



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2021 – 12:27 PM EDT

PDB ID : 7MZK
Title : SARS-CoV-2 receptor binding domain bound to Fab WCSL 129 and Fab PDI 96
Authors : Pymm, P.; Dietrich, M.H.; Tan, L.L.; Chan, L.J.; Tham, W.H.
Deposited on : 2021-05-24
Resolution : 2.25 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 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 : 2.23.2
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) : 2.23.2

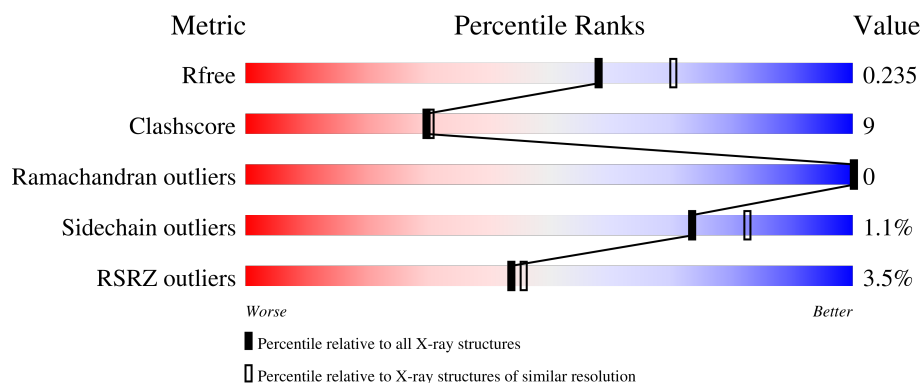
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	C	224	<div> <div>5%</div> <div>80%</div> <div>15%</div> <div>5%</div> </div>
1	F	224	<div> <div>10%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
2	A	205	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>5%</div> </div>
2	B	205	<div> <div>2%</div> <div>80%</div> <div>15%</div> <div>5%</div> </div>
3	D	216	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	216	
4	H	229	
4	N	229	
5	L	220	
5	M	220	
6	G	3	
6	I	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
9	GOL	H	301	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16846 atoms, of which 43 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 WCSL 129 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	213	Total	C	N	O	S	0	4	0
			1562	989	257	304	12			
1	F	219	Total	C	N	O	S	0	1	0
			1592	1005	265	315	7			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1521	974	253	286	8			
2	A	195	Total	C	N	O	S	0	0	0
			1524	978	252	286	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	528	GLY	-	expression tag	UNP P0DTC2
B	529	SER	-	expression tag	UNP P0DTC2
B	530	HIS	-	expression tag	UNP P0DTC2
B	531	HIS	-	expression tag	UNP P0DTC2
B	532	HIS	-	expression tag	UNP P0DTC2
B	533	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	SER	-	expression tag	UNP P0DTC2
A	530	HIS	-	expression tag	UNP P0DTC2
A	531	HIS	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is a protein called WCSL 129 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1568	985	257	322	4			
3	D	212	Total	C	N	O	S	0	0	0
			1548	972	254	318	4			

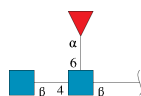
- Molecule 4 is a protein called PDI 96 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	223	Total	C	N	O	S	0	2	0
			1646	1036	273	327	10			
4	H	223	Total	C	N	O	S	0	1	0
			1615	1016	269	320	10			

- Molecule 5 is a protein called PDI 96 light chain.

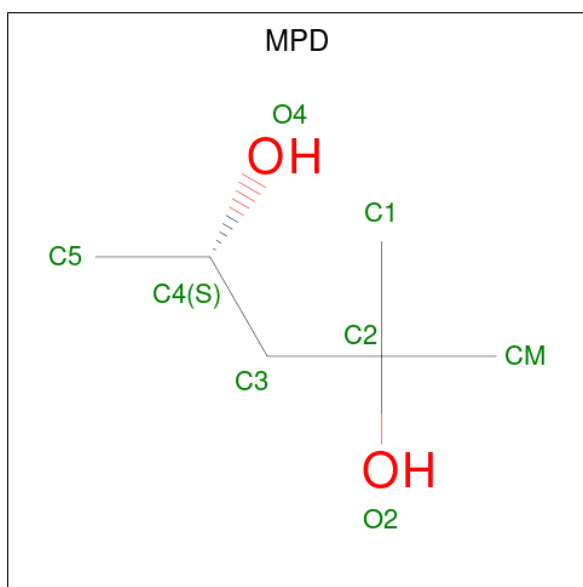
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	218	Total	C	N	O	S	0	1	0
			1670	1048	278	339	5			
5	L	219	Total	C	N	O	S	0	0	0
			1645	1033	274	333	5			

- Molecule 6 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.



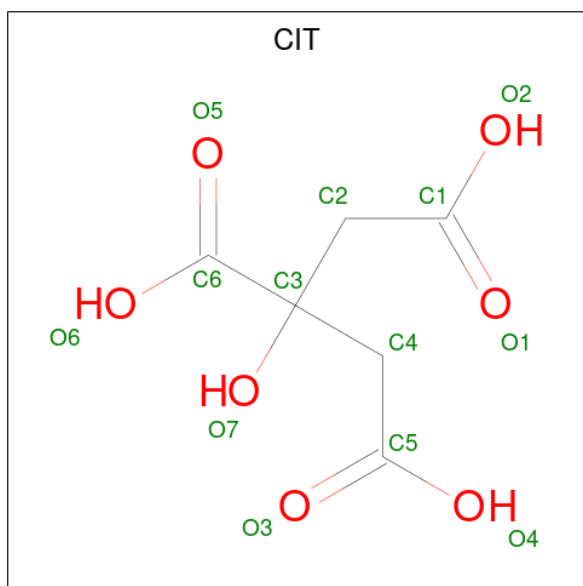
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



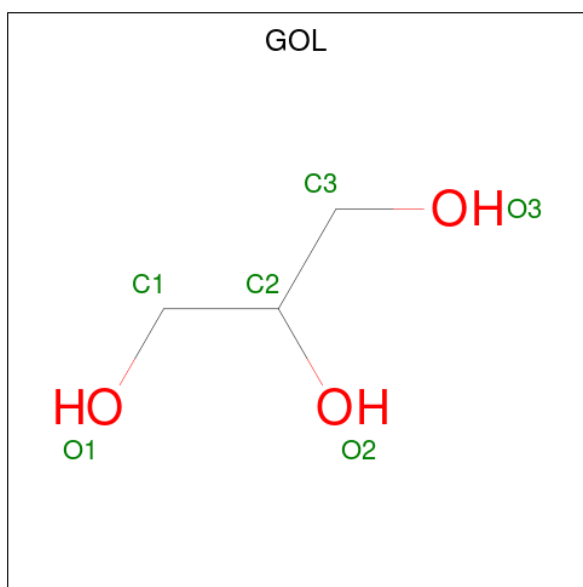
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 8 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	H	O	0	0
			14	3	8	3		
9	H	1	Total	C	H	O	0	0
			14	3	8	3		
9	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	41	Total	O	0	0
			41	41		
10	B	112	Total	O	0	0
			112	112		
10	E	123	Total	O	0	0
			123	123		
10	F	52	Total	O	0	0
			52	52		
10	A	110	Total	O	0	0
			110	110		
10	N	86	Total	O	0	0
			86	86		
10	M	84	Total	O	0	0
			84	84		
10	H	50	Total	O	0	0
			50	50		
10	L	48	Total	O	0	0
			48	48		

Continued on next page...

