



# Full wwPDB X-ray Structure Validation Report i

Nov 15, 2023 – 06:44 PM JST

PDB ID : 6JO8  
Title : The complex structure of CHIKV envelope glycoprotein bound to human MXRA8  
Authors : Song, H.; Zhao, Z.; Qi, J.; Gao, F.; Gao, F.G.  
Deposited on : 2019-03-20  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i 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](#) i) 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 : 2.36  
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) : 2.36

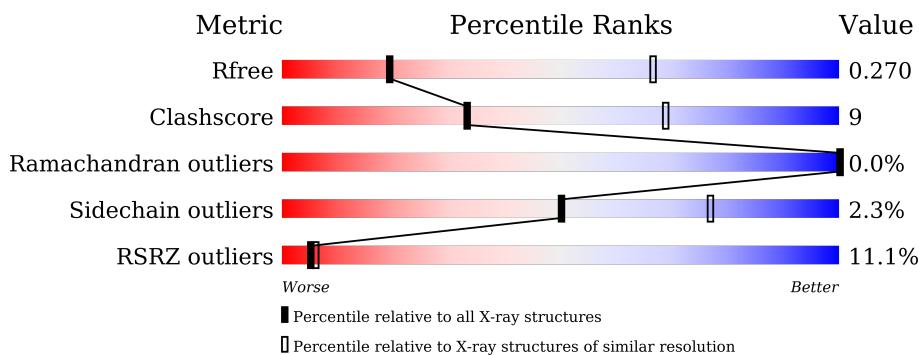
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

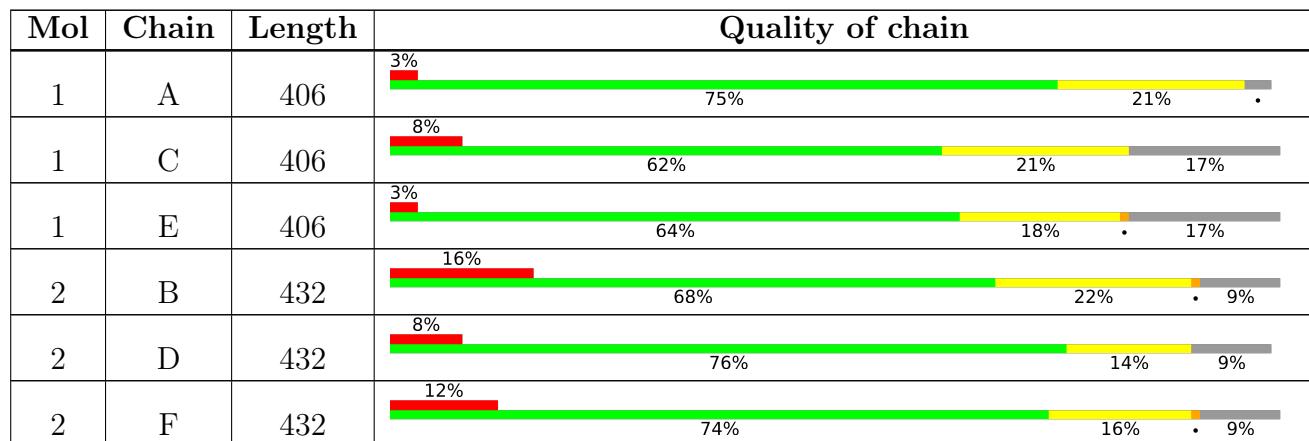
The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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.



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Mol	Chain	Length	Quality of chain			
3	M	269	3%	71%	23%	..
3	N	269	16%	72%	21%	..
3	O	269	27%	74%	22%	.
4	G	2		100%		
4	H	2		50%	50%	
4	I	2		100%		

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 23522 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 Togavirin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3092	1929	549	585	29			
1	C	338	Total	C	N	O	S	0	0	0
			2669	1664	483	502	20			
1	E	335	Total	C	N	O	S	0	0	0
			2633	1641	475	497	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP C8YZ73
C	0	MET	-	expression tag	UNP C8YZ73
E	0	MET	-	expression tag	UNP C8YZ73

- Molecule 2 is a protein called CHIKV E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	6	1	0
			2995	1893	502	576	24			
2	D	393	Total	C	N	O	S	6	1	0
			2995	1893	502	576	24			
2	F	393	Total	C	N	O	S	0	1	0
			2995	1893	502	576	24			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP A4L787
B	-18	GLY	-	expression tag	UNP A4L787
B	-17	GLY	-	expression tag	UNP A4L787
B	-16	GLY	-	expression tag	UNP A4L787
B	-15	SER	-	expression tag	UNP A4L787

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP A4L787
B	-13	GLY	-	expression tag	UNP A4L787
B	-12	GLY	-	expression tag	UNP A4L787
B	-11	GLY	-	expression tag	UNP A4L787
B	-10	SER	-	expression tag	UNP A4L787
B	-9	GLY	-	expression tag	UNP A4L787
B	-8	GLY	-	expression tag	UNP A4L787
B	-7	GLY	-	expression tag	UNP A4L787
B	-6	GLY	-	expression tag	UNP A4L787
B	-5	SER	-	expression tag	UNP A4L787
B	-4	GLY	-	expression tag	UNP A4L787
B	-3	GLY	-	expression tag	UNP A4L787
B	-2	GLY	-	expression tag	UNP A4L787
B	-1	GLY	-	expression tag	UNP A4L787
B	0	SER	-	expression tag	UNP A4L787
D	-19	GLY	-	expression tag	UNP A4L787
D	-18	GLY	-	expression tag	UNP A4L787
D	-17	GLY	-	expression tag	UNP A4L787
D	-16	GLY	-	expression tag	UNP A4L787
D	-15	SER	-	expression tag	UNP A4L787
D	-14	GLY	-	expression tag	UNP A4L787
D	-13	GLY	-	expression tag	UNP A4L787
D	-12	GLY	-	expression tag	UNP A4L787
D	-11	GLY	-	expression tag	UNP A4L787
D	-10	SER	-	expression tag	UNP A4L787
D	-9	GLY	-	expression tag	UNP A4L787
D	-8	GLY	-	expression tag	UNP A4L787
D	-7	GLY	-	expression tag	UNP A4L787
D	-6	GLY	-	expression tag	UNP A4L787
D	-5	SER	-	expression tag	UNP A4L787
D	-4	GLY	-	expression tag	UNP A4L787
D	-3	GLY	-	expression tag	UNP A4L787
D	-2	GLY	-	expression tag	UNP A4L787
D	-1	GLY	-	expression tag	UNP A4L787
D	0	SER	-	expression tag	UNP A4L787
F	-19	GLY	-	expression tag	UNP A4L787
F	-18	GLY	-	expression tag	UNP A4L787
F	-17	GLY	-	expression tag	UNP A4L787
F	-16	GLY	-	expression tag	UNP A4L787
F	-15	SER	-	expression tag	UNP A4L787
F	-14	GLY	-	expression tag	UNP A4L787
F	-13	GLY	-	expression tag	UNP A4L787

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	GLY	-	expression tag	UNP A4L787
F	-11	GLY	-	expression tag	UNP A4L787
F	-10	SER	-	expression tag	UNP A4L787
F	-9	GLY	-	expression tag	UNP A4L787
F	-8	GLY	-	expression tag	UNP A4L787
F	-7	GLY	-	expression tag	UNP A4L787
F	-6	GLY	-	expression tag	UNP A4L787
F	-5	SER	-	expression tag	UNP A4L787
F	-4	GLY	-	expression tag	UNP A4L787
F	-3	GLY	-	expression tag	UNP A4L787
F	-2	GLY	-	expression tag	UNP A4L787
F	-1	GLY	-	expression tag	UNP A4L787
F	0	SER	-	expression tag	UNP A4L787

- Molecule 3 is a protein called Matrix remodeling-associated protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	258	Total	C	N	O	S	0	0	0
			2019	1262	373	377	7			
3	N	258	Total	C	N	O	S	0	0	0
			2013	1259	370	377	7			
3	O	258	Total	C	N	O	S	0	0	0
			2013	1259	370	377	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	24	MET	-	expression tag	UNP Q9BRK3
N	24	MET	-	expression tag	UNP Q9BRK3
O	24	MET	-	expression tag	UNP Q9BRK3

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



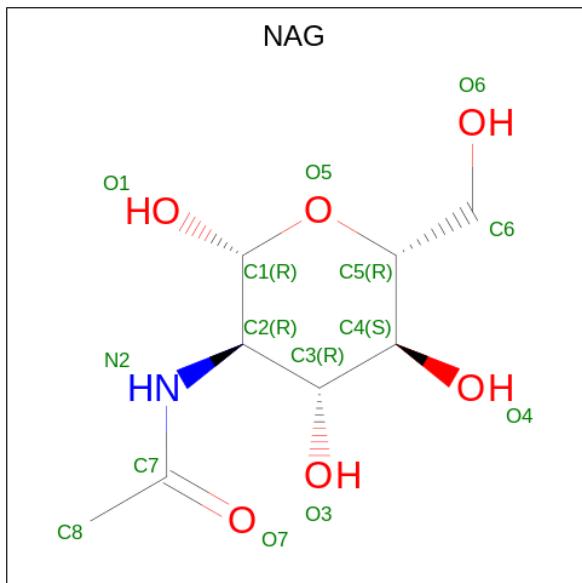
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O		0	0	0
			28	16	2	10				

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	2	Total C N O 28 16 2 10	0	0	0
4	I	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

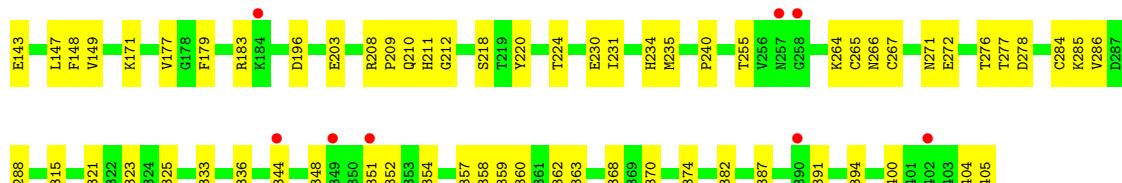
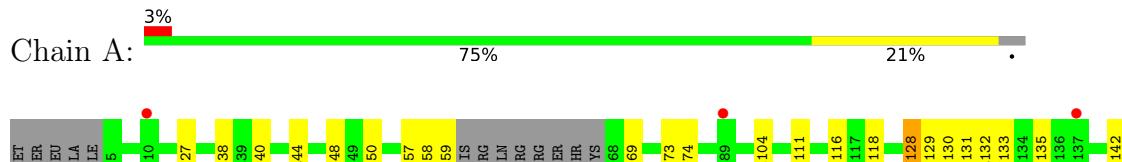


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0

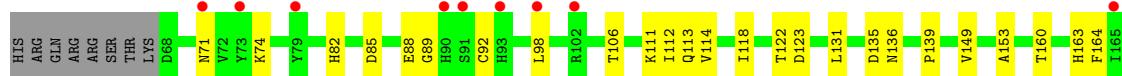
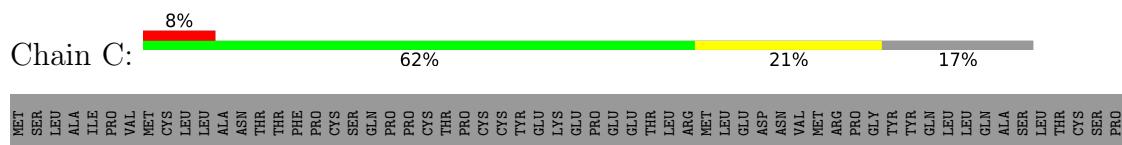
### 3 Residue-property plots [i](#)

