



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:48 AM BST

PDB ID : 5I3U  
Title : STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE N-SITE COM-  
PLEX; CATALYTIC INCORPORATION OF AZTMP to A DNA aptamer  
in CRYSTAL  
Authors : Das, K.; Arnold, E.  
Deposited on : 2016-02-11  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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  
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

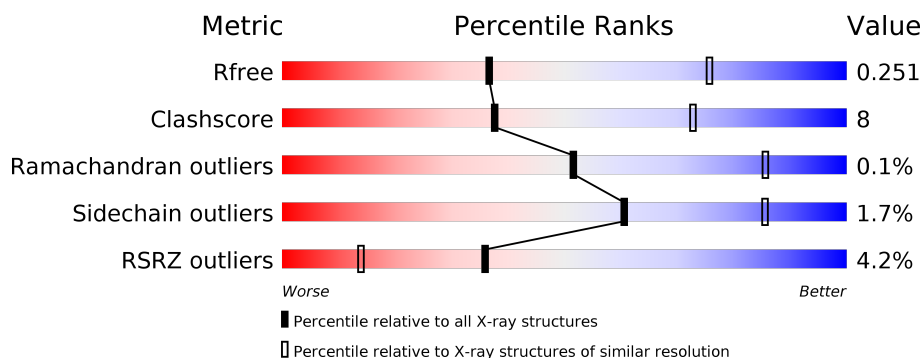
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




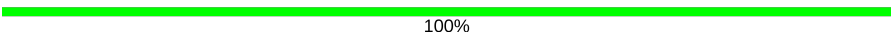
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	555	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>
1	C	555	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
2	B	444	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
2	D	444	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
3	E	39	<div> <div></div> <div> <div></div> <div>59%</div> <div>31%</div> <div>.</div> <div>8%</div> </div> </div>
3	F	39	<div> <div></div> <div> <div></div> <div>67%</div> <div>23%</div> <div>.</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	 50%50%
4	H	2	 100%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17337 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 HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4477	2898	745	827	7			
1	C	553	Total	C	N	O	S	0	0	0
			4495	2910	748	830	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3430	2234	567	622	7			
2	D	410	Total	C	N	O	S	0	1	0
			3391	2212	559	614	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P03366
B	-14	ALA	-	expression tag	UNP P03366
B	-13	HIS	-	expression tag	UNP P03366
B	-12	HIS	-	expression tag	UNP P03366
B	-11	HIS	-	expression tag	UNP P03366
B	-10	HIS	-	expression tag	UNP P03366
B	-9	HIS	-	expression tag	UNP P03366
B	-8	HIS	-	expression tag	UNP P03366
B	-7	ALA	-	expression tag	UNP P03366
B	-6	LEU	-	expression tag	UNP P03366

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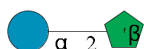
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLU	-	expression tag	UNP P03366
B	-4	VAL	-	expression tag	UNP P03366
B	-3	LEU	-	expression tag	UNP P03366
B	-2	PHE	-	expression tag	UNP P03366
B	-1	GLN	-	expression tag	UNP P03366
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	-15	MET	-	initiating methionine	UNP P03366
D	-14	ALA	-	expression tag	UNP P03366
D	-13	HIS	-	expression tag	UNP P03366
D	-12	HIS	-	expression tag	UNP P03366
D	-11	HIS	-	expression tag	UNP P03366
D	-10	HIS	-	expression tag	UNP P03366
D	-9	HIS	-	expression tag	UNP P03366
D	-8	HIS	-	expression tag	UNP P03366
D	-7	ALA	-	expression tag	UNP P03366
D	-6	LEU	-	expression tag	UNP P03366
D	-5	GLU	-	expression tag	UNP P03366
D	-4	VAL	-	expression tag	UNP P03366
D	-3	LEU	-	expression tag	UNP P03366
D	-2	PHE	-	expression tag	UNP P03366
D	-1	GLN	-	expression tag	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	36	Total	C	N	O	P	0	0	0
			742	350	135	221	36			
3	F	36	Total	C	N	O	P	0	0	0
			742	350	135	221	36			

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			

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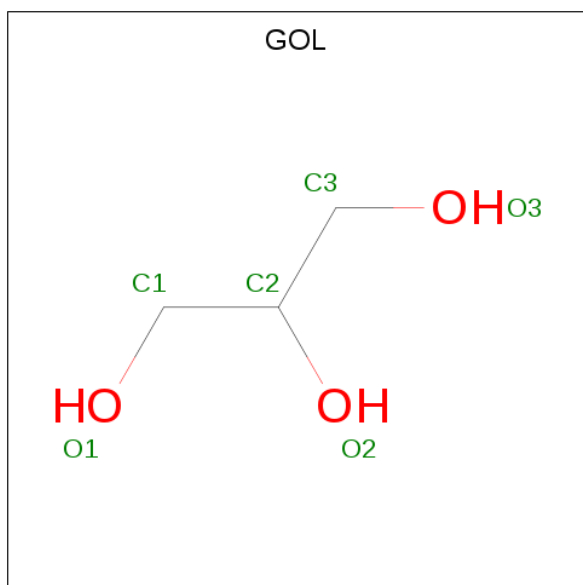
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