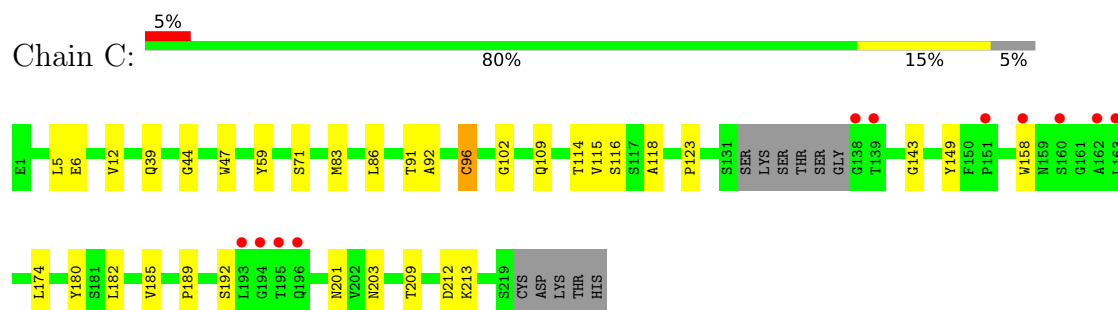
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	91	Total	O	0	0
			91	91		

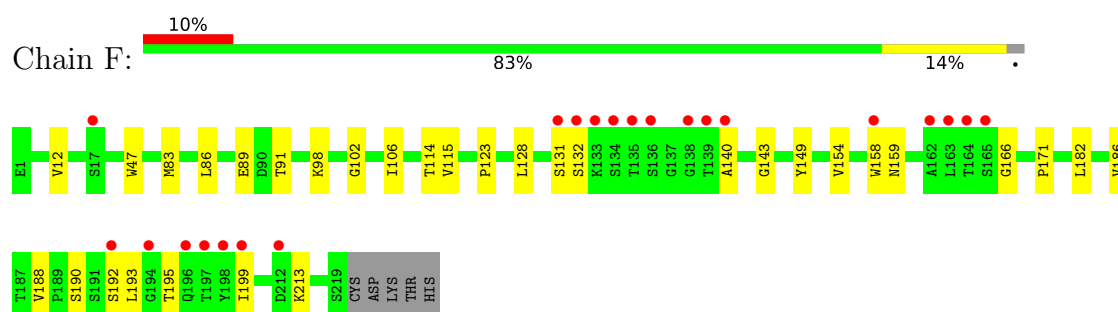
3 Residue-property plots [i](#)

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.

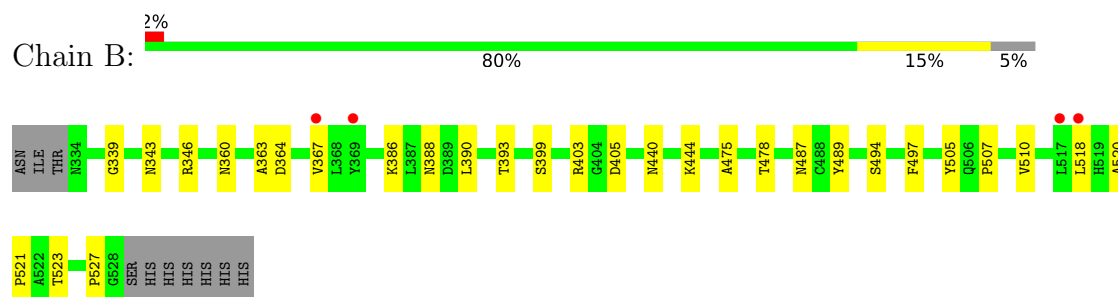
- Molecule 1: WCSL 129 heavy chain



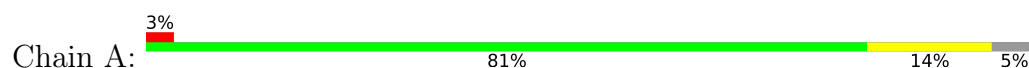
- Molecule 1: WCSL 129 heavy chain

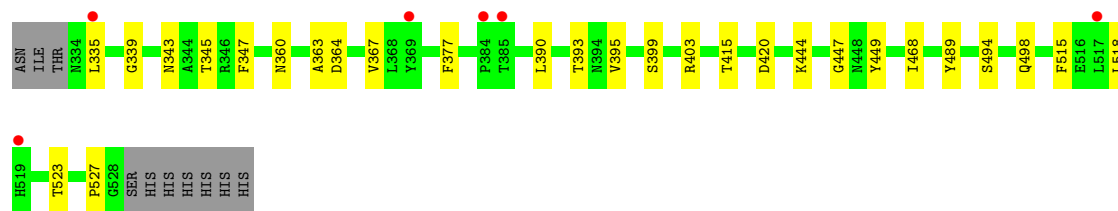


- Molecule 2: Spike protein S1

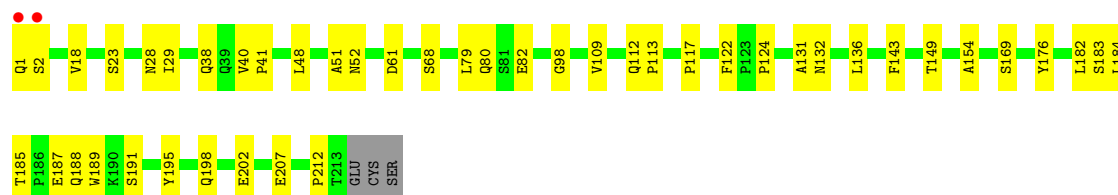
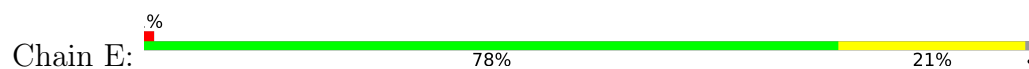


- Molecule 2: Spike protein S1

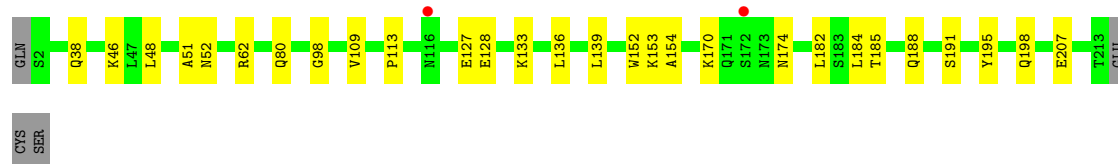
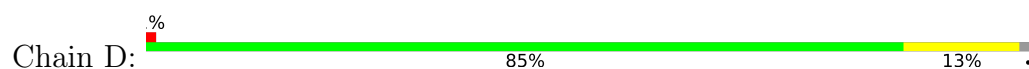




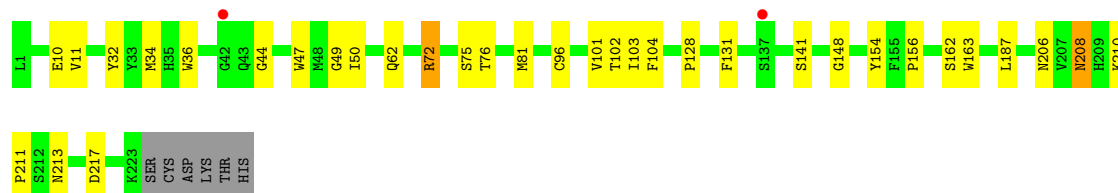
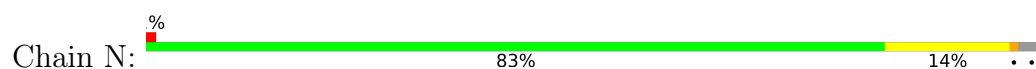
• Molecule 3: WCSL 129 light chain



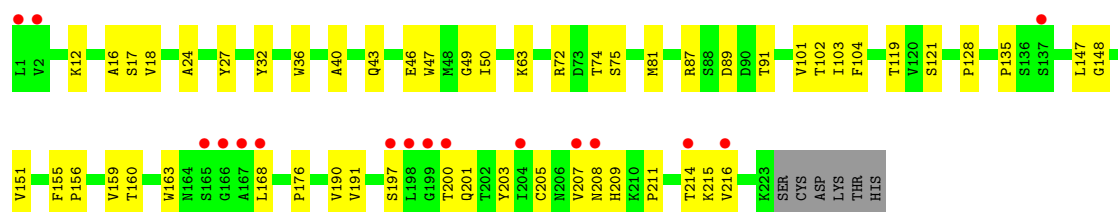
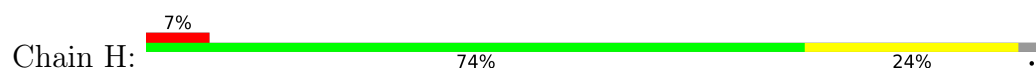
• Molecule 3: WCSL 129 light chain