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: Togavirin

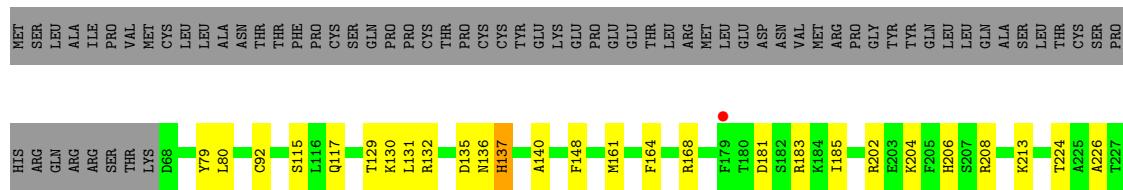


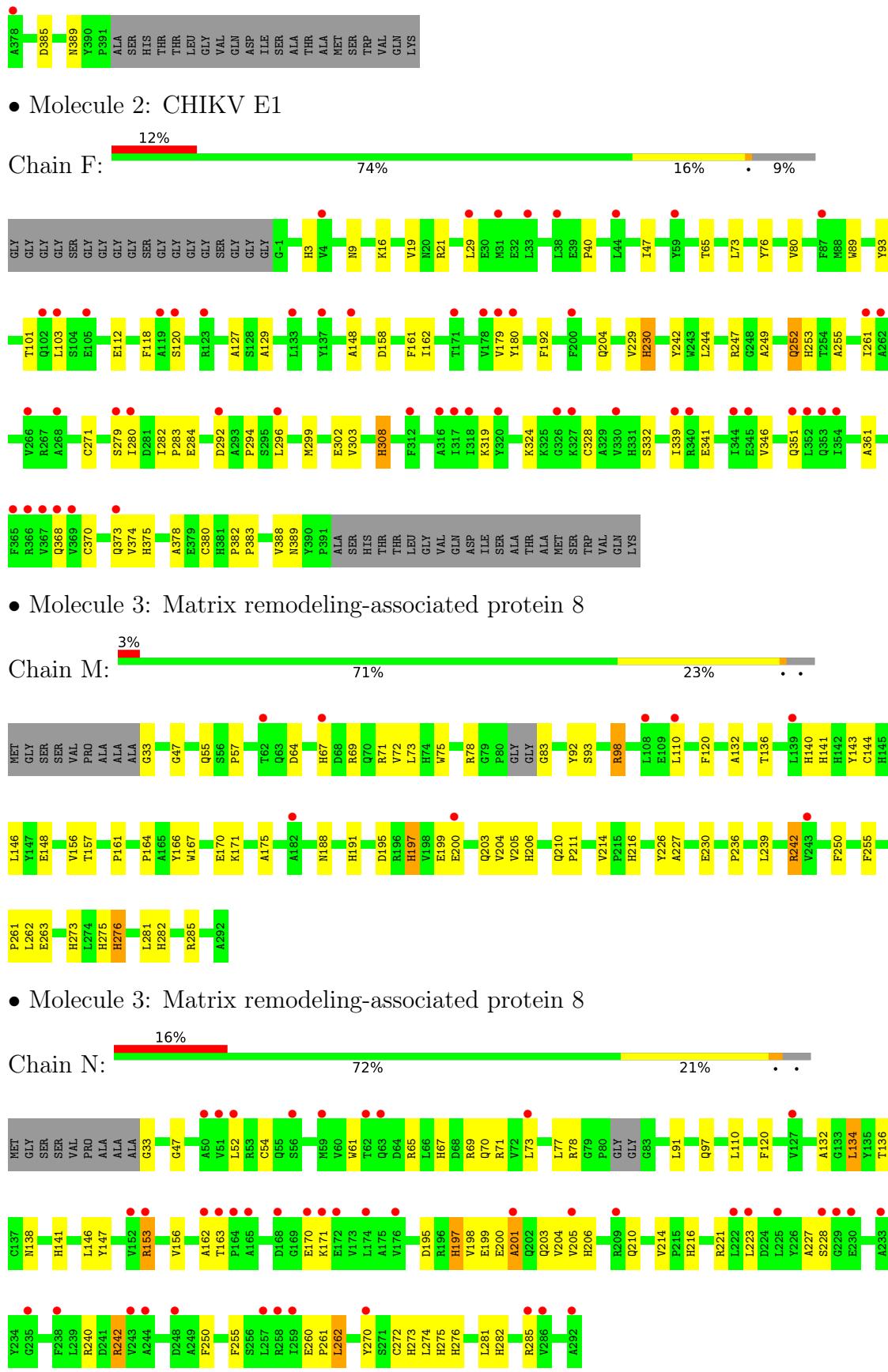
- Molecule 1: Togavirin



- Molecule 1: Togavirin







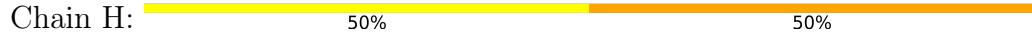
- Molecule 3: Matrix remodeling-associated protein 8



- Molecule 4: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose



- Molecule 4: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose



- Molecule 4: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.79Å 208.79Å 299.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.15 – 3.50 50.15 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.15-3.50) 99.7 (50.15-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.56 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
$R$ , $R_{free}$	0.248 , 0.271 0.247 , 0.270	Depositor DCC
$R_{free}$ test set	4649 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	144.3	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 130.6	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.43$ , $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.084 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	202.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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  $< |L| >$ ,  $< L^2 >$  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: NAG, NDG

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	0.25	0/3175	0.47	0/4325
1	C	0.24	0/2741	0.46	0/3731
1	E	0.24	0/2704	0.48	0/3683
2	B	0.25	0/3072	0.46	0/4190
2	D	0.25	0/3072	0.45	0/4190
2	F	0.25	0/3072	0.45	0/4190
3	M	0.25	0/2073	0.50	0/2826
3	N	0.24	0/2067	0.49	0/2819
3	O	0.24	0/2067	0.50	0/2819
All	All	0.25	0/24043	0.47	0/32773

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
3	N	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	228	THR	Peptide
3	N	201	ALA	Peptide

## 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	3092	0	2980	47	0
1	C	2669	0	2582	62	0
1	E	2633	0	2526	58	0
2	B	2995	0	2895	60	0
2	D	2995	0	2895	37	0
2	F	2995	0	2895	44	0
3	M	2019	0	1874	45	0
3	N	2013	0	1863	42	0
3	O	2013	0	1863	35	0
4	G	28	0	24	0	0
4	H	28	0	24	1	0
4	I	28	0	24	1	0
5	A	14	0	13	0	0
All	All	23522	0	22458	395	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 9.