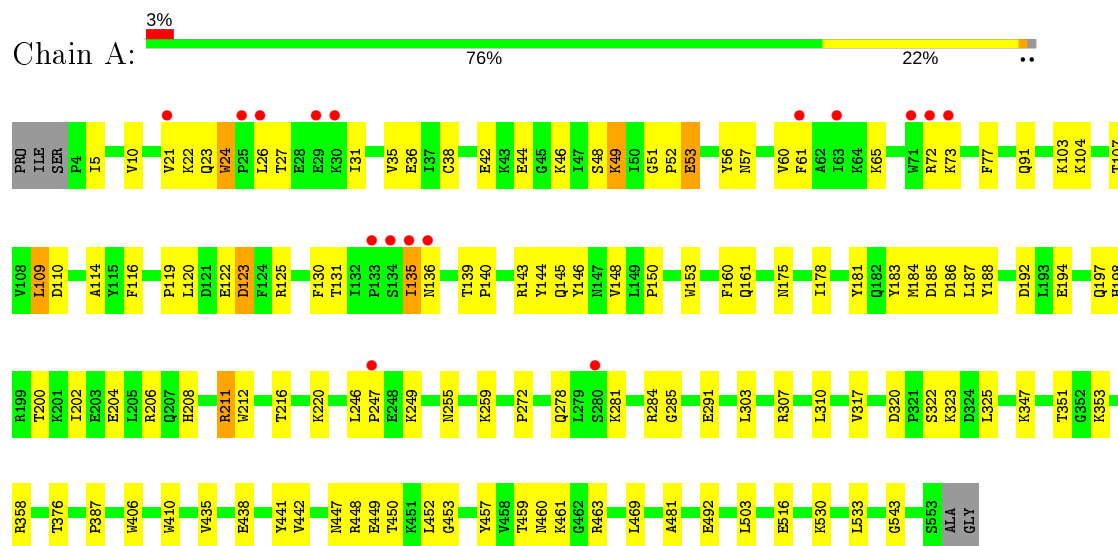


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

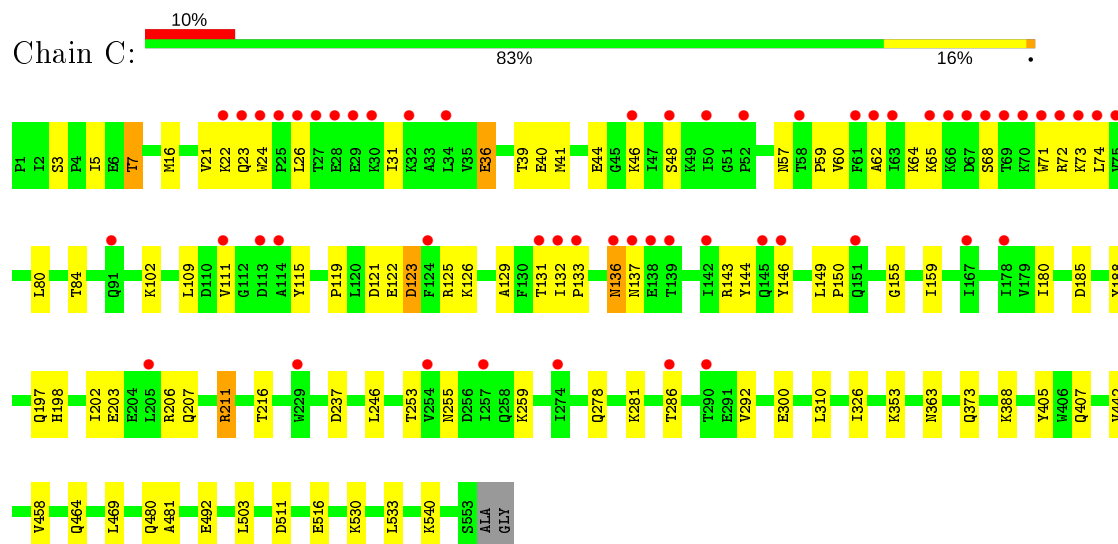
### 3 Residue-property plots [i](#)

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.

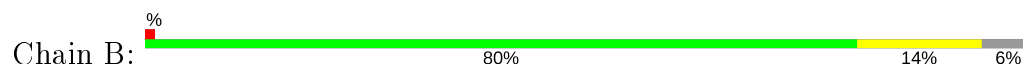
#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

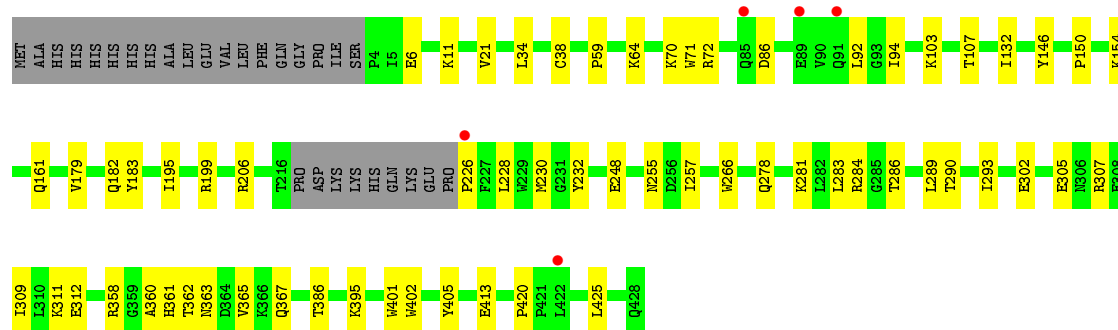


#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

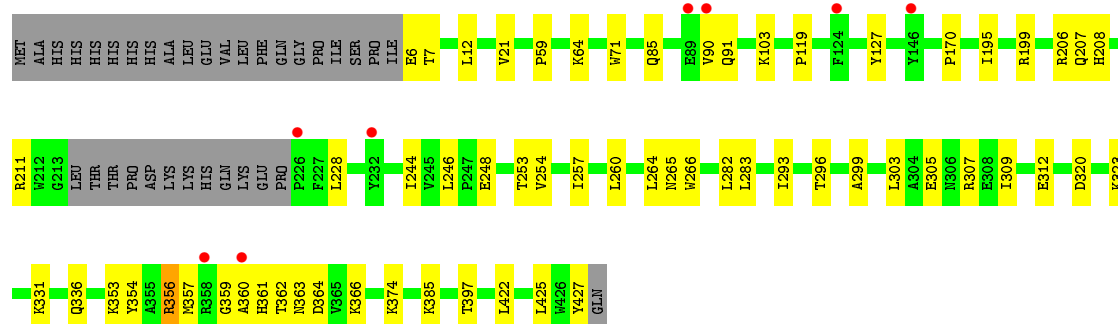
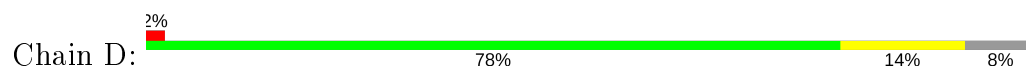


#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT





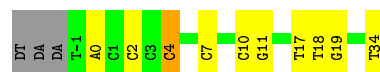
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 3: DNA (39-MER)



• Molecule 3: DNA (39-MER)



• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose





C1C1  
FR02

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.24Å 128.71Å 131.66Å 90.00° 100.84° 90.00°	Depositor
Resolution (Å)	48.10 – 3.00 80.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.10-3.00) 98.4 (80.51-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.223 , 0.254 0.223 , 0.251	Depositor DCC
$R_{free}$ test set	2343 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.5	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: OMC, GOL, MG, GLC, ATM, FRU

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	0.28	0/4594	0.46	0/6241
1	C	0.25	0/4613	0.45	0/6268
2	B	0.26	0/3528	0.44	0/4791
2	D	0.27	0/3493	0.44	0/4747
3	E	0.56	1/759 (0.1%)	1.00	3/1170 (0.3%)
3	F	0.52	0/759	0.97	0/1170
All	All	0.30	1/17746 (0.0%)	0.53	3/24387 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	19	DG	C4'-O4'	5.96	1.51	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	19	DG	O4'-C4'-C3'	-7.56	101.47	106.00
3	E	19	DG	C5'-C4'-O4'	5.99	120.67	109.30
3	E	31	DG	O4'-C4'-C3'	-5.31	102.37	104.50

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	4477	0	4524	110	0
1	C	4495	0	4549	63	1
2	B	3430	0	3460	43	0
2	D	3391	0	3411	49	1
3	E	742	0	408	15	0
3	F	742	0	408	6	0
4	G	23	0	21	2	0
4	H	23	0	21	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	12	0	16	1	0
All	All	17337	0	16818	262	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 8.