• Molecule 4: PDI 96 heavy chain

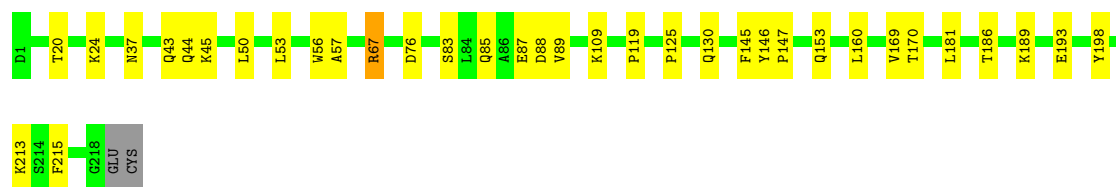


• Molecule 4: PDI 96 heavy chain



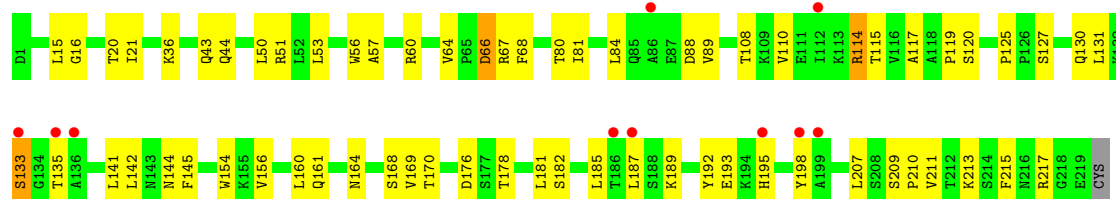
• Molecule 5: PDI 96 light chain

Chain M:  83% 15%



- Molecule 5: PDI 96 light chain

Chain L:  5% 70% 28%



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

Chain G:  100%



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

Chain I:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.90Å 103.56Å 106.29Å 103.52° 101.82° 98.20°	Depositor
Resolution (Å)	49.33 – 2.25 49.33 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.33-2.25) 98.4 (49.33-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.197 , 0.235 0.197 , 0.235	Depositor DCC
R_{free} test set	4004 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16846	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: NAG, GOL, FUC, MPD, CIT

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	C	0.25	0/1599	0.48	0/2186
1	F	0.26	0/1630	0.47	0/2226
2	A	0.26	0/1567	0.43	0/2136
2	B	0.26	0/1563	0.44	0/2129
3	D	0.27	0/1590	0.46	0/2182
3	E	0.26	0/1610	0.46	0/2206
4	H	0.25	0/1658	0.48	0/2271
4	N	0.25	0/1692	0.49	0/2312
5	L	0.25	0/1681	0.45	0/2294
5	M	0.25	0/1706	0.45	0/2324
All	All	0.26	0/16296	0.46	0/22266

There are no bond length outliers.

There are no bond angle outliers.

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	C	1562	0	1463	24	0
1	F	1592	0	1524	28	0
2	A	1524	0	1423	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1521	0	1428	21	0
3	D	1548	0	1471	23	0
3	E	1568	0	1503	30	1
4	H	1615	0	1500	53	0
4	N	1646	0	1585	30	0
5	L	1645	0	1553	50	1
5	M	1670	0	1590	24	0
6	G	38	0	34	0	0
6	I	38	0	34	0	0
7	B	8	14	14	1	0
8	E	13	5	5	1	0
9	D	6	8	8	1	0
9	H	6	8	8	11	0
9	M	6	8	8	0	0
10	A	110	0	0	5	0
10	B	112	0	0	2	0
10	C	41	0	0	1	0
10	D	91	0	0	3	0
10	E	123	0	0	4	0
10	F	52	0	0	0	0
10	H	50	0	0	3	0
10	L	48	0	0	2	0
10	M	84	0	0	3	0
10	N	86	0	0	5	0
All	All	16803	43	15151	294	1

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 9.