All (395) 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)
2:B:235:GLN:O	1:C:336:ARG:NH1	2.06	0.88
1:A:209:PRO:HG2	1:A:333:PRO:HB3	1.55	0.86
1:E:135:ASP:OD2	1:E:183:ARG:NH1	2.09	0.86
1:A:171:LYS:NZ	1:A:196:ASP:OD2	2.11	0.83
1:A:135:ASP:OD2	1:A:183:ARG:NH2	2.12	0.82
2:D:327:LYS:NZ	2:D:343:GLU:OE2	2.13	0.82
2:F:302:GLU:OE2	2:F:319:LYS:NZ	2.13	0.81
1:C:89:GLY:HA3	1:E:168:ARG:HH12	1.47	0.79
1:C:229:GLU:HB2	1:C:321:ILE:HG12	1.65	0.78
3:O:276:HIS:HB3	3:O:281:LEU:HB3	1.68	0.75
3:O:39:GLU:OE2	3:O:288:HIS:NE2	2.18	0.75
3:M:157:THR:HG21	3:M:161:PRO:HA	1.69	0.74
2:B:21:ARG:HH12	2:B:284:GLU:HG3	1.51	0.74
2:B:76:TYR:HE2	2:B:78:CYS:HB2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:SER:HB2	1:C:370:TYR:HE1	1.54	0.72
3:M:72:VAL:HG22	3:M:140:HIS:HB2	1.72	0.72
2:D:110:LYS:HG3	2:D:213:VAL:HG11	1.73	0.71
2:F:21:ARG:HH12	2:F:284:GLU:HG3	1.55	0.71
2:F:16:LYS:NZ	2:F:339:ILE:O	2.25	0.70
3:M:203:GLN:H	3:M:227:ALA:HB2	1.56	0.70
2:D:43:SER:HB3	2:D:123:ARG:HB2	1.73	0.69
3:N:204:VAL:HG13	3:N:275:HIS:HB3	1.75	0.68
1:C:203:GLU:HG2	1:C:357:THR:HG23	1.75	0.68
3:O:148:GLU:OE1	3:O:188:ASN:ND2	2.27	0.68
3:N:203:GLN:H	3:N:227:ALA:HB2	1.59	0.68
3:N:276:HIS:HB3	3:N:281:LEU:HB3	1.76	0.68
3:M:55:GLN:O	3:M:285:ARG:NH1	2.27	0.67
2:F:162:ILE:HB	2:F:279:SER:HB3	1.77	0.67
2:B:312:PHE:HA	2:B:357:SER:HB2	1.75	0.67
2:D:162:ILE:HB	2:D:279:SER:HB3	1.77	0.66
3:O:206:HIS:HB2	3:O:273:HIS:HB3	1.77	0.66
2:B:40:PRO:HA	2:B:127:ALA:HA	1.78	0.65
1:C:264:LYS:HD3	1:C:272:GLU:HB3	1.76	0.65
3:O:214:VAL:HG12	3:O:216:HIS:H	1.62	0.65
2:D:334:THR:HG22	2:D:336:ALA:H	1.61	0.65
2:F:40:PRO:HA	2:F:127:ALA:HA	1.79	0.65
1:A:57:CYS:O	1:A:69:ASN:ND2	2.26	0.64
3:M:242:ARG:NH1	3:M:263:GLU:OE1	2.30	0.64
2:D:134:ARG:NH1	2:D:141:ASN:OD1	2.29	0.64
1:E:229:GLU:HB2	1:E:321:ILE:HB	1.80	0.64
2:F:319:LYS:HG3	2:F:351:GLN:HB3	1.78	0.63
2:B:16:LYS:NZ	2:B:339:ILE:O	2.32	0.63
2:B:162:ILE:HB	2:B:279:SER:HB3	1.80	0.63
1:E:233:VAL:HG22	1:E:301:TYR:HA	1.81	0.63
3:N:214:VAL:HG12	3:N:216:HIS:H	1.62	0.63
1:E:231:ILE:HG23	1:E:319:ILE:HB	1.82	0.62
2:D:185:TYR:OH	2:D:247:ARG:NH1	2.30	0.62
3:N:162:ALA:O	3:N:163:THR:HG22	1.98	0.62
2:B:149:ASN:HA	2:B:165:PRO:HA	1.80	0.62
3:N:73:LEU:HD22	3:N:120:PHE:HD1	1.65	0.62
1:A:203:GLU:HG2	1:A:357:THR:HG23	1.82	0.62
2:F:47:ILE:HG22	2:F:120:SER:HA	1.82	0.62
2:F:294:PRO:HG3	2:F:324:LYS:HG3	1.82	0.61
1:E:348:ILE:HG13	1:E:382:VAL:HG22	1.82	0.61
1:A:266:ASN:HB3	1:A:288:GLN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:97:GLN:HG2	3:N:110:LEU:HD13	1.83	0.60
1:C:362:ARG:NH1	2:D:255:ALA:O	2.34	0.60
1:A:336:ARG:NH1	1:A:354:ASP:OD2	2.34	0.60
2:F:73:LEU:HB2	2:F:76:TYR:HB2	1.83	0.60
1:E:335:ALA:O	1:E:397:ASN:ND2	2.32	0.60
1:C:375:VAL:HG21	1:C:394:TRP:HZ3	1.66	0.60
2:F:361:ALA:HA	2:F:380:CYS:HB2	1.83	0.60
3:O:204:VAL:HG13	3:O:275:HIS:HB3	1.83	0.59
2:B:178:VAL:HG12	2:B:185:TYR:HB2	1.82	0.59
1:E:266:ASN:HB3	1:E:288:GLN:HB2	1.83	0.59
3:M:204:VAL:HG13	3:M:275:HIS:HB2	1.83	0.59
3:O:33:GLY:HA3	3:O:282:HIS:HB3	1.84	0.59
1:E:275:THR:OG1	1:E:277:THR:O	2.21	0.59
1:A:351:LEU:HD11	1:A:359:LEU:HD22	1.85	0.59
3:M:211:PRO:HG2	3:M:214:VAL:HG21	1.85	0.59
3:M:276:HIS:HB3	3:M:281:LEU:HB3	1.85	0.59
2:F:244:LEU:HA	2:F:247:ARG:HD3	1.83	0.59
1:E:228:THR:OG1	1:E:229:GLU:OE2	2.12	0.58
4:I:1:NAG:H61	4:I:2:NDG:C7	2.33	0.58
1:E:226:ALA:O	1:E:320:HIS:ND1	2.29	0.58
1:E:362:ARG:NH1	2:F:255:ALA:O	2.36	0.58
1:A:116:LEU:HD13	1:A:131:LEU:HD12	1.84	0.58
3:M:73:LEU:HG	3:M:120:PHE:HD1	1.67	0.58
1:C:118:ILE:HG21	1:C:160:THR:HB	1.86	0.58
1:A:149:VAL:HG22	1:A:177:VAL:HG22	1.84	0.58
3:M:214:VAL:HG12	3:M:216:HIS:H	1.69	0.58
2:D:47:ILE:HD13	2:D:208:PRO:HG3	1.86	0.58
3:N:272:CYS:HB3	3:N:285:ARG:HB2	1.86	0.58
2:F:332:SER:HB2	2:F:339:ILE:HG13	1.86	0.58
3:M:33:GLY:HA3	3:M:282:HIS:HB3	1.86	0.57
1:A:267:CYS:SG	1:A:288:GLN:NE2	2.77	0.57
2:F:303:VAL:HG21	2:F:378:ALA:HB2	1.85	0.57
3:N:91:LEU:HD12	3:N:97:GLN:HG3	1.86	0.57
1:E:252:VAL:HG22	1:E:281:ILE:HB	1.86	0.57
2:D:82:THR:HG22	2:D:101:THR:HG22	1.86	0.57
3:M:210:GLN:OE1	3:M:216:HIS:ND1	2.38	0.57
1:A:40:ASP:OD1	1:A:315:ARG:NH2	2.37	0.57
3:M:67:HIS:HB2	3:M:199:GLU:OE2	2.05	0.57
3:M:226:TYR:HB2	3:M:230:GLU:HB2	1.87	0.57
1:A:363:ASN:ND2	1:A:368:PRO:O	2.37	0.57
1:E:307:PRO:HD3	2:F:229:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:SER:OG	2:D:351:GLN:N	2.39	0.56
1:A:104:GLU:OE1	1:A:220:TYR:OH	2.23	0.56
2:F:129:ALA:HB1	2:F:148:ALA:HB3	1.86	0.56
3:M:206:HIS:HB2	3:M:273:HIS:HB3	1.88	0.56
2:D:40:PRO:HA	2:D:127:ALA:HA	1.87	0.56
3:N:67:HIS:ND1	3:N:70:GLN:OE1	2.38	0.56
2:B:309:SER:OG	2:B:311:ASP:OD1	2.22	0.56
3:N:260:GLU:HB2	3:N:261:PRO:HD3	1.86	0.56
1:C:149:VAL:HG22	1:C:177:VAL:HG22	1.88	0.55
1:E:245:MET:HG2	1:E:286:VAL:HG23	1.88	0.55
3:O:72:VAL:HG22	3:O:140:HIS:HB2	1.89	0.55
1:E:224:THR:H	3:N:197:HIS:HE1	1.54	0.55
3:M:143:TYR:CZ	3:M:200:GLU:HA	2.42	0.55
2:D:312:PHE:HA	2:D:357:SER:HB2	1.89	0.54
3:M:205:VAL:HG21	3:M:255:PHE:CE2	2.42	0.54
3:O:114:ALA:O	3:O:118:GLY:N	2.35	0.54
3:N:52:LEU:HD11	3:N:270:TYR:HD2	1.72	0.54
3:M:236:PRO:HD2	3:M:239:LEU:HD23	1.88	0.54
1:A:118:ILE:HA	1:A:131:LEU:HB2	1.89	0.54
1:E:79:TYR:O	1:E:115:SER:OG	2.26	0.54
1:C:242:ARG:NH1	1:C:290:HIS:HA	2.24	0.53
2:F:65:THR:HG23	2:F:101:THR:HG21	1.91	0.53
2:B:160:LYS:HB3	2:B:281:ASP:HB3	1.90	0.53
1:E:136:ASN:ND2	3:M:92:TYR:OH	2.41	0.53
1:E:236:PRO:HG3	1:E:300:GLN:HB2	1.90	0.53
1:E:181:ASP:OD2	1:E:185:ILE:HG23	2.08	0.53
1:C:234:HIS:HB3	1:C:316:LYS:HA	1.91	0.53
1:C:164:PHE:CE2	1:C:321:ILE:HB	2.43	0.53
1:C:111:LYS:NZ	1:C:323:PHE:O	2.35	0.53
2:B:134:ARG:NH1	2:B:141:ASN:OD1	2.39	0.53
2:F:29:LEU:HD11	2:F:282:ILE:HD11	1.90	0.53
1:C:232:GLU:OE1	1:C:316:LYS:NZ	2.34	0.52
1:E:213:LYS:HB3	1:E:334:LYS:HE3	1.92	0.52
1:E:229:GLU:HG3	2:F:112:GLU:HG2	1.90	0.52
3:M:239:LEU:HD12	3:M:242:ARG:HE	1.72	0.52
2:B:237:PRO:HD3	1:C:336:ARG:HH12	1.73	0.52
1:C:173:GLU:OE1	1:E:206:HIS:NE2	2.42	0.52
2:B:28:VAL:HG23	2:B:329:ALA:HB1	1.91	0.52
1:C:360:SER:HB2	1:C:370:TYR:CE1	2.40	0.52
1:E:319:ILE:HG22	1:E:320:HIS:H	1.72	0.52
3:M:148:GLU:OE1	3:M:188:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:205:VAL:HG22	3:N:274:LEU:HD23	1.92	0.52
1:C:242:ARG:HH12	1:C:290:HIS:HA	1.75	0.52
3:O:108:LEU:HD23	3:O:122:LEU:HD21	1.92	0.52
2:F:179:VAL:HG12	2:F:180:TYR:O	2.10	0.51
3:N:132:ALA:HB2	3:N:156:VAL:HG23	1.92	0.51
1:A:73:TYR:O	1:A:132:ARG:NH2	2.40	0.51
2:B:97:ASP:O	3:O:252:ARG:NH1	2.43	0.51
3:M:242:ARG:CB	3:M:261:PRO:HD2	2.40	0.51
2:F:252:GLN:HB2	2:F:261:ILE:HB	1.92	0.51
2:F:296:LEU:HD21	2:F:346:VAL:HG11	1.93	0.51
3:O:211:PRO:HG2	3:O:214:VAL:HG21	1.91	0.51
1:A:128:TRP:CD1	1:A:129:THR:HG23	2.46	0.51
1:E:238:ASP:O	1:E:240:PRO:HD3	2.10	0.51
1:E:405:GLN:HG2	2:F:383:PRO:HG3	1.93	0.51
1:A:405:GLN:OE1	2:B:310:SER:N	2.44	0.51
2:D:5:THR:HG21	2:D:31:MET:HE1	1.91	0.51
1:E:235:MET:HG2	1:E:299:TRP:CD1	2.46	0.50
1:E:251:ASN:OD1	1:E:282:ASN:HA	2.11	0.50
3:O:154:LEU:HD13	3:O:184:LEU:HD21	1.93	0.50
2:D:8:PRO:HA	2:D:275:ASN:HA	1.92	0.50
2:D:176:LYS:HB3	2:D:189:TYR:CE2	2.45	0.50
1:E:164:PHE:CZ	1:E:321:ILE:HG12	2.47	0.50
3:N:136:THR:OG1	3:N:138:ASN:ND2	2.44	0.50
1:A:285:LYS:HG2	1:A:286:VAL:H	1.77	0.50
3:M:110:LEU:H	3:M:110:LEU:HD23	1.77	0.50
3:M:170:GLU:HG2	3:M:171:LYS:H	1.74	0.50
2:F:3:HIS:CD2	2:F:19:VAL:HG22	2.46	0.50
2:B:47:ILE:HD13	2:B:208:PRO:HG3	1.93	0.49
1:E:202:ARG:NE	1:E:395:GLY:O	2.32	0.49
3:M:132:ALA:HB2	3:M:156:VAL:HG23	1.94	0.49
1:C:123:ASP:OD1	1:C:123:ASP:N	2.38	0.49
1:A:211:HIS:CG	1:A:212:GLY:H	2.30	0.49
3:N:206:HIS:HB2	3:N:273:HIS:HB3	1.93	0.49
1:A:394:TRP:HB3	1:A:400:TYR:HE2	1.77	0.49
1:E:140:ALA:HB2	3:M:98:ARG:NH2	2.28	0.49
3:M:164:PRO:HA	3:M:175:ALA:HB3	1.94	0.49
3:N:67:HIS:HB2	3:N:199:GLU:OE2	2.12	0.49
1:C:122:THR:HG22	1:C:139:PRO:HB2	1.93	0.49
3:M:47:GLY:HA2	3:M:262:LEU:H	1.77	0.49
2:B:332:SER:HB2	2:B:339:ILE:HG13	1.93	0.49
1:C:251:ASN:OD1	1:C:283:ASN:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:GLN:HB2	2:B:373:GLN:HG2	1.93	0.48
2:D:65:THR:HG23	2:D:101:THR:HG21	1.94	0.48
2:D:295:SER:O	2:D:323:SER:OG	2.30	0.48
3:M:242:ARG:HB3	3:M:261:PRO:HD2	1.95	0.48
3:O:260:GLU:HB2	3:O:261:PRO:HD3	1.96	0.48
1:C:386:PRO:HB2	1:C:388:GLU:OE1	2.14	0.48
1:A:255:THR:HG23	1:A:278:ASP:OD2	2.14	0.48
2:B:237:PRO:HG2	2:B:242:TYR:CE2	2.48	0.48
1:E:240:PRO:HG2	2:F:93:TYR:HA	1.94	0.48
2:B:76:TYR:CE2	2:B:78:CYS:HB2	2.42	0.48
1:E:80:LEU:HD12	2:F:89:TRP:CD2	2.49	0.48
1:A:234:HIS:ND1	1:A:235:MET:O	2.47	0.48
3:N:141:HIS:HB3	3:N:146:LEU:HB2	1.95	0.48
2:B:44:LEU:HA	2:B:122:TYR:HD1	1.78	0.48
1:C:114:VAL:HG11	1:C:177:VAL:HG11	1.95	0.47
1:E:265:CYS:HA	1:E:289:CYS:HA	1.95	0.47
3:N:242:ARG:CB	3:N:261:PRO:HD2	2.44	0.47
1:A:360:SER:HB2	1:A:370:TYR:CE1	2.48	0.47
1:A:362:ARG:NE	1:A:391:GLU:OE1	2.37	0.47
2:D:65:THR:HA	2:D:101:THR:HG21	1.96	0.47
1:E:137:HIS:NE2	1:E:293:VAL:HG21	2.30	0.47
1:C:106:THR:HG1	1:C:218:SER:H	1.61	0.47
3:O:242:ARG:CB	3:O:261:PRO:HD2	2.44	0.47
2:B:110:LYS:HG3	2:B:213:VAL:HG11	1.96	0.47
1:C:135:ASP:OD2	1:C:183:ARG:NH2	2.47	0.47