All (262) 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:44:GLU:CG	1:A:46:LYS:HE2	1.75	1.15
1:A:44:GLU:HG3	1:A:46:LYS:HE2	1.17	1.10
1:A:447:ASN:OD1	1:A:450:THR:N	2.02	0.92
2:D:356:ARG:HD2	2:D:361:HIS:HE1	1.35	0.92
1:A:448:ARG:HH22	3:E:18:DT:H6	1.19	0.91
1:C:122:GLU:HA	1:C:125:ARG:HE	1.36	0.91
1:A:448:ARG:NH2	3:E:18:DT:H6	1.72	0.88
1:A:450:THR:HG22	1:A:452:LEU:HG	1.57	0.86
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.76	0.85
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.10	0.85
1:A:448:ARG:NH2	3:E:18:DT:H2'	1.91	0.85
1:C:3:SER:HB2	1:C:211:ARG:HH22	1.45	0.81
2:B:206:ARG:NH2	2:B:230:MET:O	2.16	0.79
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.65	0.79
1:A:438:GLU:CD	1:A:463:ARG:HH21	1.88	0.77
1:A:447:ASN:HB3	1:A:450:THR:HB	1.66	0.76
2:B:70:LYS:HG3	2:B:226:PRO:HD2	1.67	0.75
1:A:44:GLU:HG2	1:A:46:LYS:HE2	1.66	0.72
2:D:356:ARG:HD2	2:D:361:HIS:CE1	2.22	0.72
2:D:354:TYR:HE1	2:D:374:LYS:HD2	1.56	0.71
1:A:450:THR:HG22	1:A:452:LEU:CG	2.21	0.71
3:E:18:DT:H4'	3:E:19:DG:C8	2.26	0.70
2:B:402:TRP:HE1	6:B:2003:GOL:H32	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:GLY:O	2:D:362:THR:HG22	1.90	0.69
1:A:448:ARG:NH2	3:E:18:DT:C2'	2.55	0.69
1:A:459:THR:HG22	1:A:461:LYS:H	1.58	0.69
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.57	0.69
1:C:131:THR:HG22	1:C:143:ARG:HG2	1.74	0.68
1:A:122:GLU:HA	1:A:125:ARG:HE	1.56	0.68
2:D:354:TYR:CE1	2:D:374:LYS:HD2	2.29	0.68
2:D:309:ILE:O	2:D:312:GLU:HG2	1.93	0.68
1:C:206:ARG:NH2	1:C:216:THR:O	2.26	0.68
1:C:23:GLN:HE22	1:C:60:VAL:H	1.41	0.68
1:A:91:GLN:OE1	1:A:161:GLN:NE2	2.28	0.67
1:A:56:TYR:O	1:A:143:ARG:NH1	2.25	0.65
3:F:18:DT:H4'	3:F:19:DG:C8	2.30	0.65
2:B:278:GLN:HB2	2:B:302:GLU:OE1	1.97	0.65
1:C:255:ASN:OD1	1:C:259:LYS:NZ	2.26	0.65
1:C:65:LYS:HB2	1:C:72:ARG:HG3	1.79	0.65
1:C:60:VAL:HG11	1:C:73:LYS:HE3	1.81	0.63
1:C:22:LYS:O	1:C:59:PRO:HG3	2.00	0.62
2:D:260:LEU:HD21	2:D:303:LEU:HD21	1.81	0.62
1:A:206:ARG:NH2	1:A:216:THR:O	2.33	0.61
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.83	0.61
2:B:307:ARG:O	2:B:311:LYS:HG3	2.01	0.61
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.82	0.61
1:C:278:GLN:OE1	1:C:281:LYS:NZ	2.33	0.60
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.37	0.60
1:A:185:ASP:OD1	1:A:186:ASP:N	2.35	0.59
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.27	0.59
1:C:23:GLN:HG2	1:C:133:PRO:HD3	1.84	0.59
1:A:255:ASN:OD1	1:A:259:LYS:NZ	2.31	0.59
2:D:356:ARG:CZ	2:D:361:HIS:CE1	2.85	0.59
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.83	0.58
1:A:60:VAL:HG11	1:A:73:LYS:HE3	1.85	0.58
1:C:458:VAL:HG23	1:C:464:GLN:HG2	1.86	0.58
2:B:360:ALA:O	2:B:361:HIS:HB2	2.02	0.58
2:D:362:THR:HG23	2:D:363:ASN:N	2.18	0.58
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.34	0.58
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.85	0.58
1:A:438:GLU:CG	1:A:459:THR:HG21	2.33	0.58
1:A:123:ASP:N	1:A:123:ASP:OD1	2.36	0.58
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.39	0.58
2:D:257:ILE:HD13	2:D:293:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:ARG:NH1	2:D:361:HIS:CE1	2.73	0.57
1:A:448:ARG:HH21	3:E:18:DT:C2'	2.18	0.57
2:D:305:GLU:O	2:D:309:ILE:HG13	2.06	0.56
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.39	0.55
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.88	0.55
2:D:356:ARG:CD	2:D:361:HIS:HE1	2.14	0.55
2:B:358:ARG:NH2	2:B:405:TYR:O	2.40	0.55
1:C:503:LEU:HD23	2:D:422:LEU:HD22	1.89	0.55
1:C:31:ILE:HG23	1:C:132:ILE:HD11	1.89	0.55
2:D:296:THR:HG23	2:D:299:ALA:H	1.71	0.55
2:D:323:LYS:O	2:D:385:LYS:NZ	2.39	0.55
1:A:183:TYR:OH	3:E:32:DG:N3	2.36	0.55
1:C:3:SER:CB	1:C:211:ARG:HH22	2.17	0.55
1:C:40:GLU:O	1:C:44:GLU:HG2	2.06	0.55
1:A:23:GLN:HE22	1:A:60:VAL:H	1.53	0.55
1:A:44:GLU:CG	1:A:46:LYS:CE	2.68	0.54
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.89	0.54
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.89	0.54
1:C:102:LYS:HE2	1:C:237:ASP:HA	1.89	0.54
1:A:450:THR:CG2	1:A:452:LEU:CG	2.86	0.54
2:D:6:GLU:OE1	2:D:6:GLU:N	2.41	0.54
1:A:272:PRO:HG3	1:A:351:THR:HG21	1.89	0.54
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.08	0.53
1:A:453:GLY:O	1:A:469:LEU:N	2.39	0.53
1:C:123:ASP:N	1:C:123:ASP:OD1	2.40	0.53
1:A:448:ARG:HH21	3:E:18:DT:H2''	1.72	0.53
1:A:450:THR:CG2	1:A:452:LEU:HG	2.34	0.53
2:B:309:ILE:O	2:B:312:GLU:HG2	2.09	0.53
2:B:206:ARG:NH2	2:B:228:LEU:O	2.33	0.53
1:C:3:SER:HB2	1:C:211:ARG:NH2	2.21	0.53
2:D:195:ILE:HD11	2:D:199:ARG:HE	1.73	0.53
2:D:206:ARG:HG3	2:D:228:LEU:HG	1.92	0.52
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.91	0.52
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.49	0.52
1:A:175:ASN:O	1:A:178:ILE:HG22	2.10	0.52
1:A:448:ARG:NH2	3:E:18:DT:C6	2.64	0.52
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.24	0.52
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.92	0.52
1:C:74:LEU:HD13	3:F:0:DA:C5	2.45	0.52
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.91	0.52
1:C:211:ARG:HG3	1:C:211:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PRO:HG2	1:A:53:GLU:HG2	1.92	0.51
1:A:450:THR:HG21	1:A:452:LEU:HB2	1.92	0.51
1:C:203:GLU:O	1:C:207:GLN:HG2	2.10	0.51
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.93	0.51
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.51
2:B:72:ARG:HG2	2:B:226:PRO:HB3	1.92	0.51
1:A:44:GLU:HG2	1:A:46:LYS:CE	2.37	0.51
1:A:21:VAL:O	1:A:57:ASN:ND2	2.42	0.51
1:A:65:LYS:HE3	1:A:72:ARG:NH2	2.25	0.51
1:A:438:GLU:CD	1:A:459:THR:HG21	2.31	0.51
1:A:51:GLY:O	1:A:143:ARG:HD2	2.10	0.50
2:D:320:ASP:HB3	2:D:323:LYS:HE2	1.92	0.50
1:C:65:LYS:HB3	1:C:68:SER:CB	2.41	0.50
2:D:356:ARG:CD	2:D:361:HIS:CE1	2.92	0.50
1:A:200:THR:O	1:A:204:GLU:HG3	2.10	0.50
1:A:51:GLY:H	1:A:52:PRO:CD	2.25	0.50
2:D:266:TRP:CE3	2:D:425:LEU:HD22	2.47	0.50
3:E:23:DC:H2"	3:E:24:DG:C8	2.46	0.50
1:A:38:CYS:O	1:A:42:GLU:HG3	2.13	0.49
1:A:5:ILE:HB	1:A:119:PRO:HD2	1.94	0.49
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.94	0.49
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.95	0.49
1:C:21:VAL:O	1:C:57:ASN:ND2	2.46	0.49
1:A:247:PRO:HB3	1:A:249:LYS:HE3	1.94	0.49
2:D:253:THR:O	2:D:257:ILE:HD12	2.13	0.49
2:B:6:GLU:N	2:B:6:GLU:OE1	2.40	0.49
2:B:248:GLU:OE1	2:B:307:ARG:NH2	2.45	0.49
1:C:373:GLN:NE2	2:D:397:THR:OG1	2.45	0.48