All (294) 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)
4:H:168:LEU:HD21	4:H:191:VAL:HG21	1.19	1.19
1:F:190:SER:HA	1:F:193:LEU:HD23	1.36	1.04
5:L:176:ASP:HB3	5:L:178:THR:HG22	1.45	0.97
4:N:76:THR:N	10:N:301:HOH:O	2.09	0.84
4:H:17:SER:H	9:H:301:GOL:H2	1.41	0.84
1:C:123:PRO:HB3	1:C:149:TYR:HB3	1.60	0.83
5:L:119:PRO:HB3	5:L:145:PHE:HB3	1.59	0.83
5:L:114:ARG:NH2	5:L:115:THR:O	2.12	0.82
5:L:207:LEU:HD13	5:L:211:VAL:HG23	1.59	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:PRO:O	1:C:192:SER:OG	1.96	0.82
5:L:67:ARG:NH1	5:L:88:ASP:OD2	2.11	0.80
5:L:21:ILE:HD12	5:L:108:THR:HG21	1.64	0.79
1:F:83:MET:HE2	1:F:86:LEU:HD21	1.64	0.79
4:H:128:PRO:HD2	4:H:214:THR:HG21	1.65	0.78
4:H:16:ALA:HB1	9:H:301:GOL:C2	2.14	0.78
3:E:1:GLN:HG2	3:E:2:SER:H	1.49	0.77
2:A:393:THR:HG21	2:A:518:LEU:H	1.50	0.76
1:C:83:MET:HE2	1:C:86:LEU:HD21	1.67	0.76
5:M:67:ARG:NH1	5:M:88:ASP:OD2	2.17	0.75
2:A:403:ARG:NH2	10:A:602:HOH:O	2.21	0.74
5:L:130:GLN:O	5:L:133:SER:HB3	1.87	0.74
3:E:202:GLU:OE2	10:E:401:HOH:O	2.07	0.73
3:E:188:GLN:HA	3:E:191:SER:HB3	1.71	0.72
5:L:20:THR:HG23	5:L:80:THR:HG22	1.72	0.71
5:L:120:SER:OG	10:L:301:HOH:O	2.09	0.71
4:N:210:LYS:NZ	4:N:213:ASN:HA	2.05	0.70
3:E:61:ASP:O	10:E:402:HOH:O	2.09	0.70
4:N:10:GLU:OE2	10:N:302:HOH:O	2.10	0.70
3:E:169:SER:OG	1:F:171:PRO:HG2	1.91	0.69
1:C:71:SER:OG	10:C:301:HOH:O	2.08	0.69
4:N:210:LYS:HZ2	4:N:213:ASN:HA	1.55	0.69
2:B:393:THR:HG21	2:B:518:LEU:HB2	1.75	0.68
4:N:210:LYS:HE3	4:N:210:LYS:HA	1.74	0.68
4:H:91:THR:O	10:H:401:HOH:O	2.10	0.68
1:C:201:ASN:ND2	1:C:212:ASP:OD2	2.27	0.68
1:F:190:SER:CA	1:F:193:LEU:HD23	2.20	0.67
4:H:190:VAL:HG21	5:L:141:LEU:HD22	1.75	0.67
2:A:393:THR:CG2	2:A:518:LEU:H	2.08	0.67
3:D:153:LYS:HD2	3:D:198:GLN:OE1	1.94	0.67
4:N:210:LYS:HA	4:N:210:LYS:CE	2.24	0.66
1:F:192:SER:HA	1:F:195:THR:CG2	2.26	0.66
5:M:119:PRO:HB3	5:M:145:PHE:HB3	1.77	0.66
5:M:20:THR:O	10:M:401:HOH:O	2.13	0.65
4:H:16:ALA:HB1	9:H:301:GOL:H2	1.79	0.65
1:F:123:PRO:HB3	1:F:149:TYR:HB3	1.79	0.65
5:L:114:ARG:HD3	5:L:115:THR:O	1.97	0.64
5:L:114:ARG:NH2	5:L:117:ALA:HB2	2.12	0.64
4:H:168:LEU:CD2	4:H:191:VAL:HG21	2.12	0.64
3:E:124:PRO:HD3	3:E:136:LEU:CD2	2.28	0.64
3:D:38:GLN:HB2	3:D:48:LEU:HD11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:62:GLN:NE2	10:N:303:HOH:O	2.24	0.62
3:E:68:SER:OG	10:E:403:HOH:O	2.16	0.62
3:E:1:GLN:HG2	3:E:2:SER:N	2.11	0.61
4:H:40:ALA:HB3	4:H:43:GLN:HG3	1.80	0.61
2:B:363:ALA:O	2:B:527:PRO:HD3	2.01	0.61
5:L:44:GLN:HB2	5:L:50:LEU:HD22	1.82	0.61
5:M:43:GLN:HB2	5:M:53:LEU:HD11	1.82	0.61
1:F:192:SER:HA	1:F:195:THR:HG23	1.83	0.61
5:L:185:LEU:HD11	5:L:187:LEU:CD1	2.30	0.61
1:C:5:LEU:HD23	1:C:109:GLN:HE22	1.66	0.60
5:M:67:ARG:CZ	5:M:85:GLN:HG3	2.32	0.60
5:L:15:LEU:HD23	5:L:16:GLY:N	2.16	0.60
5:L:185:LEU:HD11	5:L:187:LEU:HD11	1.83	0.59
5:L:125:PRO:HB3	5:L:215:PHE:CE1	2.36	0.59
2:A:498:GLN:NE2	10:A:606:HOH:O	2.36	0.59
1:C:185:VAL:HG21	3:D:139:LEU:CD1	2.33	0.59
2:A:335:LEU:HD12	2:A:335:LEU:O	2.02	0.59
4:H:121:SER:OG	4:H:155:PHE:CZ	2.55	0.59
3:D:185:THR:OG1	3:D:188:GLN:HG2	2.03	0.59
2:B:388:ASN:HB3	2:B:527:PRO:HD2	1.85	0.58
5:L:207:LEU:HD13	5:L:211:VAL:CG2	2.32	0.58
5:L:60:ARG:HD2	5:L:64:VAL:O	2.03	0.58
5:L:89:VAL:HG13	5:L:110:VAL:O	2.03	0.58
4:N:208:ASN:OD1	4:N:210:LYS:HD2	2.04	0.57
5:M:189:LYS:O	5:M:193:GLU:HG2	2.05	0.57
5:L:195:HIS:O	5:L:217:ARG:NH2	2.38	0.57
2:A:447:GLY:HA2	2:A:498:GLN:HG2	1.87	0.56
4:H:17:SER:N	9:H:301:GOL:H2	2.18	0.56
4:H:12:LYS:HZ2	9:H:301:GOL:HO1	1.53	0.56
4:H:17:SER:H	9:H:301:GOL:C2	2.17	0.55
1:F:140:ALA:HB2	1:F:190:SER:OG	2.07	0.55
4:H:74:THR:HG22	10:H:436:HOH:O	2.04	0.55
3:D:188:GLN:HA	3:D:191:SER:HB3	1.89	0.55
2:B:393:THR:O	2:B:523:THR:HG22	2.06	0.55
3:E:184:LEU:HB3	3:E:188:GLN:HG3	1.87	0.55
1:F:143:GLY:HA2	1:F:158:TRP:CH2	2.42	0.55
4:H:209:HIS:CD2	4:H:211:PRO:HD2	2.41	0.55
5:L:36:LYS:HG2	5:L:56:TRP:CD2	2.41	0.55
5:L:67:ARG:NH2	5:L:88:ASP:OD1	2.35	0.55
1:C:91:THR:HG23	1:C:114:THR:HA	1.88	0.55
2:B:386:LYS:O	2:B:390:LEU:HD12	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:128:PRO:HD2	4:H:214:THR:CG2	2.35	0.55
3:E:38:GLN:HB2	3:E:48:LEU:HD11	1.88	0.55
4:N:11:VAL:HG21	4:N:156:PRO:HG3	1.90	0.54
3:D:152:TRP:O	3:D:153:LYS:HG3	2.08	0.54
1:C:6:GLU:HG2	1:C:96[B]:CYS:SG	2.48	0.54
5:M:45:LYS:NZ	5:M:87:GLU:O	2.30	0.54
5:M:44:GLN:HB2	5:M:50:LEU:HD22	1.90	0.53
5:L:156:VAL:HG22	5:L:198:TYR:CD2	2.43	0.53
5:M:24:LYS:HD2	5:M:76[B]:ASP:OD1	2.08	0.53
4:H:209:HIS:N	4:H:214:THR:O	2.31	0.53
3:D:46:LYS:NZ	10:D:404:HOH:O	2.42	0.52
5:M:67:ARG:NH1	5:M:85:GLN:HG3	2.24	0.52
5:L:43:GLN:HB2	5:L:53:LEU:HD11	1.91	0.52
4:H:208:ASN:HA	4:H:214:THR:O	2.10	0.51
2:A:420:ASP:OD2	10:A:601:HOH:O	2.19	0.51
4:N:210:LYS:HE3	4:N:210:LYS:CA	2.35	0.51
4:H:148:GLY:HA2	4:H:163:TRP:CH2	2.46	0.51
4:H:160:THR:HG22	4:H:208:ASN:O	2.11	0.51
4:N:72:ARG:HD2	4:N:72:ARG:O	2.11	0.50
4:H:197:SER:HA	4:H:200:THR:CG2	2.41	0.50
1:C:12:VAL:HG13	1:C:115:VAL:HG22	1.93	0.50
2:B:497:PHE:CE2	2:B:507:PRO:HB3	2.47	0.50
3:D:128:GLU:HG2	3:D:133:LYS:HB2	1.92	0.50
3:D:80:GLN:O	3:D:109:VAL:HG21	2.11	0.50
2:B:339:GLY:O	2:B:343:ASN:HB2	2.11	0.50
4:H:17:SER:O	9:H:301:GOL:H31	2.12	0.50
4:H:47:TRP:CZ2	4:H:49:GLY:HA2	2.47	0.50
5:L:68:PHE:CE1	5:L:81:ILE:HG12	2.46	0.50
5:L:185:LEU:CD1	5:L:187:LEU:HG	2.41	0.50
2:A:449:TYR:HA	2:A:494:SER:OG	2.11	0.49
1:C:102:GLY:HA2	2:B:489:TYR:OH	2.11	0.49
4:H:16:ALA:HB1	9:H:301:GOL:O2	2.12	0.49
4:N:32:TYR:HA	4:N:102:THR:HG23	1.93	0.49
4:N:75:SER:OG	10:N:301:HOH:O	2.19	0.49
3:E:185:THR:OG1	3:E:188:GLN:HG2	2.13	0.49
5:L:169:VAL:HG22	5:L:170:THR:O	2.11	0.49
3:D:136:LEU:N	3:D:136:LEU:HD12	2.27	0.49
4:H:47:TRP:HZ2	4:H:50:ILE:HG13	1.78	0.49
2:A:339:GLY:O	2:A:343:ASN:HB2	2.13	0.49
5:L:119:PRO:CB	5:L:145:PHE:HB3	2.37	0.49
3:E:136:LEU:HD12	3:E:182:LEU:HD23	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:128:PRO:HB3	4:N:154:TYR:HB3	1.95	0.48
4:N:148:GLY:HA2	4:N:163:TRP:CH2	2.48	0.48
4:N:162:SER:OG	4:N:206:ASN:HB2	2.13	0.48
5:M:37:ASN:O	5:M:56:TRP:HA	2.13	0.48
1:F:86:LEU:HB3	1:F:115:VAL:HG21	1.95	0.48
1:F:89:GLU:CD	1:F:89:GLU:H	2.17	0.48
4:N:47:TRP:CZ2	4:N:49:GLY:HA2	2.48	0.48
4:N:44:GLY:HA3	10:M:444:HOH:O	2.14	0.48
2:B:520:ALA:HB1	2:B:521:PRO:HD2	1.94	0.48
4:H:24:ALA:HB1	4:H:27:TYR:CE1	2.49	0.48
3:E:40:VAL:HG13	3:E:41:PRO:HD2	1.95	0.48
5:L:189:LYS:O	5:L:193:GLU:HG2	2.14	0.48
5:M:146:TYR:CG	5:M:147:PRO:HA	2.49	0.48
5:L:154:TRP:O	5:L:160:LEU:HD12	2.13	0.48