1:E:233:VAL:HG13	1:E:300:GLN:O	2.13	0.47
2:B:251:LEU:HB2	2:B:261:ILE:HG13	1.96	0.47
2:F:299:MET:HA	2:F:319:LYS:O	2.14	0.47
2:B:252:GLN:NE2	2:B:260:GLN:OE1	2.37	0.47
1:A:218:SER:HB2	1:A:325:LEU:HD11	1.97	0.47
1:C:98:LEU:HD23	1:C:114:VAL:HG12	1.96	0.47
1:A:224:THR:HG22	3:M:197:HIS:CE1	2.50	0.47
1:C:233:VAL:HG12	1:C:301:TYR:HA	1.95	0.47
2:D:42:LEU:HD11	2:D:266:VAL:HB	1.96	0.47
1:E:136:ASN:O	2:F:89:TRP:HZ2	1.98	0.47
2:F:192:PHE:HA	2:F:204:GLN:NE2	2.30	0.47
2:B:222:GLN:OE1	1:C:211:HIS:ND1	2.48	0.47
1:C:88:GLU:O	1:E:168:ARG:NH1	2.48	0.47
1:C:204:LYS:HD2	1:C:356:PRO:HB2	1.97	0.47
3:N:47:GLY:HA2	3:N:262:LEU:H	1.79	0.47
3:N:205:VAL:HG21	3:N:255:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TYR:CD2	1:A:74:LYS:HG3	2.50	0.46
2:F:249:ALA:HB1	2:F:253:HIS:HB2	1.96	0.46
3:O:176:VAL:HG21	3:O:182:ALA:HB2	1.96	0.46
1:C:375:VAL:HG21	1:C:394:TRP:CZ3	2.48	0.46
2:D:59:TYR:HE2	2:D:61:LYS:HD2	1.80	0.46
1:E:229:GLU:CB	1:E:321:ILE:HB	2.45	0.46
3:M:166:TYR:CD2	3:M:167:TRP:HB2	2.50	0.46
1:C:164:PHE:CD2	1:C:322:PRO:HD2	2.51	0.46
2:B:55:ILE:HD11	2:B:233:TYR:HD2	1.80	0.46
2:D:171:THR:HG23	2:D:173:PHE:H	1.81	0.46
1:C:218:SER:HB2	1:C:325:LEU:HD11	1.96	0.46
1:C:388:GLU:OE1	1:C:388:GLU:N	2.43	0.46
1:E:224:THR:H	3:N:197:HIS:CE1	2.33	0.46
1:A:264:LYS:HD2	1:A:272:GLU:HB3	1.98	0.46
1:C:302:ASN:OD1	2:D:57:SER:N	2.34	0.46
3:N:61:TRP:CZ2	3:N:201:ALA:HB2	2.51	0.46
3:N:170:GLU:HG2	3:N:171:LYS:H	1.81	0.46
2:D:336:ALA:HB1	2:D:360:LEU:HD11	1.98	0.45
1:C:205:PHE:H	1:C:205:PHE:HD1	1.64	0.45
3:N:221:ARG:HD3	3:N:221:ARG:HA	1.61	0.45
2:D:242:TYR:CE2	1:E:378:LYS:HB2	2.52	0.45
1:A:210:GLN:HB3	2:F:230:HIS:CE1	2.52	0.45
1:A:265:CYS:O	1:A:271:ASN:HB2	2.17	0.45
1:E:287:ASP:HB3	3:M:57:PRO:HG3	1.98	0.45
3:N:33:GLY:HA3	3:N:282:HIS:HB3	1.99	0.45
3:O:194:THR:O	3:O:194:THR:OG1	2.34	0.45
2:B:203:ILE:HG13	2:B:215:ALA:HB2	1.99	0.45
2:B:250:SER:OG	2:B:251:LEU:N	2.50	0.45
2:B:8:PRO:HD2	2:B:15:TYR:CZ	2.52	0.45
1:C:82:HIS:HB3	1:C:305:LEU:HD22	1.97	0.45
3:N:163:THR:HG23	3:N:163:THR:O	2.17	0.45
2:B:24:TYR:CD1	2:B:287:PHE:HB3	2.51	0.45
1:C:307:PRO:HD3	2:D:229:VAL:HG11	1.99	0.45
1:C:312:LEU:HD13	1:C:315:ARG:HB2	1.98	0.45
1:E:329:THR:HB	3:N:228:SER:HB3	1.98	0.45
1:A:130:LYS:HE3	1:A:143:GLU:OE2	2.17	0.45
2:B:28:VAL:HB	2:B:342:ALA:HB1	1.98	0.45
2:F:368:GLN:HA	2:F:373:GLN:HA	1.97	0.45
3:M:78:ARG:HG2	3:M:83:GLY:HA2	1.98	0.44
3:O:104:ASP:HB3	3:O:108:LEU:HD13	2.00	0.44
3:O:208:ASP:HB2	3:O:271:SER:OG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG23	1:A:321:ILE:HD13	2.00	0.44
2:B:60:VAL:HG11	2:B:86:PRO:HG3	1.99	0.44
1:C:136:ASN:OD1	3:N:69:ARG:NE	2.50	0.44
1:C:294:THR:O	1:C:294:THR:OG1	2.31	0.44
1:E:135:ASP:OD1	1:E:136:ASN:ND2	2.50	0.44
3:M:141:HIS:ND1	3:M:144:CYS:HB2	2.32	0.44
3:N:134:LEU:HB2	3:N:153:ARG:HD3	1.98	0.44
3:O:84:PRO:HG2	3:O:86:ARG:HH12	1.82	0.44
2:B:81:PHE:CE1	2:B:223:ARG:HA	2.53	0.44
2:B:149:ASN:ND2	2:B:151:ASP:OD2	2.50	0.44
2:D:198:GLY:HA3	1:E:352:TYR:HE2	1.82	0.44
2:F:341:GLU:OE1	2:F:341:GLU:N	2.45	0.44
2:B:322:ALA:N	2:B:348:GLY:O	2.46	0.44
2:D:250:SER:OG	2:D:251:LEU:N	2.51	0.44
1:A:209:PRO:HG2	1:A:333:PRO:CB	2.39	0.44
1:A:352:TYR:HD2	2:F:242:TYR:HE2	1.65	0.44
1:C:118:ILE:HA	1:C:131:LEU:HB2	1.99	0.44
2:D:192:PHE:HE1	2:D:206:ARG:HG2	1.81	0.44
2:B:19:VAL:HB	2:B:27:MET:HB3	2.00	0.44
3:M:69:ARG:HD3	3:M:69:ARG:N	2.33	0.44
3:M:141:HIS:HB3	3:M:146:LEU:HB2	2.00	0.44
1:C:181:ASP:OD2	1:C:185:ILE:HB	2.18	0.44
1:C:363:ASN:HB2	1:C:368:PRO:HA	2.00	0.44
2:F:328:CYS:HB3	2:F:370:CYS:HB2	1.88	0.44
3:O:51:VAL:HG22	3:O:258:ARG:HG2	2.00	0.44
1:E:231:ILE:HD11	1:E:301:TYR:CE2	2.53	0.43
1:A:276:THR:HG23	1:A:277:THR:HG23	1.99	0.43
2:B:368:GLN:HA	2:B:373:GLN:HA	2.00	0.43
1:E:161:MET:SD	1:E:322:PRO:HG3	2.57	0.43
1:E:204:LYS:HB2	1:E:356:PRO:HB2	1.99	0.43
3:M:71:ARG:NH2	3:M:93:SER:OG	2.45	0.43
3:O:64:ASP:OD2	3:O:200:GLU:HB2	2.17	0.43
1:A:387:THR:HA	1:A:404:PRO:HG2	1.99	0.43
3:N:71:ARG:NH1	3:N:195:ASP:O	2.37	0.43
3:O:242:ARG:HB2	3:O:261:PRO:HD2	2.00	0.43
1:A:48:TYR:OH	1:A:230:GLU:OE2	2.26	0.43
1:A:240:PRO:O	2:B:90:GLY:HA3	2.18	0.43
2:B:180:TYR:O	2:B:182:GLY:N	2.50	0.43
2:B:308:HIS:O	2:B:383:PRO:HD3	2.19	0.43
3:O:84:PRO:HG2	3:O:86:ARG:NH1	2.33	0.43
1:C:238:ASP:O	1:C:240:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:65:ARG:HB2	3:N:200:GLU:OE2	2.18	0.43
1:A:348:ILE:HG13	1:A:382:VAL:HG22	2.00	0.43
2:B:18:LEU:HD13	2:B:331:HIS:CG	2.54	0.43
1:C:204:LYS:HE2	1:C:204:LYS:HB3	1.92	0.43
1:C:309:ASN:HB3	1:C:312:LEU:HG	2.00	0.43
3:M:199:GLU:C	3:M:200:GLU:HG2	2.39	0.43
3:N:54:CYS:O	3:N:255:PHE:HB2	2.18	0.43
3:N:260:GLU:HB2	3:N:261:PRO:CD	2.48	0.43
2:B:66:ALA:HB1	2:B:103:LEU:HD12	2.01	0.43
2:D:173:PHE:CE2	2:D:268:ALA:HB2	2.54	0.43
1:C:136:ASN:ND2	3:N:69:ARG:HH11	2.16	0.43
1:E:117:GLN:OE1	1:E:132:ARG:NE	2.43	0.43
3:O:144:CYS:SG	3:O:276:HIS:NE2	2.83	0.43
2:B:85:TYR:O	2:B:227:GLY:HA2	2.17	0.43
2:B:178:VAL:HG21	2:B:200:PHE:CZ	2.54	0.43
1:A:133:TYR:HE2	1:A:142:ALA:HB2	1.82	0.42
2:B:89:TRP:O	3:O:65:ARG:NH1	2.52	0.42
2:B:341:GLU:HG2	2:B:354:ILE:HG22	2.01	0.42
3:O:107:ARG:HD3	3:O:126:ALA:O	2.19	0.42
1:C:71:ASN:HB3	1:C:74:LYS:HB3	2.01	0.42
2:B:146:ALA:HB2	2:B:154:VAL:CG2	2.49	0.42
2:B:190:PRO:HA	2:B:191:PRO:HD3	1.89	0.42
1:C:342:TYR:HD1	2:D:385:ASP:HB3	1.84	0.42
1:E:129:THR:OG1	1:E:130:LYS:NZ	2.46	0.42
1:E:365:GLY:HA3	1:E:388:GLU:HG2	2.01	0.42
2:F:158:ASP:HB3	2:F:283:PRO:HG3	2.00	0.42
1:A:358:LEU:HD13	1:A:374:TRP:CD2	2.55	0.42
2:B:28:VAL:HG22	2:B:331:HIS:HB2	2.01	0.42
1:C:327:ASN:OD1	1:C:327:ASN:N	2.45	0.42
3:M:71:ARG:HE	3:M:71:ARG:HB2	1.70	0.42
2:B:18:LEU:HD22	2:B:331:HIS:CE1	2.54	0.42
2:D:76:TYR:HE2	2:D:78:CYS:HB2	1.85	0.42
3:O:66:LEU:O	3:O:68:ASP:N	2.53	0.42
3:O:73:LEU:HD22	3:O:120:PHE:HD1	1.84	0.42
2:F:9:ASN:ND2	2:F:271:CYS:O	2.52	0.42
3:M:255:PHE:N	3:M:255:PHE:CD1	2.88	0.42
1:A:111:LYS:HE3	1:A:323:PHE:O	2.19	0.42
1:C:351:LEU:HB3	1:C:394:TRP:CH2	2.55	0.42
3:M:191:HIS:CE1	3:M:195:ASP:OD2	2.72	0.42
1:C:85:ASP:OD1	1:C:89:GLY:HA2	2.20	0.42
2:D:320:TYR:CE1	2:D:346:VAL:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:242:ARG:HH12	3:M:263:GLU:HB2	1.85	0.42
1:A:38:LEU:HD23	1:A:50:LEU:HD23	2.02	0.42
1:C:254:ILE:HG21	1:C:275:THR:HG21	2.01	0.42
3:M:75:TRP:HA	3:M:136:THR:O	2.20	0.42
3:N:210:GLN:OE1	3:N:216:HIS:ND1	2.52	0.42
1:C:285:LYS:HG2	1:C:286:VAL:H	1.86	0.41
3:N:242:ARG:H	3:N:242:ARG:HD3	1.85	0.41
3:O:124:ILE:HD11	3:O:135:TYR:HE2	1.85	0.41
1:A:27:TYR:HD2	1:A:74:LYS:HG3	1.84	0.41
1:A:58:SER:HA	1:A:59:PRO:HD3	1.90	0.41
2:B:317:ILE:HG12	2:B:353:GLN:HG3	2.02	0.41
2:D:31:MET:HG2	2:D:135:VAL:HG22	2.03	0.41
1:E:135:ASP:CG	1:E:183:ARG:HH12	2.11	0.41
1:E:234:HIS:NE2	1:E:302:ASN:HB2	2.34	0.41
3:N:242:ARG:HB3	3:N:261:PRO:HD2	2.03	0.41
1:C:112:ILE:HD13	1:C:175:LEU:HD21	2.01	0.41
1:C:305:LEU:HA	2:D:229:VAL:O	2.21	0.41
1:E:231:ILE:HB	1:E:321:ILE:HD11	2.02	0.41
2:F:374:VAL:HG22	2:F:375:HIS:H	1.85	0.41
2:F:388:VAL:HG22	2:F:389:ASN:H	1.85	0.41
3:O:124:ILE:O	3:O:181:PRO:HA	2.20	0.41
2:B:21:ARG:NH1	2:B:284:GLU:HG3	2.27	0.41
1:E:234:HIS:HB3	1:E:315:ARG:C	2.41	0.41
3:N:77:LEU:HD23	3:N:78:ARG:N	2.35	0.41
1:A:147:LEU:HD12	1:A:179:PHE:HB3	2.03	0.41
2:B:9:ASN:O	2:B:272:ALA:HA	2.21	0.41
2:B:167:SER:HG	2:B:275:ASN:H	1.63	0.41
2:D:76:TYR:CE2	2:D:78:CYS:HB2	2.55	0.41
3:M:33:GLY:N	3:M:275:HIS:HE2	2.19	0.41
3:N:197:HIS:CG	3:N:198:VAL:H	2.38	0.41
3:N:223:LEU:HD23	3:N:223:LEU:HA	1.89	0.41
4:H:1:NAG:H61	4:H:2:NDG:C8	2.50	0.41
2:B:306:CYS:SG	2:B:307:THR:N	2.94	0.41
3:M:242:ARG:HB2	3:M:261:PRO:HD2	2.03	0.41
1:C:113:GLN:HA	1:C:163:HIS:O	2.21	0.40
1:E:231:ILE:CG2	1:E:319:ILE:HB	2.49	0.40
2:F:161:PHE:CD1	2:F:280:ILE:HG12	2.55	0.40
2:F:308:HIS:CD2	2:F:382:PRO:HA	2.56	0.40
3:O:209:ARG:HG3	3:O:270:TYR:CE1	2.56	0.40
2:B:55:ILE:HD11	2:B:233:TYR:CD2	2.56	0.40
2:B:65:THR:HG23	2:B:101:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:PRO:HG3	1:E:375:VAL:HG12	2.02	0.40
2:F:161:PHE:HD1	2:F:280:ILE:HG12	1.87	0.40
1:C:153:ALA:HB3	1:C:170:PRO:HG3	2.03	0.40
1:E:362:ARG:HH12	2:F:255:ALA:HB3	1.86	0.40
1:C:181:ASP:OD1	1:C:185:ILE:N	2.42	0.40
1:C:368:PRO:HG3	2:D:256:PRO:HG3	2.03	0.40
2:F:80:VAL:HG22	2:F:103:LEU:HD12	2.04	0.40
3:O:233:ALA:O	3:O:240:ARG:NH2	2.55	0.40
2:B:159:ALA:HA	2:B:283:PRO:HD3	2.04	0.40
2:B:176:LYS:HB3	2:B:189:TYR:CE2	2.57	0.40
3:O:74:HIS:HE1	3:O:76:ASP:OD2	2.04	0.40
3:O:222:LEU:HD12	3:O:243:VAL:HG11	2.03	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	389/406 (96%)	357 (92%)	32 (8%)	0	100 100
1	C	336/406 (83%)	316 (94%)	19 (6%)	1 (0%)	41 75
1	E	331/406 (82%)	294 (89%)	37 (11%)	0	100 100
2	B	392/432 (91%)	378 (96%)	14 (4%)	0	100 100
2	D	392/432 (91%)	377 (96%)	15 (4%)	0	100 100
2	F	392/432 (91%)	374 (95%)	18 (5%)	0	100 100
3	M	254/269 (94%)	220 (87%)	34 (13%)	0	100 100
3	N	254/269 (94%)	229 (90%)	25 (10%)	0	100 100
3	O	254/269 (94%)	229 (90%)	25 (10%)	0	100 100
All	All	2994/3321 (90%)	2774 (93%)	219 (7%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	377	HIS