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.95	0.48
1:C:64:LYS:HB2	1:C:71:TRP:CE2	2.48	0.48
1:A:450:THR:HG22	1:A:452:LEU:CB	2.43	0.48
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.13	0.48
2:B:362:THR:HG23	2:B:363:ASN:N	2.29	0.48
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.49	0.48
3:F:17:DT:C5'	3:F:17:DT:H6	2.27	0.48
2:D:85:GLN:HE21	2:D:90:VAL:HG21	1.79	0.47
1:A:503:LEU:HD11	1:A:533:LEU:HB3	1.94	0.47
4:G:1:GLC:H62	4:G:2:FRU:H61	1.96	0.47
1:A:109:LEU:HD12	1:A:187:LEU:HB2	1.96	0.47
1:A:208:HIS:O	1:A:212:TRP:HD1	1.98	0.47
1:A:438:GLU:CG	1:A:459:THR:CG2	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:O	1:A:284:ARG:HG2	2.15	0.47
1:A:450:THR:HG21	1:A:452:LEU:HD12	1.96	0.47
1:A:202:ILE:O	1:A:206:ARG:HG3	2.15	0.47
1:A:26:LEU:O	1:A:31:ILE:HD11	2.15	0.47
2:B:255:ASN:HB2	2:B:289:LEU:HB3	1.97	0.47
1:C:133:PRO:HB3	1:C:137:ASN:H	1.80	0.46
1:C:180:ILE:HA	1:C:188:TYR:O	2.14	0.46
2:D:282:LEU:HD21	2:D:296:THR:HG22	1.97	0.46
1:A:278:GLN:OE1	1:A:281:LYS:NZ	2.48	0.46
1:A:194:GLU:HB3	1:A:197:GLN:HG3	1.97	0.46
2:B:305:GLU:O	2:B:309:ILE:HG13	2.15	0.46
1:C:211:ARG:HH11	1:C:211:ARG:HG3	1.80	0.46
2:B:257:ILE:HD12	2:B:293:ILE:HD11	1.98	0.46
1:C:246:LEU:HD11	1:C:310:LEU:HD12	1.98	0.46
1:C:60:VAL:HG11	1:C:73:LYS:CE	2.43	0.46
2:D:207:GLN:O	2:D:211:ARG:HG3	2.15	0.46
2:B:266:TRP:CZ3	2:B:425:LEU:HD21	2.51	0.46
1:C:253:THR:HA	1:C:292:VAL:HA	1.98	0.46
1:C:129:ALA:HA	1:C:144:TYR:O	2.16	0.46
2:D:336:GLN:OE1	2:D:353:LYS:HE2	2.16	0.45
1:A:27:THR:O	1:A:31:ILE:HG13	2.17	0.45
1:A:320:ASP:OD1	1:A:322:SER:OG	2.28	0.45
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.81	0.45
1:C:326:ILE:HD13	1:C:388:LYS:HB2	1.99	0.45
1:A:543:GLY:N	2:B:283:LEU:O	2.50	0.45
2:D:362:THR:CG2	2:D:363:ASN:N	2.79	0.45
1:A:23:GLN:NE2	1:A:60:VAL:H	2.15	0.45
2:D:331:LYS:NZ	2:D:364:ASP:OD2	2.34	0.45
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.81	0.45
2:D:357:MET:O	2:D:360:ALA:HB2	2.16	0.45
1:A:24:TRP:CH2	3:E:-1:DT:H2'	2.53	0.44
2:B:360:ALA:HA	2:B:367:GLN:CD	2.37	0.44
1:C:115:TYR:HB3	1:C:149:LEU:HB2	2.00	0.44
1:C:155:GLY:O	1:C:159:ILE:HG12	2.16	0.44
1:C:80:LEU:O	1:C:84:THR:OG1	2.28	0.44
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.99	0.44
1:A:459:THR:HG22	1:A:461:LYS:N	2.30	0.44
1:A:184:MET:HG2	3:E:33:DG:H2''	1.98	0.44
1:A:353:LYS:NZ	3:E:7:DC:OP1	2.50	0.44
2:B:281:LYS:O	2:B:284:ARG:HG3	2.17	0.44
1:C:503:LEU:HD11	1:C:533:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ALA:HA	1:C:73:LYS:HA	2.00	0.44
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.18	0.44
1:A:459:THR:HG22	1:A:460:ASN:N	2.32	0.44
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.52	0.44
1:C:146:TYR:CG	1:C:150:PRO:HB3	2.53	0.44
2:D:363:ASN:OD1	2:D:366:LYS:N	2.27	0.43
2:B:395:LYS:NZ	4:G:2:FRU:O4	2.48	0.43
1:C:36:GLU:O	1:C:40:GLU:HG2	2.18	0.43
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.83	0.43
2:D:7:THR:HG22	2:D:119:PRO:HB2	1.99	0.43
1:A:49:LYS:HA	1:A:144:TYR:CD1	2.54	0.43
3:F:10:DC:H2"	3:F:11:DG:C8	2.53	0.43
1:C:3:SER:CB	1:C:211:ARG:HH12	2.31	0.43
1:C:540:LYS:HE3	2:D:265:ASN:OD1	2.18	0.43
1:A:325:LEU:HB3	1:A:387:PRO:HB3	2.00	0.43
1:C:26:LEU:HD22	1:C:133:PRO:HD2	2.00	0.43
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.54	0.43
1:A:146:TYR:CG	1:A:150:PRO:HB3	2.54	0.43
2:B:103:LYS:HE2	2:B:179:VAL:HG23	2.00	0.43
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.54	0.42
1:A:448:ARG:CZ	3:E:18:DT:H2'	2.48	0.42
1:A:110:ASP:HB2	1:A:220:LYS:HD3	2.01	0.42
1:A:51:GLY:H	1:A:52:PRO:HD3	1.84	0.42
2:D:360:ALA:O	2:D:361:HIS:HB2	2.20	0.42
2:D:244:ILE:HD13	2:D:425:LEU:HD11	2.00	0.42
2:B:86:ASP:OD1	2:B:154:LYS:NZ	2.52	0.42
2:B:92:LEU:O	2:B:161:GLN:NE2	2.53	0.42
1:C:123:ASP:O	1:C:126:LYS:HE3	2.20	0.42
1:C:136:ASN:N	1:C:136:ASN:OD1	2.53	0.42
2:D:254:VAL:HG13	2:D:283:LEU:HD22	2.01	0.42
2:D:354:TYR:HE1	2:D:374:LYS:CD	2.31	0.42
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.55	0.42
1:A:317:VAL:HG11	1:A:347:LYS:HB3	2.01	0.42
1:A:447:ASN:OD1	1:A:449:GLU:N	2.53	0.42
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.84	0.42
1:C:253:THR:HG22	1:C:292:VAL:HG22	2.01	0.42
2:D:360:ALA:C	2:D:361:HIS:HD1	2.23	0.42
2:B:183:TYR:OH	2:B:386:THR:HG23	2.19	0.42
1:A:303:LEU:O	1:A:307:ARG:HG2	2.19	0.41
1:A:51:GLY:HA3	1:A:143:ARG:HB2	2.02	0.41
2:D:360:ALA:C	2:D:361:HIS:ND1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LYS:HB3	2:B:11:LYS:HE3	1.82	0.41
1:C:5:ILE:HB	1:C:119:PRO:HD2	2.02	0.41
1:C:353:LYS:NZ	3:F:7:DC:OP1	2.53	0.41
1:A:410:TRP:CD1	2:B:363:ASN:HA	2.55	0.41
1:A:441:TYR:CD1	2:B:286:THR:HG23	2.55	0.41
1:A:503:LEU:HA	1:A:503:LEU:HD12	1.84	0.41
2:B:290:THR:HG22	2:B:290:THR:O	2.19	0.41
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.84	0.41
1:C:121:ASP:O	1:C:125:ARG:HG3	2.19	0.41
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.55	0.41
1:C:64:LYS:HG3	1:C:65:LYS:O	2.21	0.41
1:C:300:GLU:HG2	1:C:300:GLU:H	1.68	0.41
1:A:198:HIS:O	1:A:202:ILE:HG12	2.20	0.41
1:A:492:GLU:HG2	1:A:530:LYS:HB2	2.01	0.41
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.55	0.41
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.51	0.41
2:B:107:THR:HA	2:B:232:TYR:O	2.20	0.41
2:B:266:TRP:CE3	2:B:425:LEU:HD21	2.56	0.41
1:A:450:THR:HG22	1:A:452:LEU:HB2	2.03	0.41
1:C:469:LEU:HD11	1:C:480:GLN:HG2	2.03	0.41
1:A:285:GLY:N	3:E:9:DT:OP1	2.54	0.41
2:D:246:LEU:HD13	2:D:260:LEU:HD11	2.03	0.41
3:F:4:OMC:H1'	3:F:4:OMC:HM23	1.85	0.41
1:A:31:ILE:O	1:A:35:VAL:HG23	2.20	0.41
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.56	0.41
1:A:120:LEU:H	1:A:148:VAL:HA	1.85	0.40
1:A:51:GLY:N	1:A:52:PRO:CD	2.83	0.40
1:C:7:THR:OG1	1:C:121:ASP:HA	2.21	0.40
1:C:198:HIS:O	1:C:202:ILE:HG12	2.21	0.40
1:C:540:LYS:HA	1:C:540:LYS:HD3	1.83	0.40
1:A:48:SER:HB3	1:A:145:GLN:HG2	2.02	0.40
2:B:94:ILE:HD13	2:B:182:GLN:HB3	2.04	0.40
2:D:103:LYS:HA	2:D:103:LYS:HD3	1.94	0.40
2:D:356:ARG:HD2	2:D:356:ARG:HA	1.86	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)
1:C:197:GLN:NE2	2:D:91:GLN:OE1[2_657]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	548/555 (99%)	533 (97%)	14 (3%)	1 (0%)	47	82
1	C	551/555 (99%)	534 (97%)	17 (3%)	0	100	100
2	B	412/444 (93%)	402 (98%)	10 (2%)	0	100	100
2	D	407/444 (92%)	398 (98%)	9 (2%)	0	100	100
All	All	1918/1998 (96%)	1867 (97%)	50 (3%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ILE