1:C:59:TYR:HE2	2:B:478:THR:HG21	1.79	0.47
4:N:36:TRP:CE2	4:N:81:MET:HB2	2.49	0.47
4:N:148:GLY:HA2	4:N:163:TRP:CZ2	2.49	0.47
5:L:160:LEU:HD12	5:L:161:GLN:N	2.29	0.47
2:B:520:ALA:HB1	2:B:521:PRO:CD	2.44	0.47
4:H:12:LYS:HE2	4:H:18:VAL:HG23	1.96	0.47
5:M:198:TYR:HB2	5:M:215:PHE:CE1	2.49	0.47
1:C:116:SER:OG	1:C:118:ALA:HB2	2.14	0.47
4:N:131:PHE:CE2	5:M:130:GLN:HG3	2.50	0.47
4:N:206:ASN:ND2	4:N:217:ASP:OD1	2.35	0.47
5:M:169:VAL:HG12	5:M:170:THR:O	2.15	0.47
4:H:12:LYS:CE	4:H:18:VAL:HG23	2.44	0.47
1:F:154:VAL:CG2	1:F:182:LEU:HD21	2.45	0.47
2:B:403:ARG:NH1	2:B:405:ASP:OD2	2.48	0.47
1:F:159:ASN:HA	1:F:199:ILE:HG12	1.96	0.47
4:H:135:PRO:HD3	4:H:147:LEU:HB2	1.96	0.47
5:L:141:LEU:HD12	5:L:181:LEU:O	2.14	0.47
1:C:44:GLY:HA3	10:D:428:HOH:O	2.15	0.46
2:B:364:ASP:OD2	2:B:367:VAL:HG23	2.14	0.46
3:E:154:ALA:HB2	3:E:195:TYR:CE1	2.50	0.46
4:H:163:TRP:CZ3	4:H:205:CYS:HB3	2.50	0.46
4:H:208:ASN:HA	4:H:215:LYS:HA	1.95	0.46
3:D:127:GLU:OE1	3:D:127:GLU:N	2.47	0.46
3:D:184:LEU:HB3	3:D:188:GLN:HG3	1.97	0.46
2:A:363:ALA:O	2:A:527:PRO:HD3	2.15	0.46
4:H:46:GLU:OE2	4:H:63:LYS:HD2	2.15	0.46
3:E:198:GLN:HG3	3:E:207:GLU:HG3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:VAL:HG22	1:F:182:LEU:HD21	1.97	0.46
5:M:186:THR:HG23	10:M:460:HOH:O	2.15	0.46
4:H:201:GLN:HG2	4:H:203:TYR:CZ	2.51	0.46
5:L:133:SER:OG	5:L:135:THR:HG22	2.16	0.46
1:F:182:LEU:C	1:F:182:LEU:HD12	2.36	0.46
2:A:447:GLY:CA	2:A:498:GLN:HG2	2.46	0.46
1:F:143:GLY:HA2	1:F:158:TRP:CZ2	2.50	0.46
5:L:56:TRP:O	5:L:57:ALA:HB3	2.16	0.46
3:E:117:PRO:HB3	3:E:143:PHE:HB3	1.97	0.46
1:C:182:LEU:HD12	1:C:182:LEU:C	2.37	0.45
1:C:47:TRP:CE3	3:D:98:GLY:HA3	2.50	0.45
1:C:174:LEU:HD13	1:C:180:TYR:CE1	2.51	0.45
4:H:87:ARG:HG3	4:H:89:ASP:OD1	2.15	0.45
3:E:176:TYR:HE2	8:E:301:CIT:H42	1.81	0.45
2:B:475:ALA:O	2:B:487:ASN:HB2	2.17	0.45
4:N:76:THR:HG23	10:N:301:HOH:O	2.17	0.45
3:E:189:TRP:CZ2	3:E:212:PRO:HA	2.51	0.45
1:F:166:GLY:O	1:F:186:VAL:HA	2.16	0.45
2:A:395:VAL:HG22	2:A:515:PHE:HD1	1.82	0.45
4:N:187:LEU:HD12	4:N:187:LEU:C	2.37	0.45
1:F:186:VAL:HG22	1:F:188:VAL:HG13	1.98	0.45
5:M:125:PRO:HB3	5:M:215:PHE:CE2	2.52	0.45
5:L:60:ARG:CZ	5:L:66:ASP:HA	2.47	0.45
5:L:144:ASN:HA	5:L:178:THR:OG1	2.17	0.45
5:L:176:ASP:HB3	5:L:178:THR:CG2	2.33	0.45
3:E:98:GLY:HA3	1:F:47:TRP:CZ3	2.52	0.45
2:A:468:ILE:HD11	3:D:62:ARG:HB3	1.98	0.45
4:H:12:LYS:HD2	9:H:301:GOL:O1	2.16	0.45
4:H:36:TRP:CE2	4:H:81:MET:HB2	2.52	0.45
4:H:207:VAL:O	4:H:216:VAL:N	2.49	0.45
3:D:198:GLN:HG3	3:D:207:GLU:HG3	1.98	0.45
2:B:399:SER:HA	2:B:510:VAL:O	2.17	0.45
3:E:189:TRP:O	3:E:212:PRO:HG3	2.16	0.45
2:A:364:ASP:OD2	2:A:367:VAL:HG21	2.17	0.45
1:C:39:GLN:C	1:C:92:ALA:HB1	2.37	0.45
4:H:135:PRO:HD3	4:H:147:LEU:CB	2.47	0.45
1:C:47:TRP:CZ3	3:D:98:GLY:HA3	2.52	0.44
4:H:155:PHE:CE1	4:H:156:PRO:HB3	2.52	0.44
2:A:360:ASN:H	2:A:523:THR:HB	1.82	0.44
5:L:161:GLN:OE1	5:L:164:ASN:ND2	2.50	0.44
3:E:131:ALA:O	3:E:132:ASN:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:364:ASP:HB2	2:A:367:VAL:HG23	2.00	0.44
4:H:163:TRP:CH2	4:H:205:CYS:HB3	2.52	0.44
5:L:44:GLN:HB2	5:L:50:LEU:CD2	2.47	0.44
3:D:170:LYS:HE2	3:D:174:ASN:O	2.17	0.44
3:D:136:LEU:HD11	3:D:184:LEU:HD12	1.98	0.44
5:L:84:LEU:HD12	5:L:88:ASP:HB2	1.99	0.44
1:C:143:GLY:HA2	1:C:158:TRP:CZ2	2.52	0.44
5:L:156:VAL:HG22	5:L:198:TYR:HD2	1.81	0.44
9:D:301:GOL:O1	10:D:401:HOH:O	2.21	0.44
2:B:346:ARG:HB3	10:B:794:HOH:O	2.18	0.44
3:E:80:GLN:O	3:E:109:VAL:HG21	2.17	0.44
5:M:153:GLN:HB3	5:M:160:LEU:HD21	1.99	0.44
3:D:154:ALA:HB2	3:D:195:TYR:CE1	2.52	0.44
3:E:28:ASN:OD1	3:E:29:ILE:N	2.44	0.44
4:H:160:THR:CG2	4:H:208:ASN:OD1	2.66	0.44
3:D:51:ALA:O	3:D:52:ASN:HB2	2.17	0.44
1:C:143:GLY:HA2	1:C:158:TRP:CH2	2.53	0.43
2:B:440:ASN:HA	4:N:104:PHE:CG	2.53	0.43
4:N:47:TRP:HZ2	4:N:50:ILE:HG13	1.84	0.43
5:M:67:ARG:HH12	5:M:88:ASP:CG	2.13	0.43
5:L:51:ARG:HA	10:L:306:HOH:O	2.18	0.43
3:E:124:PRO:HD3	3:E:136:LEU:HD23	1.98	0.43
1:F:12:VAL:O	1:F:115:VAL:HA	2.18	0.43
2:A:390:LEU:HD12	2:A:390:LEU:HA	1.70	0.43
5:L:185:LEU:HD13	5:L:187:LEU:HG	2.01	0.43
4:N:34:MET:SD	4:N:96[B]:CYS:SG	3.16	0.43
4:N:101:VAL:HG23	4:N:103:ILE:H	1.84	0.43
4:H:148:GLY:HA2	4:H:163:TRP:CZ2	2.53	0.43
5:L:192:TYR:HA	5:L:198:TYR:OH	2.18	0.43
1:F:98:LYS:HB3	1:F:106:ILE:CG2	2.48	0.43
2:A:393:THR:HG21	2:A:518:LEU:N	2.26	0.43
5:M:56:TRP:O	5:M:57:ALA:HB3	2.19	0.43
1:C:213:LYS:HA	1:C:213:LYS:HD3	1.64	0.42
4:H:32:TYR:HA	4:H:102:THR:HG23	2.00	0.42
5:L:131:LEU:HB3	5:L:189:LYS:HG3	2.01	0.42
2:B:360:ASN:H	2:B:523:THR:HG23	1.84	0.42
4:H:12:LYS:NZ	9:H:301:GOL:O1	2.40	0.42
4:H:91:THR:HG23	4:H:119:THR:HA	2.00	0.42
7:B:601:MPD:H52	7:B:601:MPD:O2	2.20	0.42
2:A:444:LYS:HD3	10:A:690:HOH:O	2.19	0.42
5:M:89:VAL:HG13	5:M:109:LYS:NZ	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:136:LEU:HB2	3:D:182:LEU:HB3	2.01	0.42
2:B:494:SER:O	10:B:701:HOH:O	2.22	0.42
4:N:210:LYS:N	4:N:211:PRO:CD	2.82	0.42
1:F:131:SER:OG	1:F:132:SER:N	2.53	0.42
4:H:17:SER:O	9:H:301:GOL:H2	2.20	0.42
4:H:87:ARG:NH2	10:H:404:HOH:O	2.48	0.42
2:B:444:LYS:HB2	2:B:444:LYS:HE3	1.77	0.42
1:F:91:THR:HG23	1:F:114:THR:HA	2.01	0.42
3:E:136:LEU:HB2	3:E:182:LEU:HB3	2.01	0.41
3:E:149:THR:HG23	10:E:485:HOH:O	2.19	0.41
4:H:151:VAL:HG11	4:H:159:VAL:HG21	2.02	0.41
5:L:141:LEU:HD12	5:L:142:LEU:N	2.35	0.41
2:B:403:ARG:HD2	2:B:505:TYR:HA	2.02	0.41
1:F:193:LEU:HD22	1:F:193:LEU:N	2.35	0.41
4:H:40:ALA:CB	4:H:43:GLN:HG3	2.50	0.41
2:A:364:ASP:HB2	2:A:367:VAL:CG2	2.50	0.41
1:C:91:THR:O	1:C:92:ALA:HB2	2.20	0.41
1:F:102:GLY:HA2	2:A:489:TYR:OH	2.20	0.41
4:H:160:THR:HG21	4:H:208:ASN:OD1	2.21	0.41
3:D:191:SER:O	3:D:191:SER:OG	2.38	0.41
5:M:89:VAL:HG13	5:M:109:LYS:HZ2	1.86	0.41
5:M:181:LEU:C	5:M:181:LEU:HD23	2.41	0.41
5:L:209:SER:OG	5:L:210:PRO:HD2	2.21	0.41
3:E:51:ALA:O	3:E:52:ASN:HB2	2.20	0.41
2:A:415:THR:HG22	10:A:638:HOH:O	2.20	0.41
1:C:203:ASN:ND2	1:C:209:THR:O	2.45	0.41
1:F:98:LYS:HB3	1:F:106:ILE:HG22	2.02	0.41
2:A:347:PHE:CE2	2:A:399:SER:HB2	2.56	0.41
4:N:210:LYS:HZ1	4:N:213:ASN:CG	2.25	0.41
4:H:155:PHE:HA	4:H:156:PRO:HA	1.84	0.41
1:F:83:MET:HE2	1:F:86:LEU:CD2	2.41	0.41
3:E:122:PHE:CD2	1:F:128:LEU:HD13	2.56	0.40
3:E:18:VAL:HB	3:E:79:LEU:HD11	2.03	0.40
5:M:213:LYS:HD3	5:M:213:LYS:HA	1.90	0.40
3:E:112:GLN:HB2	3:E:113:PRO:CD	2.52	0.40
2:A:345:THR:OG1	3:D:113:PRO:HD3	2.22	0.40
4:H:101:VAL:HG23	4:H:103:ILE:H	1.87	0.40
4:H:176:PRO:HD2	5:L:168:SER:OG	2.22	0.40
5:L:185:LEU:HD11	5:L:187:LEU:HG	2.02	0.40