### 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	351/364 (96%)	345 (98%)	6 (2%)	60 82
1	C	300/364 (82%)	293 (98%)	7 (2%)	50 77
1	E	295/364 (81%)	288 (98%)	7 (2%)	49 76
2	B	329/349 (94%)	321 (98%)	8 (2%)	49 76
2	D	329/349 (94%)	320 (97%)	9 (3%)	44 73
2	F	329/349 (94%)	324 (98%)	5 (2%)	65 84
3	M	204/217 (94%)	198 (97%)	6 (3%)	42 71
3	N	203/217 (94%)	195 (96%)	8 (4%)	32 64
3	O	203/217 (94%)	200 (98%)	3 (2%)	65 84
All	All	2543/2790 (91%)	2484 (98%)	59 (2%)	50 77

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	128	TRP
1	A	148	PHE
1	A	208	ARG
1	A	284	CYS
1	A	344	LYS
2	B	85	TYR
2	B	87	PHE
2	B	151	ASP
2	B	158	ASP
2	B	230	HIS
2	B	233	TYR

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Mol	Chain	Res	Type
2	B	292	ASP
2	B	366	ARG
1	C	92	CYS
1	C	179	PHE
1	C	284	CYS
1	C	299	TRP
1	C	336	ARG
1	C	350	LEU
1	C	378	LYS
2	D	1	TYR
2	D	85	TYR
2	D	95	PHE
2	D	125	HIS
2	D	151	ASP
2	D	192	PHE
2	D	230	HIS
2	D	242	TYR
2	D	389	ASN
1	E	92	CYS
1	E	131	LEU
1	E	137	HIS
1	E	148	PHE
1	E	208	ARG
1	E	262	ARG
1	E	320	HIS
2	F	118	PHE
2	F	230	HIS
2	F	252	GLN
2	F	292	ASP
2	F	308	HIS
3	M	64	ASP
3	M	98	ARG
3	M	197	HIS
3	M	242	ARG
3	M	250	PHE
3	M	276	HIS
3	N	134	LEU
3	N	147	TYR
3	N	153	ARG
3	N	197	HIS
3	N	240	ARG
3	N	242	ARG

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Mol	Chain	Res	Type
3	N	250	PHE
3	N	262	LEU
3	O	97	GLN
3	O	242	ARG
3	O	250	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	136	ASN
1	E	282	ASN
2	F	3	HIS
2	F	204	GLN
3	N	63	GLN
3	N	197	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
4	NAG	G	1	2,4	14,14,15	0.55	0	17,19,21	1.02	2 (11%)
4	NDG	G	2	4	14,14,15	0.97	1 (7%)	17,19,21	2.35	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	H	1	2,4	14,14,15	0.42	0	17,19,21	0.67	0
4	NDG	H	2	4	14,14,15	1.22	1 (7%)	17,19,21	1.93	3 (17%)
4	NAG	I	1	2,4	14,14,15	0.97	1 (7%)	17,19,21	1.59	3 (17%)
4	NDG	I	2	4	14,14,15	1.14	1 (7%)	17,19,21	2.44	4 (23%)

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	NAG	G	1	2,4	-	0/6/23/26	0/1/1/1
4	NDG	G	2	4	-	1/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	2/6/23/26	0/1/1/1
4	NDG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	2,4	-	2/6/23/26	0/1/1/1
4	NDG	I	2	4	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NDG	C1-C2	4.00	1.58	1.52
4	I	2	NDG	C1-C2	3.76	1.58	1.52
4	G	2	NDG	C1-C2	3.16	1.57	1.52
4	I	1	NAG	O5-C1	2.98	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NDG	C1-O5-C5	7.48	122.33	112.19
4	I	2	NDG	C1-O5-C5	7.41	122.24	112.19
4	H	2	NDG	C1-C2-N2	5.72	120.25	110.49
4	I	1	NAG	C1-O5-C5	4.87	118.79	112.19
4	I	2	NDG	C1-C2-N2	4.49	118.15	110.49
4	H	2	NDG	C1-O5-C5	3.49	116.92	112.19
4	G	2	NDG	O5-C1-C2	2.89	115.85	111.29
4	G	1	NAG	O4-C4-C3	2.78	116.78	110.35
4	I	2	NDG	C3-C4-C5	-2.68	105.47	110.24
4	I	1	NAG	O4-C4-C3	2.52	116.17	110.35
4	G	2	NDG	C3-C4-C5	-2.51	105.77	110.24
4	I	1	NAG	O4-C4-C5	2.48	115.44	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	G	2	NDG	C1-C2-N2	2.23	114.29	110.49
4	G	2	NDG	C8-C7-N2	-2.14	112.47	116.10
4	G	2	NDG	O4-C4-C3	-2.14	105.41	110.35
4	I	2	NDG	C8-C7-N2	-2.05	112.62	116.10
4	H	2	NDG	C3-C4-C5	-2.02	106.64	110.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