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/495 (99%)	476 (97%)	14 (3%)	42	76
1	C	493/495 (100%)	481 (98%)	12 (2%)	49	79
2	B	376/403 (93%)	375 (100%)	1 (0%)	92	97
2	D	371/403 (92%)	369 (100%)	2 (0%)	88	96
All	All	1730/1796 (96%)	1701 (98%)	29 (2%)	60	85

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	36	GLU
1	A	49	LYS
1	A	53	GLU
1	A	61	PHE
1	A	77	PHE
1	A	109	LEU
1	A	123	ASP
1	A	135	ILE
1	A	136	ASN
1	A	211	ARG
1	A	291	GLU
1	A	358	ARG
1	A	516	GLU
2	B	413	GLU
1	C	7	THR
1	C	16	MET
1	C	24	TRP
1	C	36	GLU
1	C	39	THR
1	C	48	SER
1	C	109	LEU
1	C	123	ASP
1	C	136	ASN
1	C	211	ARG
1	C	286	THR
1	C	516	GLU
2	D	356	ARG
2	D	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	161	GLN
2	B	161	GLN
2	B	175	ASN
1	C	330	GLN
1	C	332	GLN
1	C	340	GLN
1	C	545	ASN
2	D	361	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ATM	E	34	3	16,23,24	1.30	1 (6%)	17,32,35	1.78	2 (11%)
3	OMC	E	2	3	15,22,23	3.23	6 (40%)	17,31,34	1.39	2 (11%)
3	OMC	F	2	3	15,22,23	3.31	6 (40%)	17,31,34	1.44	2 (11%)
3	ATM	F	34	3	16,23,24	1.29	1 (6%)	17,32,35	1.76	2 (11%)
3	OMC	F	4	3	15,22,23	3.20	6 (40%)	17,31,34	1.33	2 (11%)
3	OMC	E	4	3	15,22,23	3.25	6 (40%)	17,31,34	1.33	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
3	ATM	E	34	3	-	0/7/24/25	0/2/2/2
3	OMC	E	2	3	-	0/7/27/28	0/2/2/2
3	OMC	F	2	3	-	0/7/27/28	0/2/2/2
3	ATM	F	34	3	-	0/7/24/25	0/2/2/2
3	OMC	F	4	3	-	0/7/27/28	0/2/2/2
3	OMC	E	4	3	-	0/7/27/28	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	OMC	C6-N1	8.00	1.45	1.35
3	E	4	OMC	C6-N1	7.84	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C6-N1	7.82	1.45	1.35
3	F	4	OMC	C6-N1	7.69	1.45	1.35
3	F	2	OMC	C4-N3	5.96	1.45	1.35
3	E	4	OMC	C4-N3	5.92	1.45	1.35
3	E	2	OMC	C4-N3	5.88	1.45	1.35
3	F	4	OMC	C4-N3	5.84	1.45	1.35
3	F	2	OMC	C2-N3	5.04	1.48	1.38
3	E	4	OMC	C6-C5	5.00	1.49	1.38
3	E	4	OMC	C2-N3	4.91	1.47	1.38
3	E	2	OMC	C2-N3	4.91	1.47	1.38
3	F	4	OMC	C6-C5	4.88	1.48	1.38
3	F	4	OMC	C2-N3	4.88	1.47	1.38
3	E	2	OMC	C6-C5	4.88	1.48	1.38
3	F	2	OMC	C6-C5	4.88	1.48	1.38
3	F	34	ATM	C4-N3	4.34	1.40	1.33
3	E	34	ATM	C4-N3	4.30	1.40	1.33
3	E	4	OMC	C5-C4	2.52	1.47	1.41
3	F	2	OMC	C5-C4	2.48	1.47	1.41
3	F	4	OMC	C5-C4	2.46	1.47	1.41
3	E	2	OMC	C5-C4	2.37	1.46	1.41
3	E	4	OMC	C4-N4	2.30	1.41	1.35
3	F	4	OMC	C4-N4	2.24	1.41	1.35
3	F	2	OMC	C4-N4	2.21	1.41	1.35
3	E	2	OMC	C4-N4	2.17	1.41	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	34	ATM	C4-N3-C2	5.64	119.91	115.14
3	E	34	ATM	C4-N3-C2	5.45	119.75	115.14
3	F	2	OMC	C2-N3-C4	4.39	120.79	116.34
3	E	4	OMC	C2-N3-C4	4.32	120.72	116.34
3	F	4	OMC	C2-N3-C4	4.31	120.71	116.34
3	E	2	OMC	C2-N3-C4	4.28	120.68	116.34
3	F	34	ATM	C2'-C1'-N1	-2.66	108.13	114.27
3	E	34	ATM	C5-C6-N1	-2.15	119.88	122.19
3	F	2	OMC	N4-C4-N3	2.15	119.89	116.49
3	E	2	OMC	N4-C4-N3	2.14	119.88	116.49
3	E	4	OMC	N4-C4-N3	2.12	119.84	116.49
3	F	4	OMC	N4-C4-N3	2.06	119.74	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	OMC	1	0