All (1) 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)
3:E:187:GLU:OE1	5:L:213:LYS:NZ[1_566]	2.10	0.10

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	C	214/224 (96%)	208 (97%)	6 (3%)	0	100	100
1	F	218/224 (97%)	212 (97%)	6 (3%)	0	100	100
2	A	193/205 (94%)	185 (96%)	8 (4%)	0	100	100
2	B	193/205 (94%)	187 (97%)	6 (3%)	0	100	100
3	D	210/216 (97%)	205 (98%)	5 (2%)	0	100	100
3	E	211/216 (98%)	203 (96%)	8 (4%)	0	100	100
4	H	222/229 (97%)	215 (97%)	7 (3%)	0	100	100
4	N	223/229 (97%)	219 (98%)	4 (2%)	0	100	100
5	L	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
5	M	217/220 (99%)	210 (97%)	7 (3%)	0	100	100
All	All	2118/2188 (97%)	2053 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	164/184 (89%)	162 (99%)	2 (1%)	71	80
1	F	171/184 (93%)	170 (99%)	1 (1%)	86	91
2	A	162/177 (92%)	161 (99%)	1 (1%)	86	91
2	B	163/177 (92%)	163 (100%)	0	100	100
3	D	172/181 (95%)	172 (100%)	0	100	100
3	E	175/181 (97%)	172 (98%)	3 (2%)	60	71
4	H	169/194 (87%)	166 (98%)	3 (2%)	59	68
4	N	183/194 (94%)	180 (98%)	3 (2%)	62	73
5	L	180/194 (93%)	175 (97%)	5 (3%)	43	52
5	M	185/194 (95%)	183 (99%)	2 (1%)	73	82
All	All	1724/1860 (93%)	1704 (99%)	20 (1%)	73	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	96[A]	CYS
1	C	96[B]	CYS
3	E	23	SER
3	E	82	GLU
3	E	183	SER
1	F	213	LYS
2	A	377	PHE
4	N	72	ARG
4	N	141	SER
4	N	208	ASN
5	M	67	ARG
5	M	83	SER
4	H	72	ARG
4	H	75	SER
4	H	104	PHE
5	L	66	ASP
5	L	114	ARG
5	L	127	SER
5	L	133	SER
5	L	182	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
5	M	153	GLN
4	H	213	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 ⓘ

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	$\# Z > 2$
6	NAG	G	1	2,6	14,14,15	0.37	0	17,19,21	0.38	0
6	NAG	G	2	6	14,14,15	0.21	0	17,19,21	0.40	0
6	FUC	G	3	6	10,10,11	0.77	0	14,14,16	0.80	0
6	NAG	I	1	2,6	14,14,15	0.38	0	17,19,21	0.48	0
6	NAG	I	2	6	14,14,15	0.28	0	17,19,21	0.40	0
6	FUC	I	3	6	10,10,11	0.77	0	14,14,16	0.96	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
6	NAG	G	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	FUC	G	3	6	-	-	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

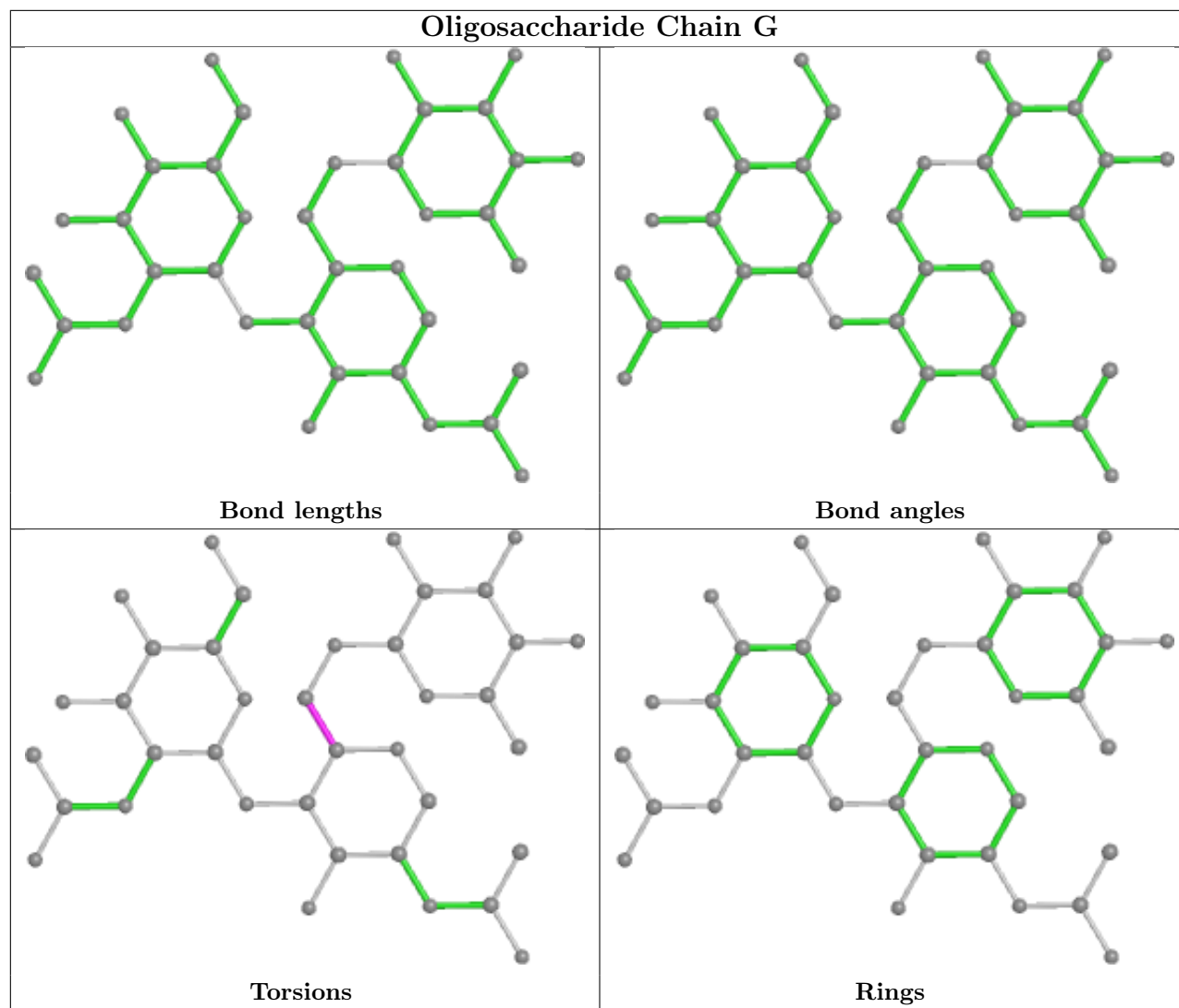
All (2) torsion outliers are listed below:

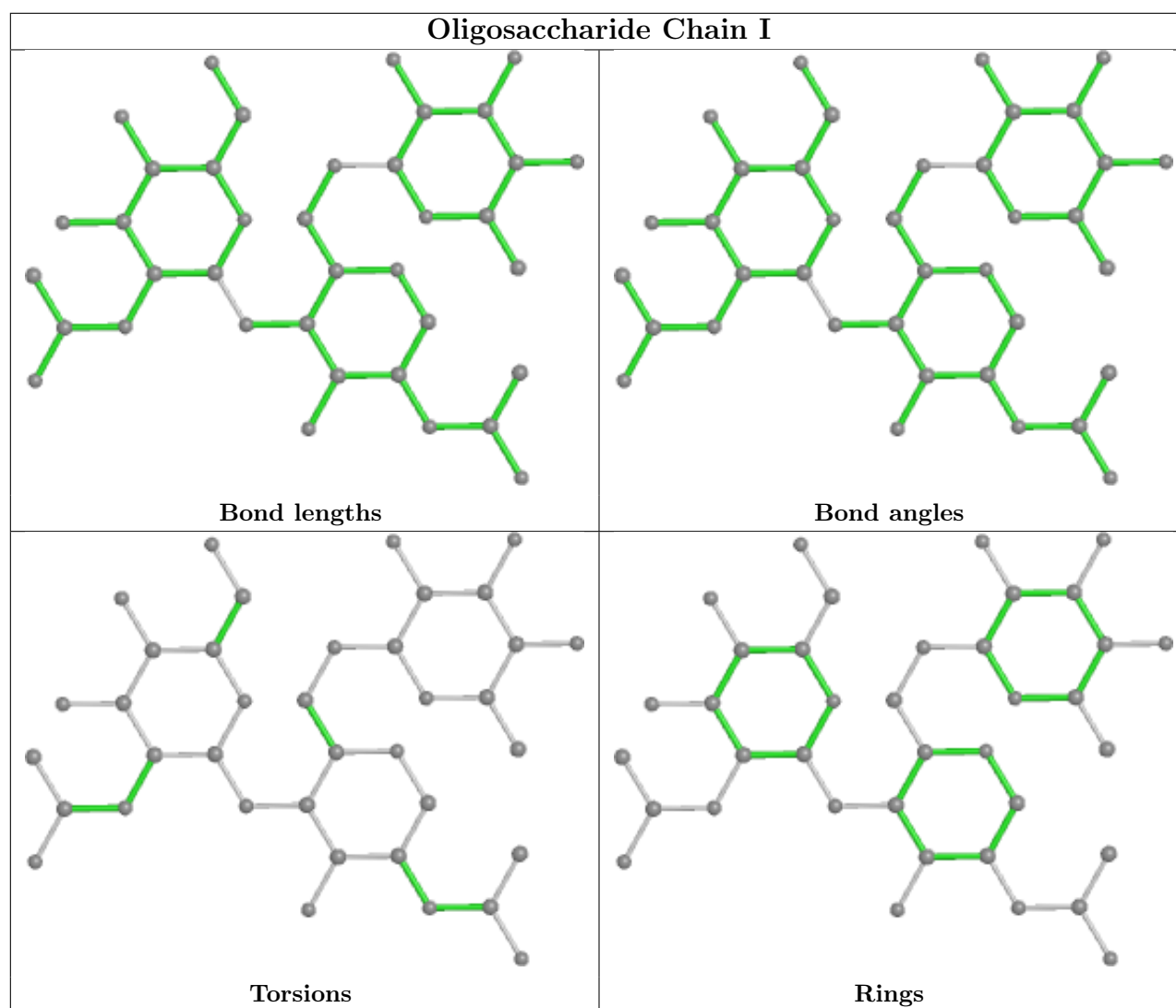
Mol	Chain	Res	Type	Atoms
6	G	1	NAG	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6

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](#)

5 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	MPD	B	601	-	7,7,7	0.25	0	9,10,10	0.38	0
9	GOL	M	301	-	5,5,5	0.76	0	5,5,5	1.06	0
8	CIT	E	301	-	3,12,12	1.32	0	3,17,17	2.22	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	H	301	-	5,5,5	0.95	0	5,5,5	1.11	1 (20%)
9	GOL	D	301	-	5,5,5	0.96	0	5,5,5	1.14	1 (20%)

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	MPD	B	601	-	-	1/5/5/5	-
9	GOL	M	301	-	-	1/4/4/4	-
8	CIT	E	301	-	-	1/6/16/16	-
9	GOL	H	301	-	-	1/4/4/4	-
9	GOL	D	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	E	301	CIT	C3-C2-C1	-2.88	110.37	114.98
8	E	301	CIT	C3-C4-C5	-2.13	111.58	114.98
9	D	301	GOL	C3-C2-C1	-2.06	103.71	111.70
9	H	301	GOL	C3-C2-C1	-2.02	103.84	111.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	301	GOL	O2-C2-C3-O3
9	M	301	GOL	O2-C2-C3-O3
9	H	301	GOL	O2-C2-C3-O3
8	E	301	CIT	O7-C3-C4-C5
9	D	301	GOL	C1-C2-C3-O3
7	B	601	MPD	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	601	MPD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	301	CIT	1	0
9	H	301	GOL	11	0
9	D	301	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	213/224 (95%)	0.11	11 (5%) 27 30	30, 56, 87, 99	0
1	F	219/224 (97%)	0.20	22 (10%) 7 7	29, 52, 91, 102	0
2	A	195/205 (95%)	0.26	6 (3%) 49 52	27, 35, 81, 91	0
2	B	195/205 (95%)	0.05	4 (2%) 63 66	23, 35, 80, 91	0
3	D	212/216 (98%)	-0.21	2 (0%) 84 85	26, 41, 58, 71	0
3	E	213/216 (98%)	-0.27	2 (0%) 84 85	26, 38, 65, 77	0
4	H	223/229 (97%)	0.31	16 (7%) 15 16	30, 61, 95, 102	0
4	N	223/229 (97%)	-0.09	2 (0%) 84 85	28, 47, 72, 88	0
5	L	219/220 (99%)	0.22	10 (4%) 32 35	31, 64, 91, 101	0
5	M	218/220 (99%)	-0.30	0 100 100	28, 48, 70, 83	0
All	All	2130/2188 (97%)	0.03	75 (3%) 44 46	23, 48, 86, 102	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	199	GLY	6.6
4	N	137	SER	4.9
4	H	168	LEU	4.7
1	C	193	LEU	4.4
1	C	162	ALA	4.3
2	A	369	TYR	4.0
1	C	163	LEU	4.0
1	F	198	TYR	4.0
5	L	198	TYR	4.0
5	L	136	ALA	3.9
5	L	86	ALA	3.8
1	C	194	GLY	3.7
4	H	166	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	139	THR	3.6
1	F	132	SER	3.6
2	A	519	HIS	3.4
1	F	162	ALA	3.4
1	F	138	GLY	3.2
1	C	151	PRO	3.2
1	F	135	THR	3.2
2	B	518	LEU	3.2
1	F	165	SER	3.1
1	F	194	GLY	3.1
4	H	137	SER	3.1
1	F	134	SER	2.9
3	E	1	GLN	2.8
1	C	160	SER	2.8
1	F	158	TRP	2.8
1	F	131	SER	2.8
1	F	140	ALA	2.8
4	H	1	LEU	2.7
2	B	517	LEU	2.7
1	F	192	SER	2.7
2	A	384	PRO	2.7
2	B	369	TYR	2.7
4	H	2	VAL	2.6
1	F	196	GLN	2.6
5	L	133	SER	2.6
5	L	195	HIS	2.6
4	H	208	ASN	2.5
4	H	167	ALA	2.5
2	A	385	THR	2.5
1	F	136	SER	2.5
1	F	197	THR	2.5
3	D	116	ASN	2.5
4	H	204	ILE	2.4
1	F	164	THR	2.4
4	H	216	VAL	2.4
2	A	517	LEU	2.4
2	B	367	VAL	2.4
1	C	196	GLN	2.4
4	N	42	GLY	2.4
4	H	165	SER	2.4
4	H	214	THR	2.3
1	C	158	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	L	199	ALA	2.3
1	F	163	LEU	2.3
4	H	200	THR	2.3
5	L	135	THR	2.3
4	H	197	SER	2.3
1	F	212	ASP	2.3
5	L	112	ILE	2.2
5	L	186	THR	2.2
3	D	172	SER	2.2
2	A	335	LEU	2.2
3	E	2	SER	2.1
1	F	199	ILE	2.0
5	L	187	LEU	2.0
1	C	138	GLY	2.0
4	H	207	VAL	2.0
4	H	198	LEU	2.0
1	C	195	THR	2.0
1	F	139	THR	2.0
1	F	17	SER	2.0
1	F	133	LYS	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.