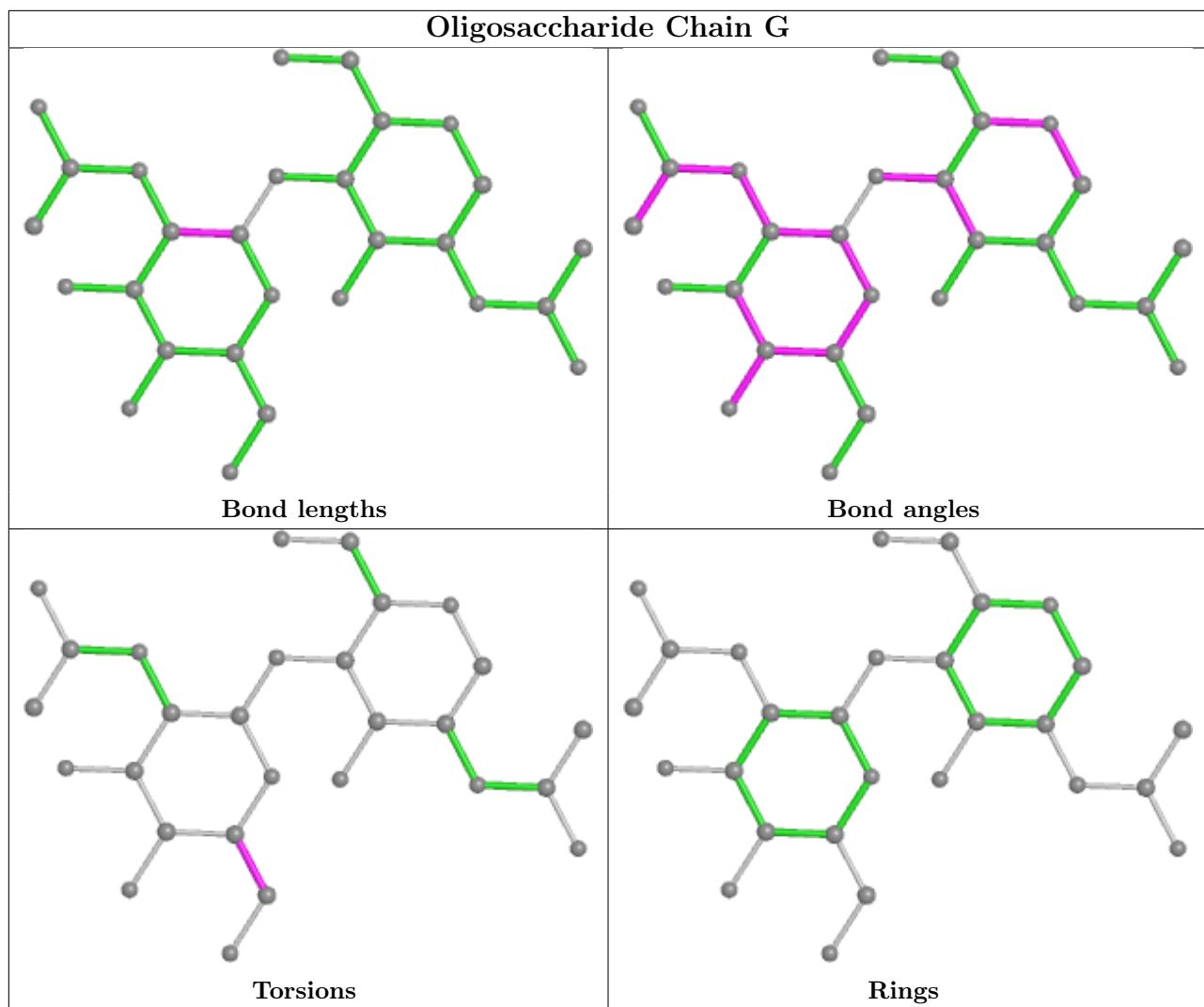
Mol	Chain	Res	Type	Atoms
4	I	2	NDG	O5-C5-C6-O6
4	H	2	NDG	O5-C5-C6-O6
4	I	2	NDG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	2	NDG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

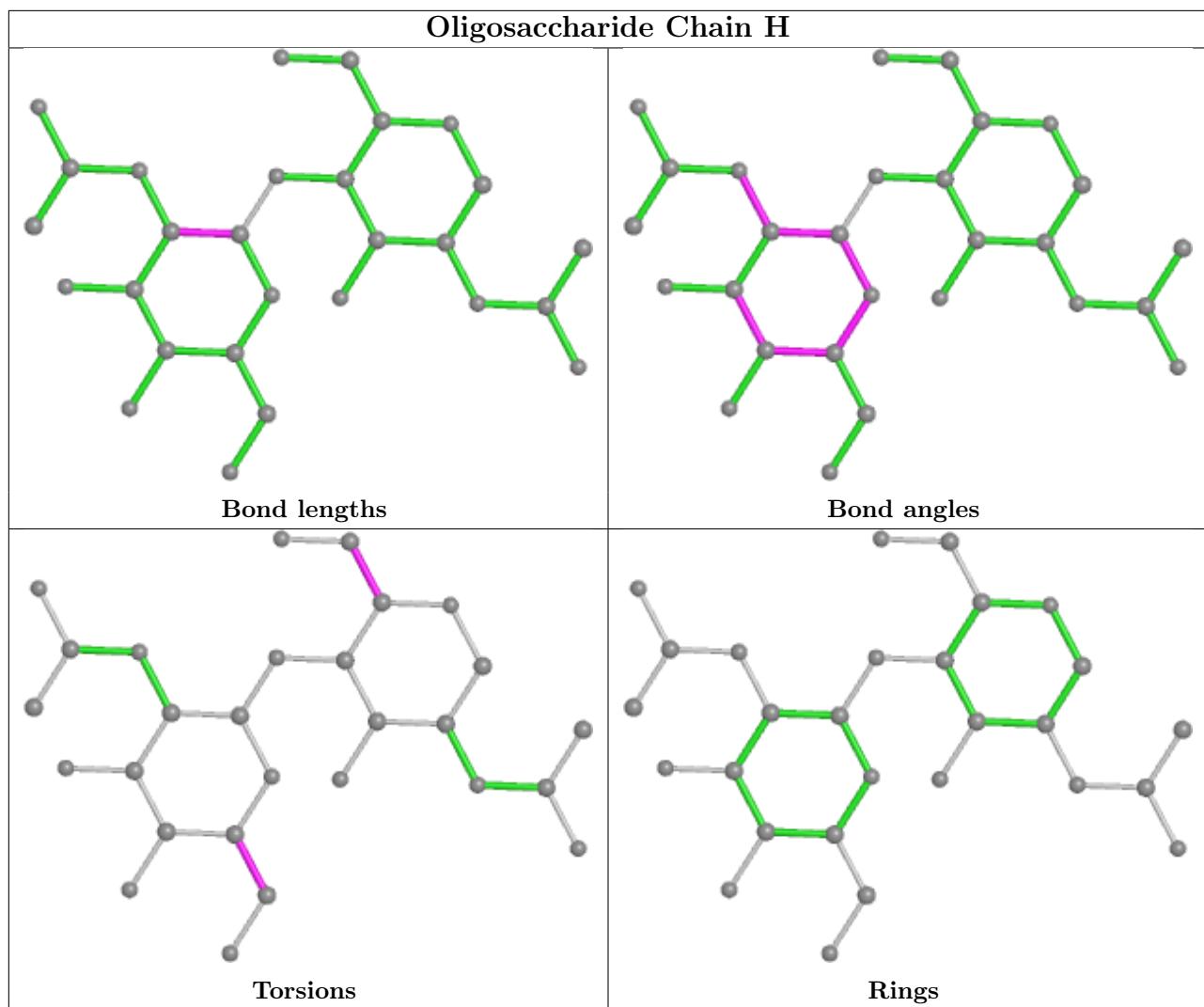
There are no ring outliers.

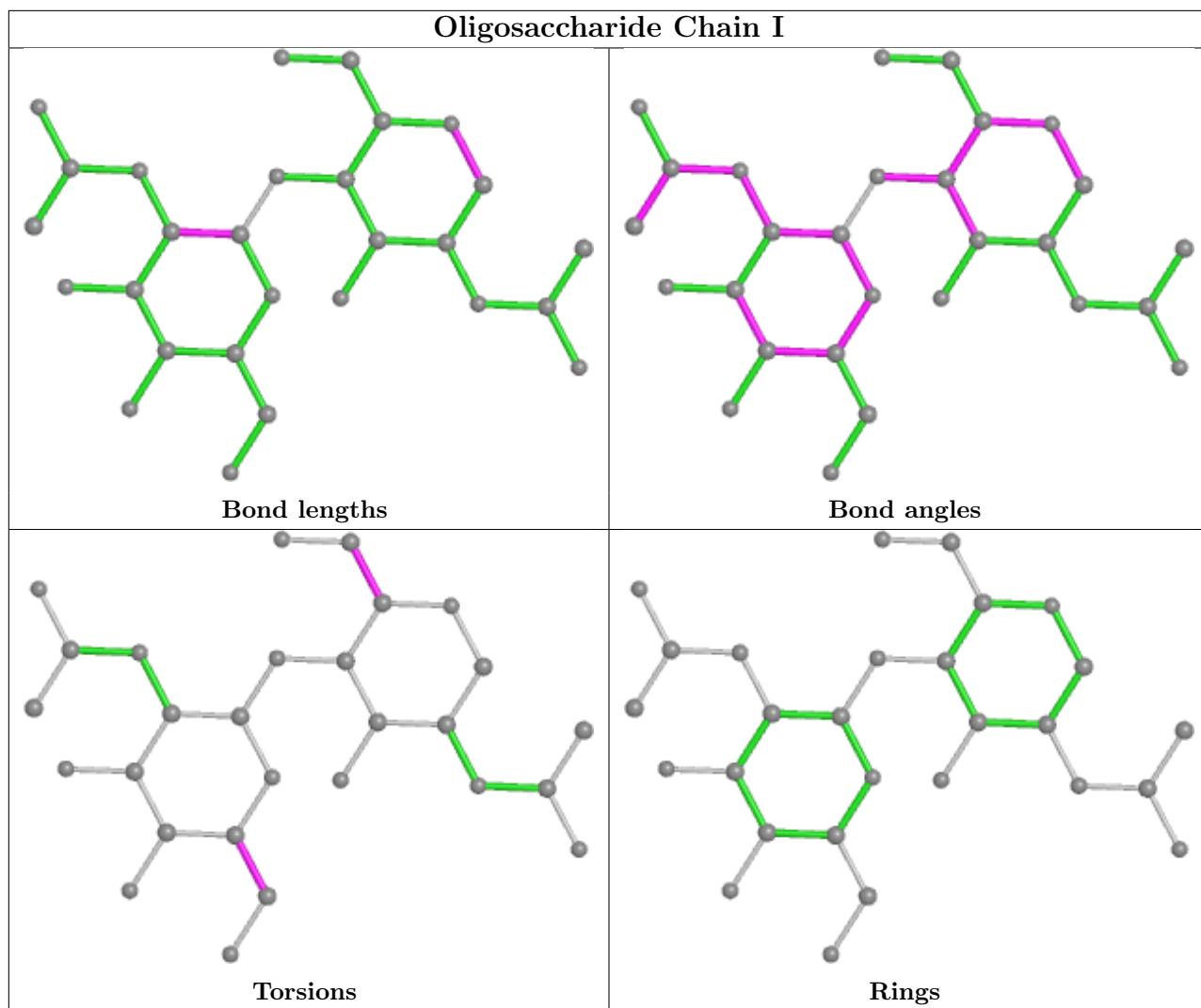
4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	H	2	NDG	1	0
4	I	2	NDG	1	0
4	H	1	NAG	1	0