## 5.5 Carbohydrates

4 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	$\# Z  > 2$
4	GLC	G	1	4	11,11,12	0.53	0	15,15,17	0.98	2 (13%)
4	FRU	G	2	4	11,12,12	0.53	0	10,18,18	0.64	0
4	GLC	H	1	4	11,11,12	0.57	0	15,15,17	0.75	0
4	FRU	H	2	4	11,12,12	0.50	0	10,18,18	0.71	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
4	GLC	G	1	4	-	2/2/19/22	0/1/1/1
4	FRU	G	2	4	-	3/5/24/24	0/1/1/1
4	GLC	H	1	4	-	0/2/19/22	0/1/1/1
4	FRU	H	2	4	-	2/5/24/24	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	2.27	115.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	O5-C5-C6	2.03	110.38	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	FRU	O5-C5-C6-O6
4	H	2	FRU	C4-C5-C6-O6
4	G	1	GLC	C4-C5-C6-O6
4	G	2	FRU	C4-C5-C6-O6
4	G	2	FRU	O5-C5-C6-O6
4	G	1	GLC	O5-C5-C6-O6
4	G	2	FRU	O1-C1-C2-C3

There are no ring outliers.

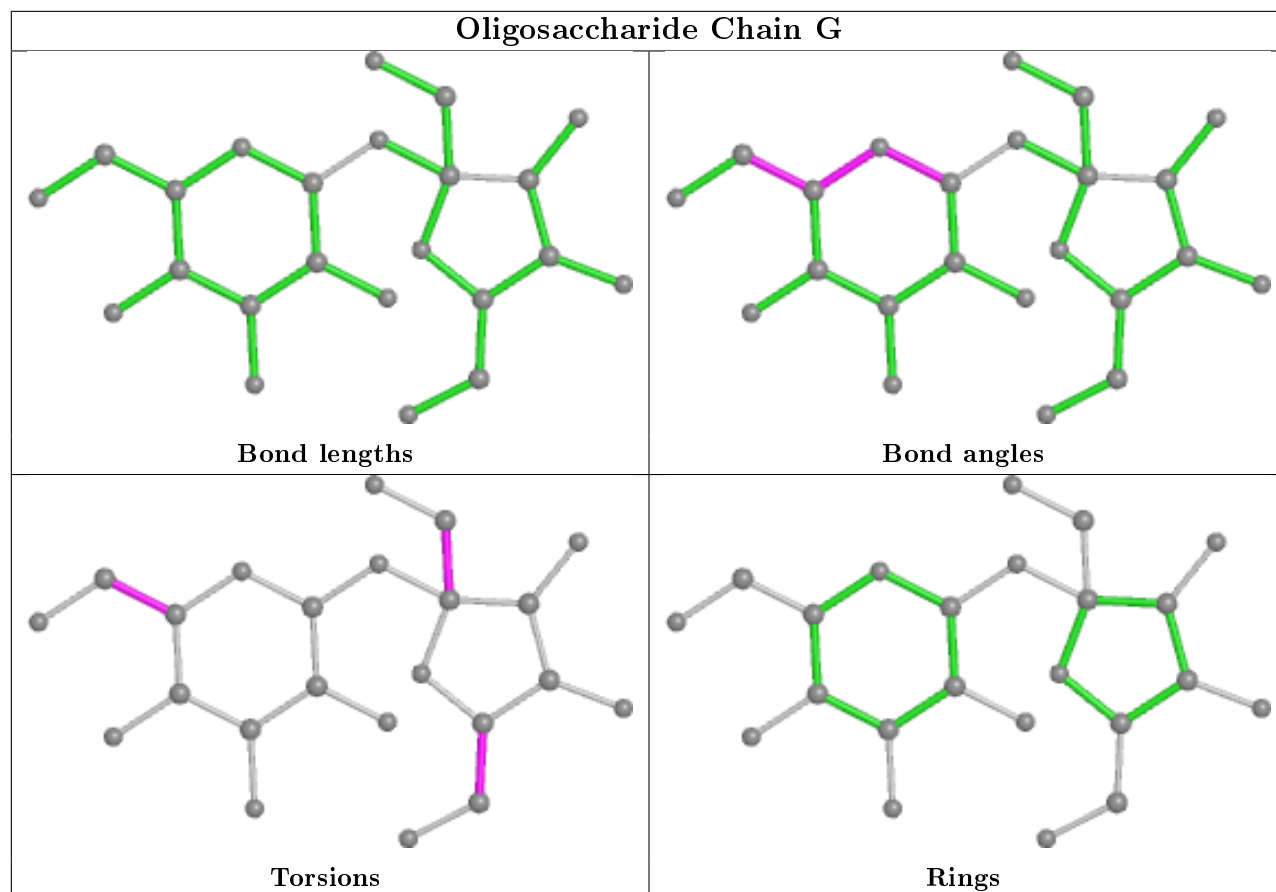
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	1	0
4	G	2	FRU	2	0