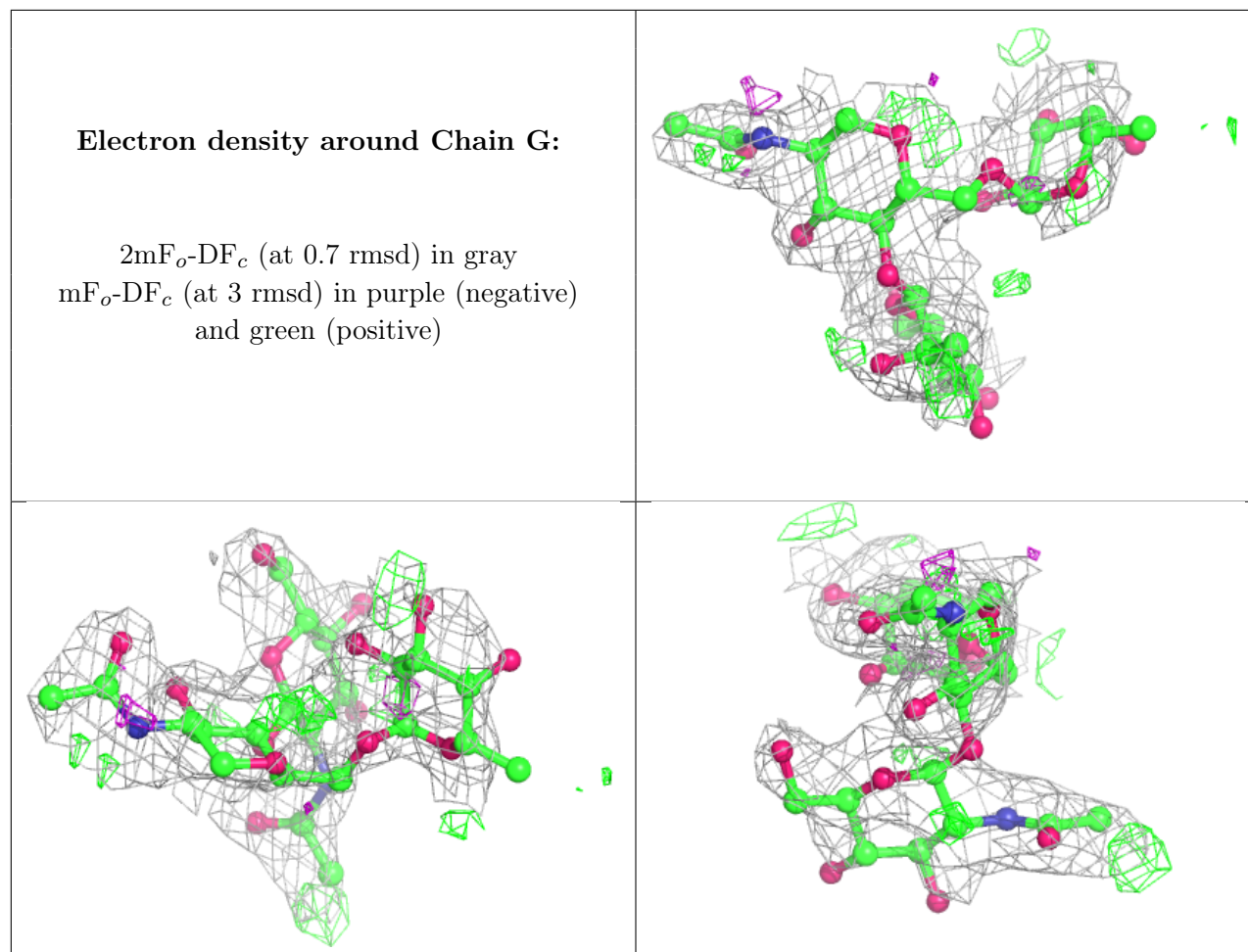
6.3 Carbohydrates [i](#)

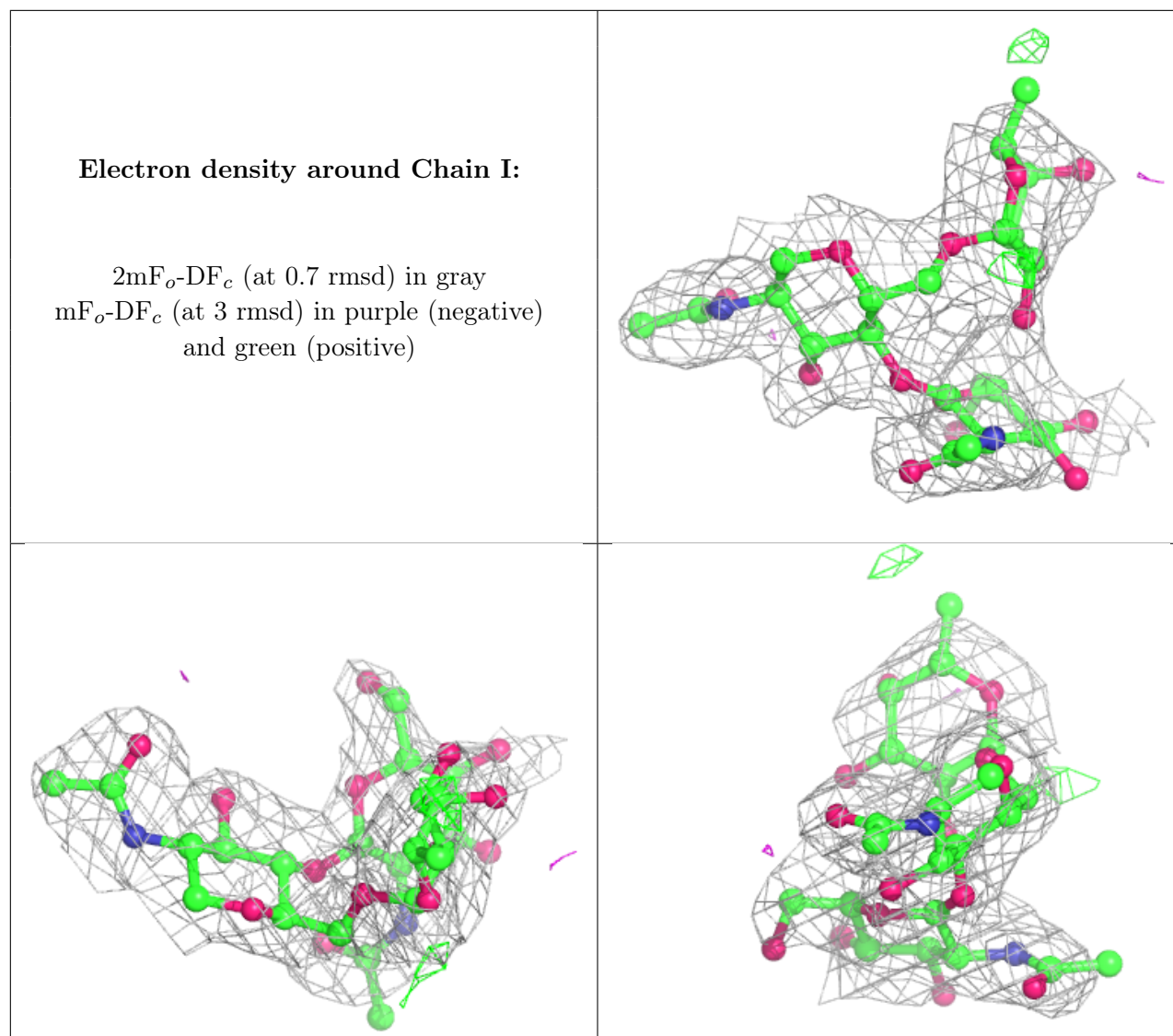
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	FUC	G	3	10/11	0.70	0.31	99,102,106,108	0
6	NAG	G	2	14/15	0.74	0.24	76,94,103,104	0
6	NAG	I	2	14/15	0.75	0.29	81,92,99,104	0
6	NAG	G	1	14/15	0.82	0.20	51,70,93,97	0
6	FUC	I	3	10/11	0.85	0.21	86,94,98,100	0
6	NAG	I	1	14/15	0.91	0.12	43,67,86,93	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CIT	E	301	13/13	0.77	0.21	54,75,92,100	0
9	GOL	H	301	6/6	0.79	0.31	55,73,89,89	0
9	GOL	D	301	6/6	0.86	0.21	56,72,78,86	0
7	MPD	B	601	8/8	0.87	0.22	48,64,72,87	0
9	GOL	M	301	6/6	0.88	0.20	48,65,78,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.