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







## 5.6 Ligand geometry (i)

1 ligand is 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	A	1101	1	14,14,15	0.30	0	17,19,21	0.61	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1101	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	1101	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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	393/406 (96%)	0.31	11 (2%) 53 47	82, 148, 246, 355	0
1	C	338/406 (83%)	0.55	32 (9%) 8 8	115, 174, 332, 460	0
1	E	335/406 (82%)	0.35	11 (3%) 46 41	115, 171, 231, 309	0
2	B	393/432 (90%)	0.90	70 (17%) 1 1	105, 202, 387, 479	0
2	D	393/432 (90%)	0.41	36 (9%) 9 9	133, 188, 251, 340	0
2	F	393/432 (90%)	0.71	52 (13%) 3 4	117, 221, 327, 418	0
3	M	258/269 (95%)	0.23	8 (3%) 49 43	107, 160, 226, 325	0
3	N	258/269 (95%)	0.89	43 (16%) 1 2	155, 235, 327, 492	0
3	O	258/269 (95%)	1.24	73 (28%) 0 0	159, 255, 333, 379	0
All	All	3019/3321 (90%)	0.61	336 (11%) 5 6	82, 190, 324, 492	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	163	THR	15.8
2	B	369	VAL	12.3
2	B	354	ILE	12.1
2	B	27	MET	11.5
2	B	367	VAL	10.9
2	B	330	VAL	10.8
2	B	353	GLN	9.0
2	B	352	LEU	8.6
2	F	352	LEU	8.3
3	O	52	LEU	8.1
2	F	353	GLN	7.6
2	F	296	LEU	7.5
3	N	50	ALA	7.1
3	N	171	LYS	7.0
2	B	318	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	19	VAL	6.8
2	B	29	LEU	6.8
2	F	148	ALA	6.7
2	B	345	GLU	6.6
3	N	162	ALA	6.5
1	C	311	GLU	6.4
2	F	38	LEU	6.3
2	F	318	ILE	6.0
2	B	326	GLY	5.8
3	O	151	ALA	5.7
3	N	172	GLU	5.7
1	C	282	ASN	5.7
2	F	31	MET	5.6
1	C	245	MET	5.5
2	B	325	LYS	5.5
2	B	316	ALA	5.5
2	B	329	ALA	5.4
3	O	59	MET	5.4
2	F	266	VAL	5.3
2	F	367	VAL	5.3
2	F	261	ILE	5.3
3	N	259	ILE	5.3
2	F	368	GLN	5.2
2	B	317	ILE	5.2
2	B	31	MET	5.1
3	O	245	VAL	5.1
2	D	67	GLU	5.1
2	F	316	ALA	5.1
2	F	137	TYR	5.1
2	F	369	VAL	5.0
2	F	317	ILE	4.9
3	N	170	GLU	4.8
3	O	154	LEU	4.8
1	C	281	ILE	4.8
1	C	274	LEU	4.8
2	F	330	VAL	4.8
3	O	200	GLU	4.7
3	N	292	ALA	4.7
1	E	349	MET	4.7
2	F	354	ILE	4.6
3	N	52	LEU	4.6
3	N	62	THR	4.5

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Mol	Chain	Res	Type	RSRZ
3	O	201	ALA	4.5
2	B	28	VAL	4.5
3	O	152	VAL	4.5
3	O	49	ARG	4.4
3	N	51	VAL	4.3
3	O	139	LEU	4.3
2	B	315	VAL	4.3
2	B	278	ILE	4.3
2	F	33	LEU	4.3
3	N	258	ARG	4.3
3	N	56	SER	4.3
3	N	63	GLN	4.3
1	C	310	ALA	4.2
1	E	327	ASN	4.2
3	O	108	LEU	4.2
3	O	62	THR	4.2
1	E	351	LEU	4.2
3	O	250	PHE	4.2
2	F	262	ALA	4.2
3	O	50	ALA	4.2
3	N	233	ALA	4.1
3	O	207	TRP	4.1
2	D	103	LEU	4.1
2	B	280	ILE	4.1
2	D	80	VAL	4.1
3	O	122	LEU	4.1
2	B	285	ALA	4.1
1	C	269	GLY	4.0
2	B	331	HIS	4.0
1	C	317	GLY	4.0
2	D	93	TYR	4.0
3	N	228	SER	4.0
2	F	180	TYR	3.9
3	O	184	LEU	3.9
2	D	66	ALA	3.9
2	D	84	VAL	3.9
3	O	48	ALA	3.9
3	N	225	LEU	3.9
3	O	51	VAL	3.9
2	B	292	ASP	3.9
1	C	283	ASN	3.8
2	F	120	SER	3.8

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Mol	Chain	Res	Type	RSRZ
3	O	259	ILE	3.8
3	O	292	ALA	3.8
3	O	67	HIS	3.8
3	O	262	LEU	3.8
3	N	168	ASP	3.8
2	D	106	ALA	3.8
2	F	327	LYS	3.7
2	B	137	TYR	3.7
2	F	179	VAL	3.7
3	O	183	LEU	3.6
3	O	289	LEU	3.6
2	B	282	ILE	3.6
3	O	257	LEU	3.6
3	O	243	VAL	3.5
2	F	268	ALA	3.5
3	O	264	VAL	3.5
2	B	302	GLU	3.5
1	A	349	MET	3.5
2	B	351	GLN	3.4
2	F	292	ASP	3.4
3	N	257	LEU	3.4
1	C	327	ASN	3.4
3	O	63	GLN	3.4
2	F	320	TYR	3.4
3	N	165	ALA	3.4
2	F	200	PHE	3.4
2	B	350	SER	3.3
2	B	355	SER	3.3
3	O	56	SER	3.3
3	O	222	LEU	3.3
3	O	44	TRP	3.3
3	O	182	ALA	3.3
3	O	249	ALA	3.3
3	O	278	TYR	3.3
3	O	156	VAL	3.3
1	E	254	ILE	3.3
2	B	372	THR	3.3
3	M	200	GLU	3.3
3	N	235	GLY	3.3
3	O	244	ALA	3.3
2	B	370	CYS	3.3
2	B	135	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	26	PRO	3.2
1	C	316	LYS	3.2
2	F	344	ILE	3.2
3	O	223	LEU	3.2
2	D	108	VAL	3.2
2	B	161	PHE	3.2
3	N	230	GLU	3.2
2	D	200	PHE	3.2
2	B	288	THR	3.2
2	D	177	ILE	3.2
1	C	254	ILE	3.2
3	N	270	TYR	3.2
2	B	296	LEU	3.2
2	D	60	VAL	3.2
3	M	67	HIS	3.1
3	N	223	LEU	3.1
2	F	326	GLY	3.1
2	B	327	LYS	3.1
3	N	285	ARG	3.1
1	C	167	ALA	3.1
3	O	43	SER	3.1
2	F	345	GLU	3.1
1	C	314	ASP	3.1
1	A	402	TYR	3.1
2	F	312	PHE	3.1
3	O	291	VAL	3.1
3	N	229	GLY	3.0
3	O	40	SER	3.0
2	F	59	TYR	3.0
2	B	266	VAL	3.0
2	B	374	VAL	3.0
2	D	102	GLN	3.0
3	N	243	VAL	3.0
1	C	73	TYR	3.0
2	B	371	SER	3.0
3	O	58	ARG	3.0
2	B	148	ALA	3.0
2	D	86	PRO	3.0
2	B	286	ALA	2.9
3	M	62	THR	2.9
1	C	347	VAL	2.9
2	B	38	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	339	ILE	2.9
3	O	146	LEU	2.9
3	N	59	MET	2.9
1	C	270	SER	2.9
2	B	342	ALA	2.9
3	N	127	VAL	2.9
3	O	270	TYR	2.9
2	B	133	LEU	2.9
1	C	79	TYR	2.8
2	B	33	LEU	2.8
3	O	73	LEU	2.8
2	D	38	LEU	2.8
2	D	296	LEU	2.8
3	O	258	ARG	2.8
3	N	201	ALA	2.8
2	D	54	VAL	2.8
2	B	184	VAL	2.7
2	B	173	PHE	2.7
2	F	119	ALA	2.7
3	O	140	HIS	2.7
2	B	303	VAL	2.7
2	B	20	ASN	2.7
3	N	222	LEU	2.7
3	M	243	VAL	2.7
2	B	391	PRO	2.7
1	E	329	THR	2.7
1	C	394	TRP	2.6
2	D	161	PHE	2.6
2	D	27	MET	2.6
2	F	178	VAL	2.6
1	E	342	TYR	2.6
2	F	280	ILE	2.6
2	F	103	LEU	2.6
3	O	164	PRO	2.6
1	A	351	LEU	2.6
3	O	143	TYR	2.6
3	O	199	GLU	2.6
2	D	104	SER	2.6
2	F	105	GLU	2.6
1	C	308	ARG	2.6
1	E	352	TYR	2.6
2	B	271	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	O	287	PHE	2.5
3	N	164	PRO	2.5
3	N	238	PHE	2.5
2	D	31	MET	2.5
3	O	132	ALA	2.5
2	F	366	ARG	2.5
3	N	248	ASP	2.5
2	D	107	HIS	2.5
3	O	206	HIS	2.5
1	C	297	LYS	2.5
3	O	110	LEU	2.5
1	A	344	LYS	2.5
1	A	258	GLY	2.5
2	B	346	VAL	2.5
3	N	176	VAL	2.5
3	O	286	VAL	2.5
3	M	182	ALA	2.4
2	B	344	ILE	2.4
2	B	294	PRO	2.4
3	N	174	LEU	2.4
1	C	91	SER	2.4
2	D	90	GLY	2.4
1	A	10	LEU	2.4
2	D	85	TYR	2.4
3	M	139	LEU	2.4
3	O	75	TRP	2.4
3	O	248	ASP	2.4
2	D	163	VAL	2.4
3	N	286	VAL	2.4
2	B	9	ASN	2.3
1	C	318	LYS	2.3
2	D	178	VAL	2.3
2	B	17	THR	2.3
2	F	29	LEU	2.3
2	F	279	SER	2.3
1	A	89	GLY	2.3
2	B	15	TYR	2.3
3	O	71	ARG	2.3
2	B	273	VAL	2.3
1	E	179	PHE	2.3
2	D	294	PRO	2.3
3	N	73	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	165	ILE	2.3
1	E	350	LEU	2.3
2	B	200	PHE	2.3
3	O	39	GLU	2.2
3	O	272	CYS	2.2
3	N	244	ALA	2.2
2	B	301	CYS	2.2
2	F	102	GLN	2.2
3	O	97	GLN	2.2
1	C	98	LEU	2.2
2	F	133	LEU	2.2
3	O	255	PHE	2.2
1	C	71	ASN	2.2
1	A	137	HIS	2.2
3	O	212	PRO	2.2
3	O	150	LEU	2.2
2	F	351	GLN	2.2
2	F	171	THR	2.2
2	B	3	HIS	2.2
2	B	166	MET	2.2
2	D	184	VAL	2.2
2	F	4	VAL	2.2
3	N	209	ARG	2.2
3	O	274	LEU	2.2
2	F	373	GLN	2.2
1	C	375	VAL	2.2
2	B	276	MET	2.2
1	C	93	HIS	2.2
2	D	28	VAL	2.2
2	D	119	ALA	2.1
3	O	185	THR	2.1
3	O	205	VAL	2.1
3	M	108	LEU	2.1
2	B	328	CYS	2.1
3	O	193	TRP	2.1
1	A	184	LYS	2.1
2	B	304	PRO	2.1
2	D	33	LEU	2.1
2	D	378	ALA	2.1
2	F	340	ARG	2.1
3	N	205	VAL	2.1
1	E	330	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	330	VAL	2.1
2	D	367	VAL	2.1
1	C	291	ALA	2.1
1	E	331	ARG	2.1
2	F	123	ARG	2.1
1	C	90	HIS	2.1
1	A	257	ASN	2.1
3	O	148	GLU	2.1
1	A	390	LEU	2.1
3	O	246	GLY	2.1
2	D	162	ILE	2.0
1	C	102	ARG	2.0
2	F	87	PHE	2.0
2	F	365	PHE	2.0
2	B	347	GLU	2.0
3	O	119	ASN	2.0
3	N	153	ARG	2.0
3	O	275	HIS	2.0
2	D	133	LEU	2.0
3	M	110	LEU	2.0
2	D	105	GLU	2.0
2	B	281	ASP	2.0
3	O	121	SER	2.0
3	N	152	VAL	2.0
2	F	44	LEU	2.0
2	B	365	PHE	2.0
1	C	276	THR	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.