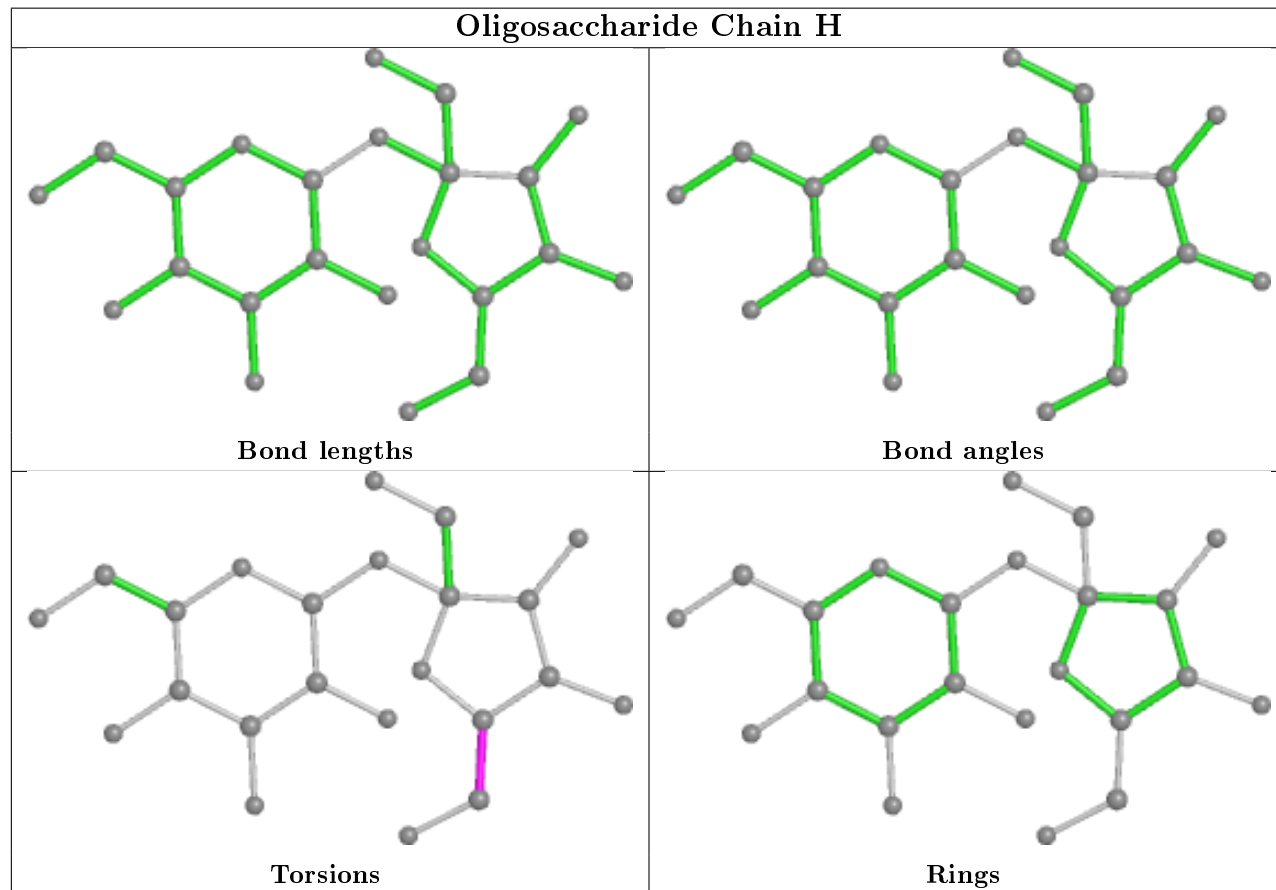
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## Oligosaccharide Chain G



## Oligosaccharide Chain H



## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	B	2003	-	5,5,5	0.42	0	5,5,5	0.17	0
6	GOL	B	2002	-	5,5,5	0.37	0	5,5,5	0.19	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	GOL	B	2003	-	-	3/4/4/4	-
6	GOL	B	2002	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2003	GOL	O1-C1-C2-O2
6	B	2003	GOL	O1-C1-C2-C3
6	B	2002	GOL	O1-C1-C2-C3
6	B	2002	GOL	O1-C1-C2-O2
6	B	2003	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2003	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	550/555 (99%)	0.15	16 (2%) 51 23	46, 101, 164, 191	0
1	C	553/555 (99%)	0.53	55 (9%) 7 2	43, 113, 171, 193	0
2	B	416/444 (93%)	-0.08	5 (1%) 79 54	48, 84, 127, 144	0
2	D	410/444 (92%)	0.08	8 (1%) 65 36	46, 93, 135, 175	0
3	E	33/39 (84%)	-0.41	0 100 100	78, 103, 120, 162	0
3	F	33/39 (84%)	-0.22	0 100 100	83, 118, 135, 173	0
All	All	1995/2076 (96%)	0.18	84 (4%) 36 14	43, 95, 162, 193	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	ASN	9.2
1	C	26	LEU	8.5
1	C	137	ASN	8.3
1	C	67	ASP	6.7
1	A	133	PRO	6.4
1	A	26	LEU	5.6
1	A	73	LYS	5.2
1	A	134	SER	4.9
1	C	25	PRO	4.9
1	C	63	ILE	4.9
1	C	28	GLU	4.8
2	D	358	ARG	4.7
1	C	66	LYS	4.7
1	C	68	SER	4.7
1	C	69	THR	4.7
1	C	70	LYS	4.6
1	C	254	VAL	4.5
1	C	133	PRO	4.3
1	C	257	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	30	LYS	4.1
1	C	73	LYS	4.1
1	C	72	ARG	4.0
1	C	74	LEU	4.0
1	C	75	VAL	3.9
1	A	71	TRP	3.9
2	B	89	GLU	3.7
1	C	62	ALA	3.7
1	C	27	THR	3.7
1	C	111	VAL	3.7
1	A	135	ILE	3.6
1	C	34	LEU	3.6
1	C	114	ALA	3.6
1	A	61	PHE	3.5
1	A	29	GLU	3.5
1	C	205	LEU	3.4
2	D	360	ALA	3.4
1	C	142	ILE	3.3
1	C	132	ILE	3.1
1	C	71	TRP	3.1
1	C	229	TRP	3.1
1	C	124	PHE	3.0
1	C	24	TRP	3.0
1	A	136	ASN	2.9
1	C	29	GLU	2.9
1	C	145	GLN	2.9
1	C	138	GLU	2.8
1	C	52	PRO	2.8
2	B	226	PRO	2.7
1	C	167	ILE	2.7
1	C	61	PHE	2.7
1	C	139	THR	2.6
1	A	25	PRO	2.6
2	D	226	PRO	2.6
1	C	48	SER	2.6
1	C	65	LYS	2.6
1	A	21	VAL	2.5
1	C	131	THR	2.5
1	C	178	ILE	2.5
1	C	91	GLN	2.5
1	C	22	LYS	2.5
1	A	63	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	422	LEU	2.4
1	C	290	THR	2.4
1	C	113	ASP	2.4
1	C	274	ILE	2.3
1	C	146	TYR	2.3
1	A	72	ARG	2.3
1	C	23	GLN	2.3
1	C	46	LYS	2.3
2	D	89	GLU	2.3
2	D	146	TYR	2.3
1	C	30	LYS	2.2
1	A	280	SER	2.2
2	B	85	GLN	2.2
1	C	58	THR	2.2
1	A	247	PRO	2.2
2	B	91	GLN	2.2
1	C	151	GLN	2.1
2	D	90	VAL	2.1
1	C	286	THR	2.1
2	D	232	TYR	2.1
1	C	32	LYS	2.1
1	C	50	ILE	2.0
2	D	124	PHE	2.0

