15	0.85	0.28	125,129,137,140	0
5	NAG	J	1	14/15	0.86	0.31	104,125,140,141	0
5	FUC	J	3	10/11	0.89	0.37	118,142,149,153	0
5	NAG	I	2	14/15	0.90	0.23	121,129,135,135	0
5	FUC	I	3	10/11	0.91	0.30	134,143,160,165	0
5	NAG	I	1	14/15	0.95	0.21	96,107,124,133	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



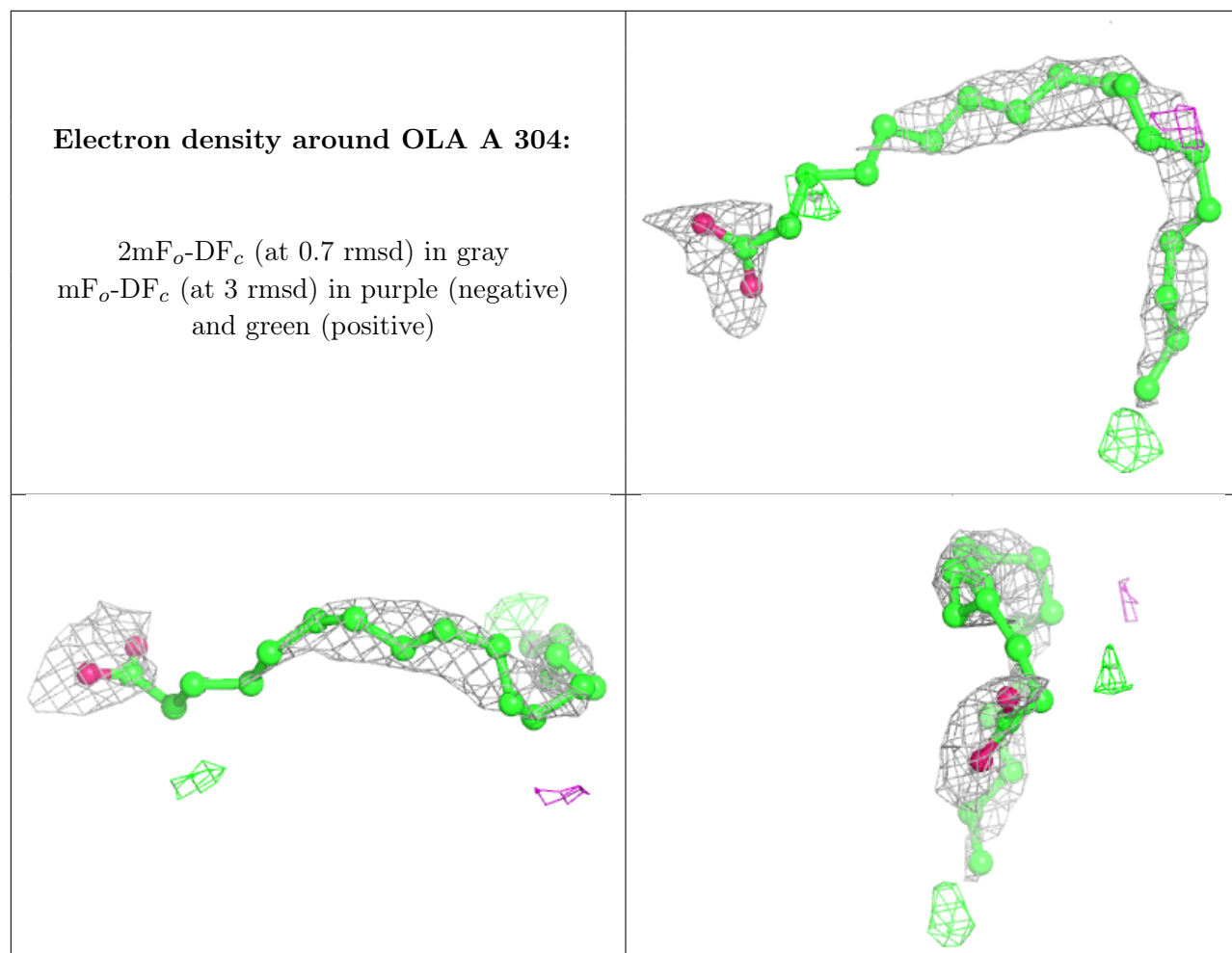


## 6.4 Ligands [i](#)

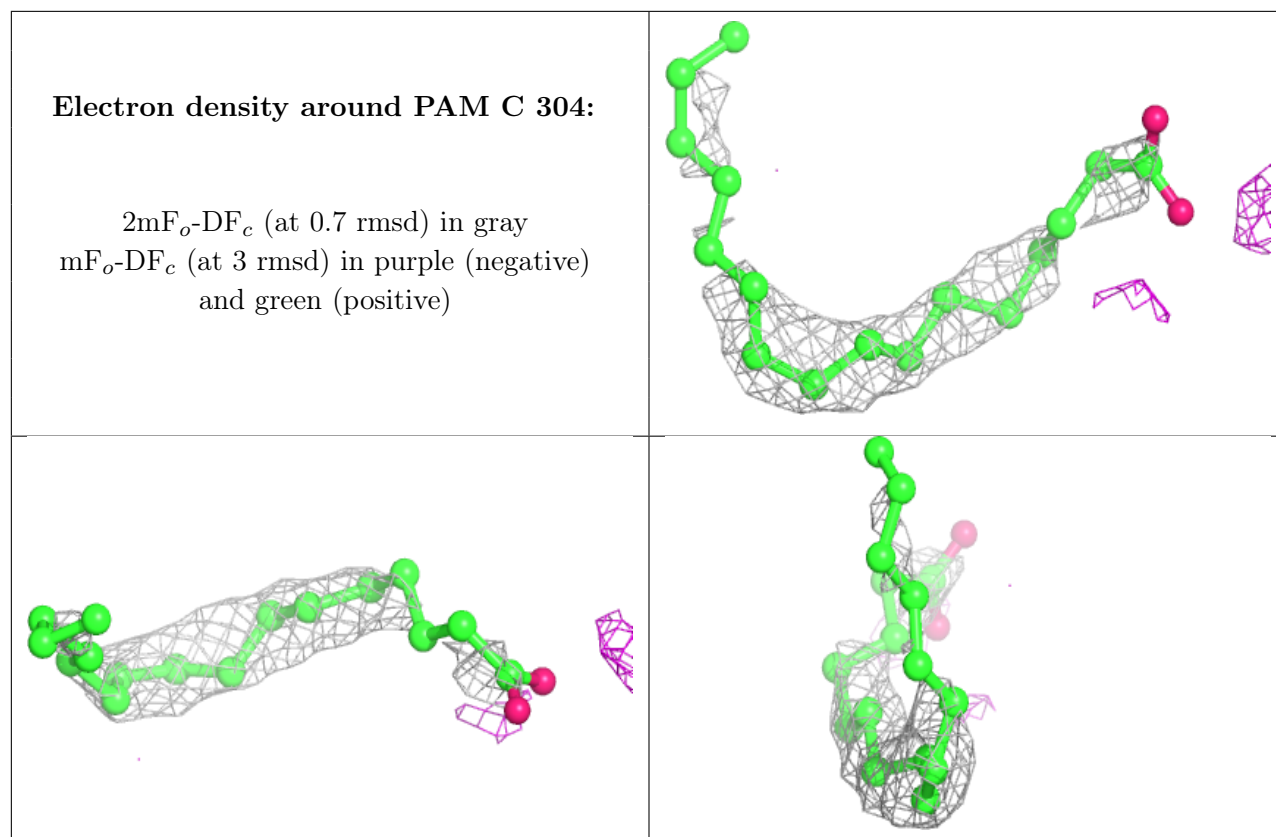
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	OLA	A	304	20/20	0.83	0.49	75,88,133,134	0
7	PAM	C	304	18/18	0.83	0.71	78,90,159,163	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 [i](#)

There are no such residues in this entry.