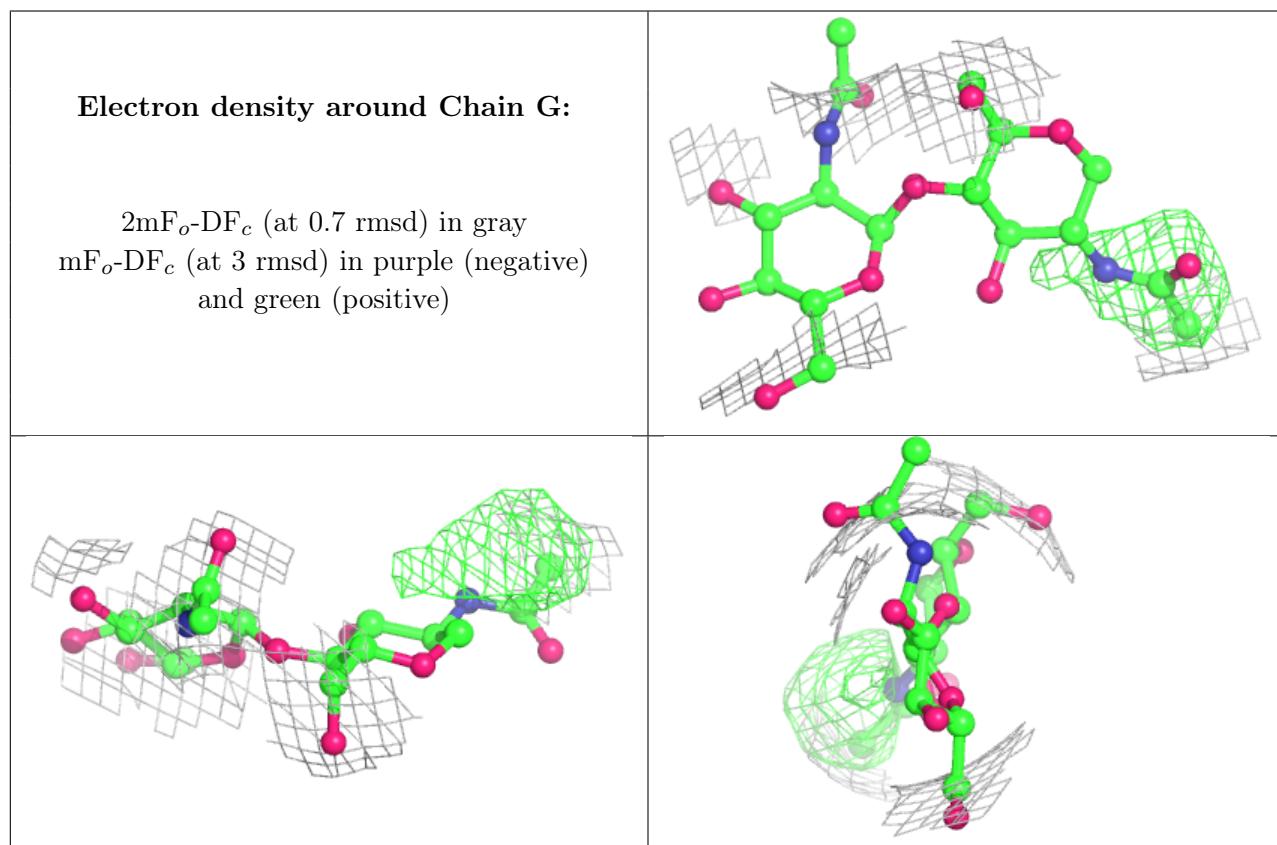
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NDG	G	2	14/15	0.82	0.24	276,282,286,291	0

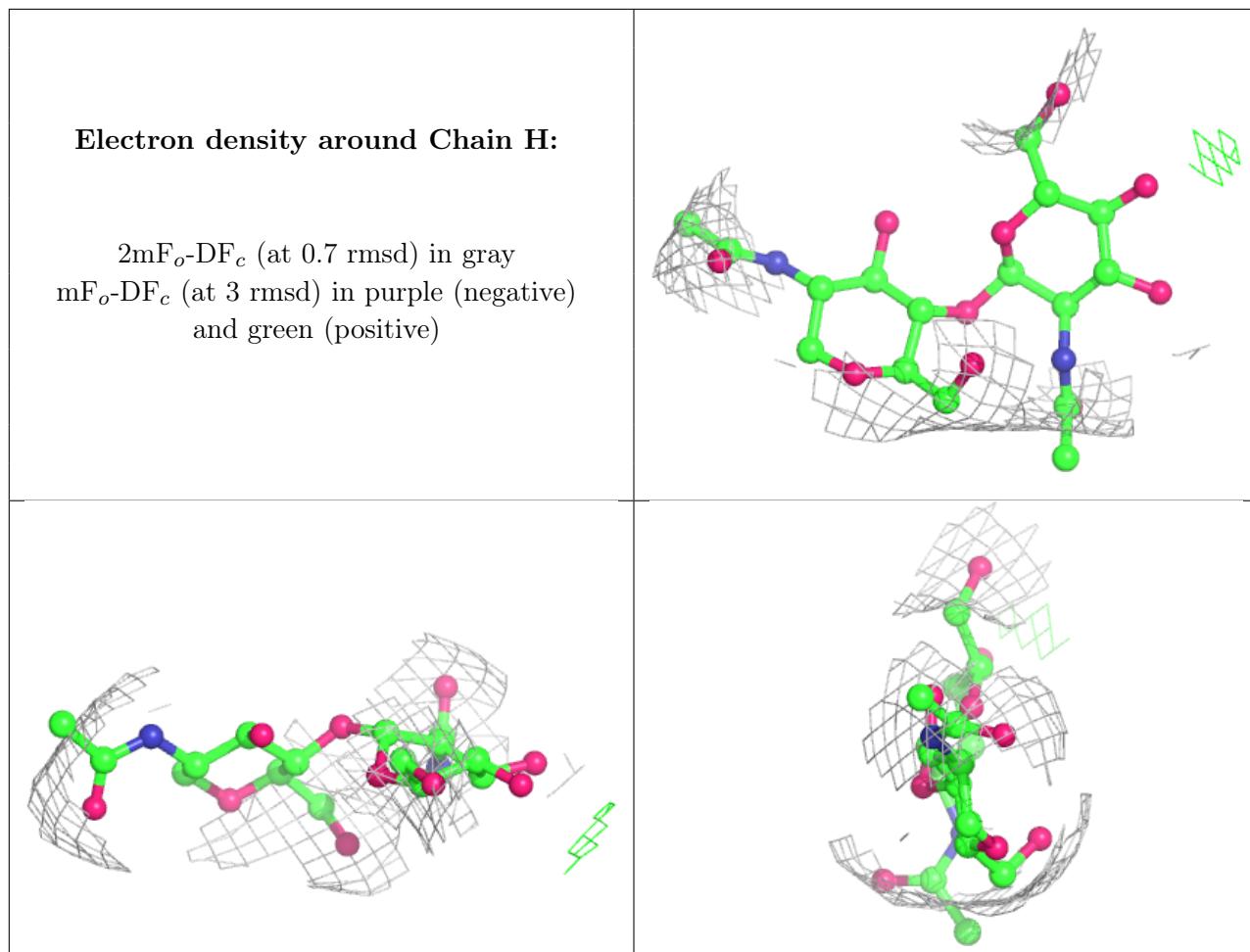
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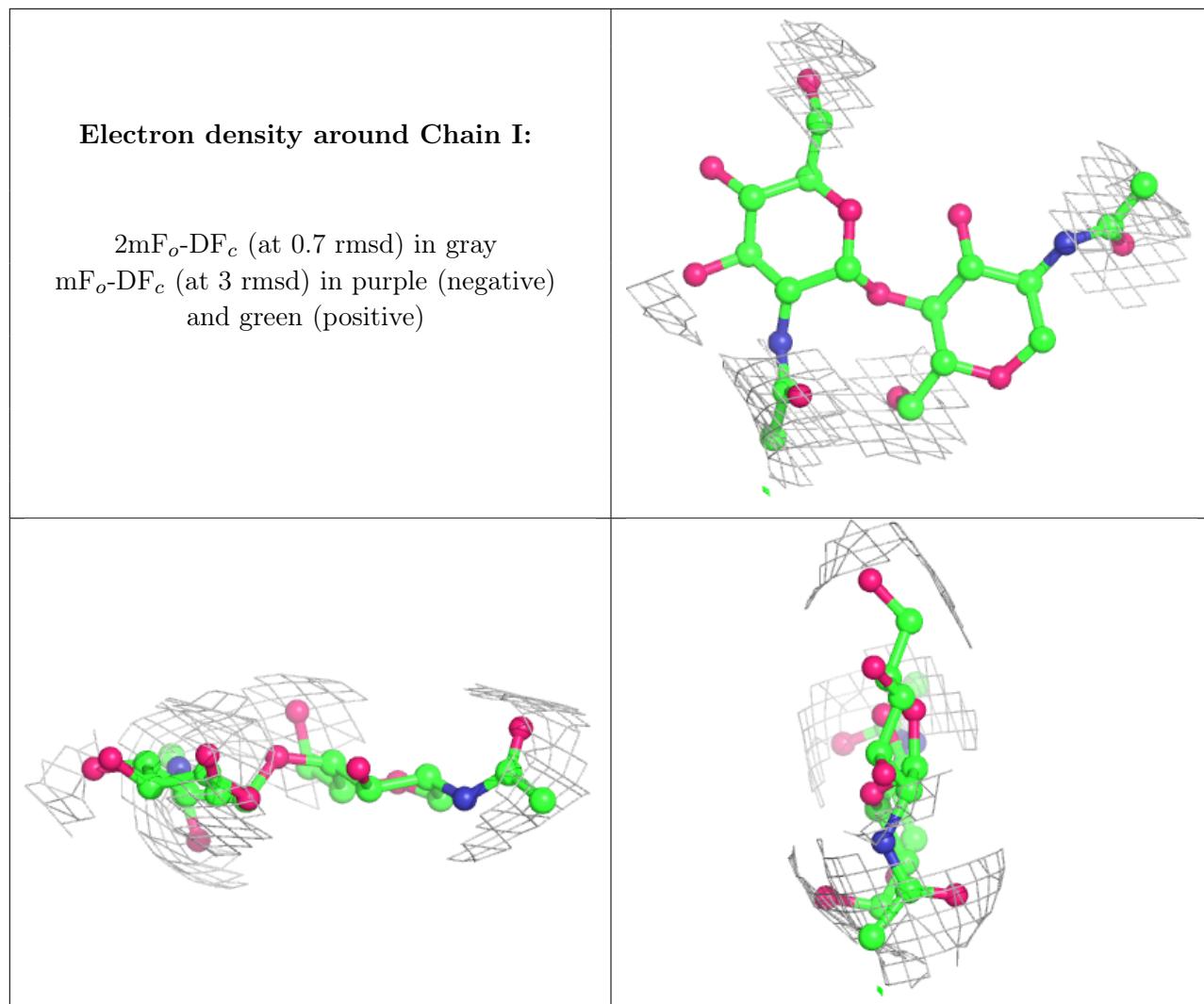
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	G	1	14/15	0.86	0.16	241,245,251,252	0
4	NDG	H	2	14/15	0.86	0.49	249,258,262,265	0
4	NAG	H	1	14/15	0.88	0.29	176,183,198,199	0
4	NAG	I	1	14/15	0.93	0.23	241,247,252,255	0
4	NDG	I	2	14/15	0.94	0.39	274,280,282,282	0

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







## 6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	1101	14/15	0.83	0.34	147,156,165,171	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.