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

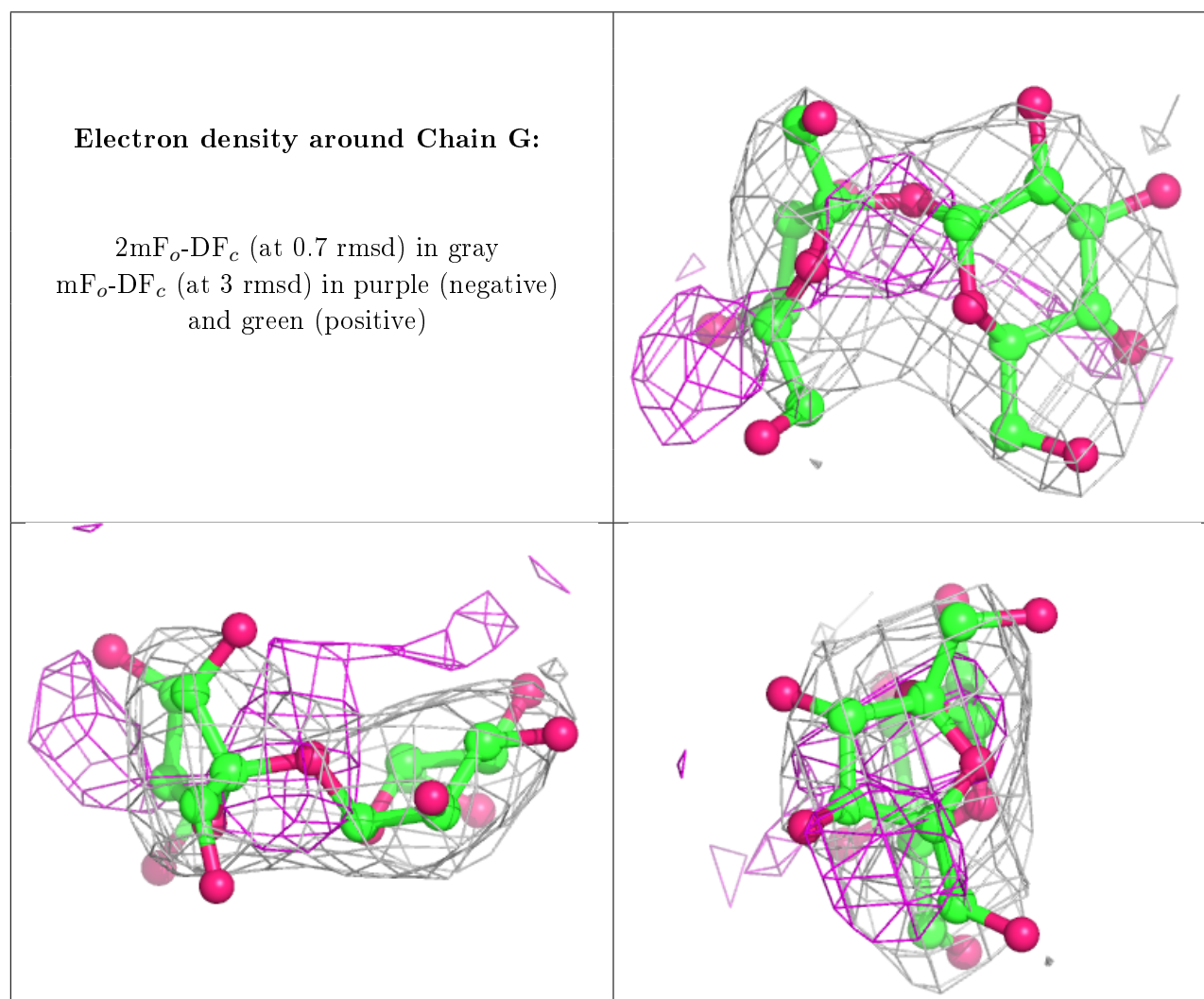
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATM	F	34	22/23	0.82	0.39	113,137,153,167	0
3	ATM	E	34	22/23	0.84	0.24	108,121,136,141	0
3	OMC	F	2	21/22	0.92	0.16	90,105,112,115	0
3	OMC	F	4	21/22	0.93	0.20	91,96,103,109	0
3	OMC	E	2	21/22	0.94	0.18	87,93,100,104	0
3	OMC	E	4	21/22	0.95	0.21	69,78,85,87	0

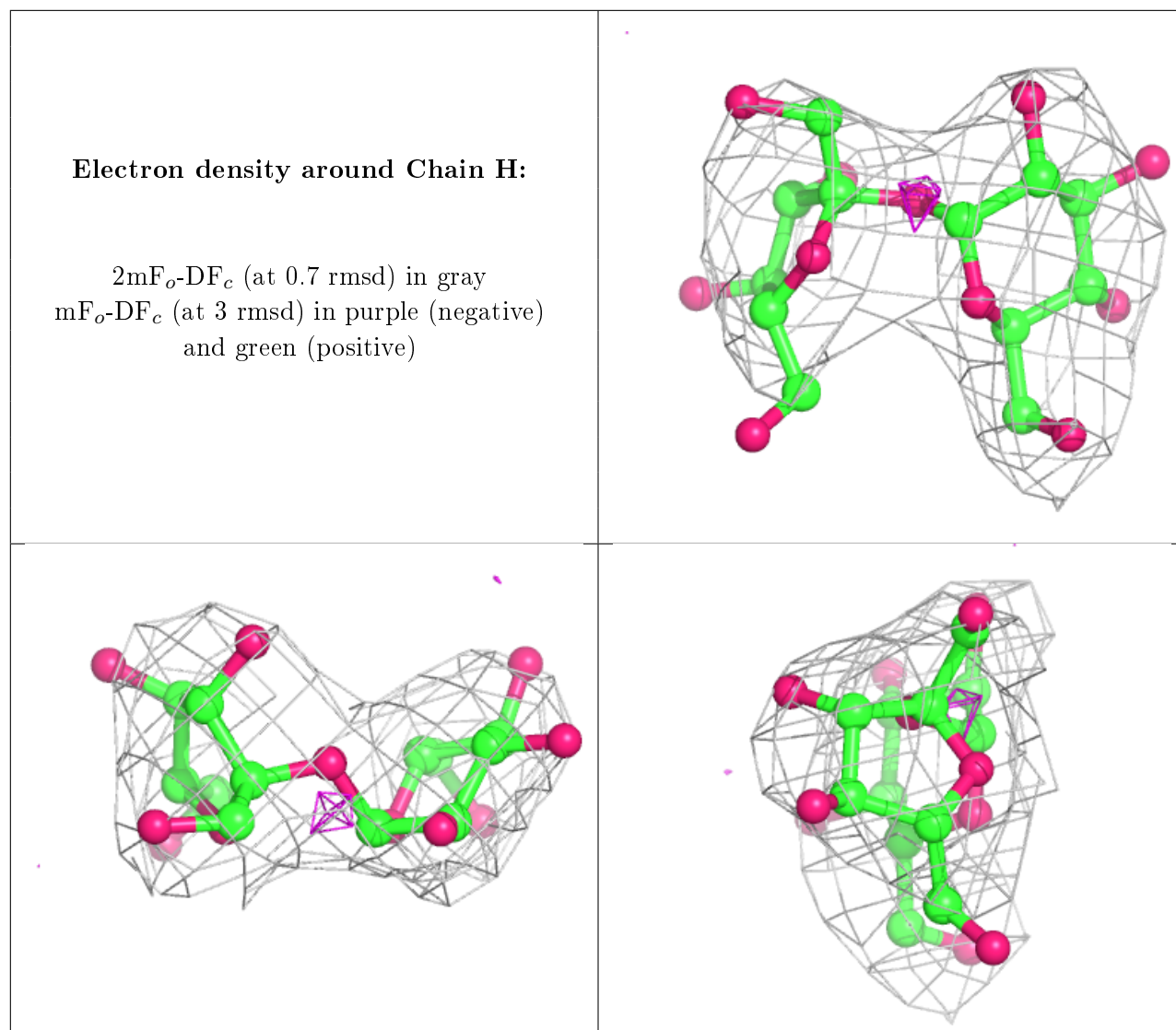
### 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	Q<0.9
4	GLC	H	1	11/12	0.90	0.28	74,91,101,102	0
4	FRU	G	2	12/12	0.91	0.48	82,101,104,105	0
4	FRU	H	2	12/12	0.92	0.31	87,100,103,103	0
4	GLC	G	1	11/12	0.94	0.36	72,87,96,98	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 ⓘ

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	MG	C	601	1/1	0.68	0.24	80,80,80,80	0
5	MG	A	601	1/1	0.82	0.23	79,79,79,79	0
6	GOL	B	2002	6/6	0.87	0.22	74,84,84,85	0
6	GOL	B	2003	6/6	0.94	0.45	65,72,79,81	0



## 6.5 Other polymers

There are no such residues in this entry.