



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:36 AM UTC

PDB ID : 6E3K / pdb_00006e3k
Title : Interferon gamma signalling complex with IFNGR1 and IFNGR2
Authors : Jude, K.M.; Mendoza, J.L.; Garcia, K.C.
Deposited on : 2018-07-14
Resolution : 3.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

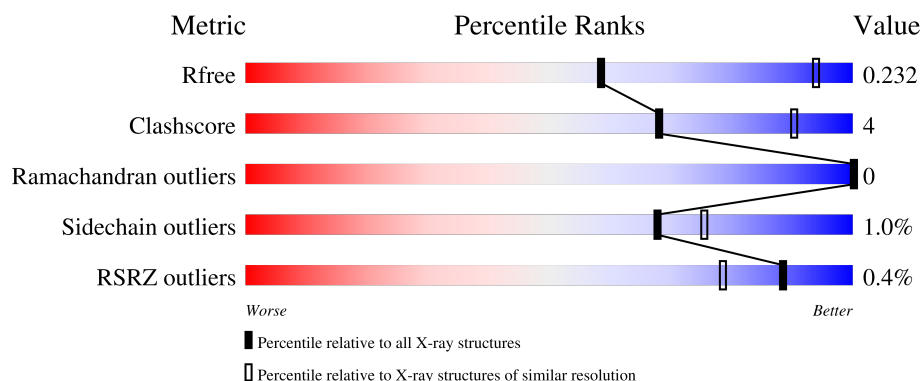
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	148	% 75% 9% 16%
1	B	148	78% 7% 15%
2	C	242	77% 8% 14%
2	D	242	% 73% 11% 16%
3	E	233	82% 9% 9%

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Mol	Chain	Length	Quality of chain
3	I	233	 81% 10% 9%
4	F	2	 100%
5	G	5	 60% 40%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8966 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 Interferon gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1027	653	173	198	3			
1	B	126	Total	C	N	O	S	0	0	0
			1020	647	171	199	3			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P01579
A	-2	PRO	-	expression tag	UNP P01579
A	-1	GLY	-	expression tag	UNP P01579
A	0	SER	-	expression tag	UNP P01579
A	134	ALA	-	expression tag	UNP P01579
A	135	ALA	-	expression tag	UNP P01579
A	136	ALA	-	expression tag	UNP P01579
A	137	HIS	-	expression tag	UNP P01579
A	138	HIS	-	expression tag	UNP P01579
A	139	HIS	-	expression tag	UNP P01579
A	140	HIS	-	expression tag	UNP P01579
A	141	HIS	-	expression tag	UNP P01579
A	142	HIS	-	expression tag	UNP P01579
A	143	HIS	-	expression tag	UNP P01579
A	144	HIS	-	expression tag	UNP P01579
B	-3	GLY	-	expression tag	UNP P01579
B	-2	PRO	-	expression tag	UNP P01579
B	-1	GLY	-	expression tag	UNP P01579
B	0	SER	-	expression tag	UNP P01579
B	134	ALA	-	expression tag	UNP P01579
B	135	ALA	-	expression tag	UNP P01579
B	136	ALA	-	expression tag	UNP P01579
B	137	HIS	-	expression tag	UNP P01579
B	138	HIS	-	expression tag	UNP P01579
B	139	HIS	-	expression tag	UNP P01579

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Chain	Residue	Modelled	Actual	Comment	Reference
B	140	HIS	-	expression tag	UNP P01579
B	141	HIS	-	expression tag	UNP P01579
B	142	HIS	-	expression tag	UNP P01579
B	143	HIS	-	expression tag	UNP P01579
B	144	HIS	-	expression tag	UNP P01579

- Molecule 2 is a protein called Interferon gamma receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1649	1049	274	315	11			
2	D	203	Total	C	N	O	S	0	0	0
			1577	999	263	305	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P15260
C	0	SER	-	expression tag	UNP P15260
C	149	ILE	THR	engineered mutation	UNP P15260
C	161	LYS	MET	engineered mutation	UNP P15260
C	167	LYS	GLN	engineered mutation	UNP P15260
C	174	ASN	LYS	engineered mutation	UNP P15260
C	182	ARG	GLN	engineered mutation	UNP P15260
C	205	ASN	HIS	engineered mutation	UNP P15260
C	230	ALA	-	expression tag	UNP P15260
C	231	ALA	-	expression tag	UNP P15260
C	232	ALA	-	expression tag	UNP P15260
C	233	HIS	-	expression tag	UNP P15260
C	234	HIS	-	expression tag	UNP P15260
C	235	HIS	-	expression tag	UNP P15260
C	236	HIS	-	expression tag	UNP P15260
C	237	HIS	-	expression tag	UNP P15260
C	238	HIS	-	expression tag	UNP P15260
C	239	HIS	-	expression tag	UNP P15260
C	240	HIS	-	expression tag	UNP P15260
D	-1	GLY	-	expression tag	UNP P15260
D	0	SER	-	expression tag	UNP P15260
D	149	ILE	THR	engineered mutation	UNP P15260
D	161	LYS	MET	engineered mutation	UNP P15260
D	167	LYS	GLN	engineered mutation	UNP P15260
D	174	ASN	LYS	engineered mutation	UNP P15260

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Chain	Residue	Modelled	Actual	Comment	Reference
D	182	ARG	GLN	engineered mutation	UNP P15260
D	205	ASN	HIS	engineered mutation	UNP P15260
D	230	ALA	-	expression tag	UNP P15260
D	231	ALA	-	expression tag	UNP P15260
D	232	ALA	-	expression tag	UNP P15260
D	233	HIS	-	expression tag	UNP P15260
D	234	HIS	-	expression tag	UNP P15260
D	235	HIS	-	expression tag	UNP P15260
D	236	HIS	-	expression tag	UNP P15260
D	237	HIS	-	expression tag	UNP P15260
D	238	HIS	-	expression tag	UNP P15260
D	239	HIS	-	expression tag	UNP P15260
D	240	HIS	-	expression tag	UNP P15260

- Molecule 3 is a protein called Interferon gamma receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1692	1087	283	313	9			
3	I	213	Total	C	N	O	S	0	0	0
			1698	1090	286	313	9			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	26	GLY	-	expression tag	UNP P38484
E	27	SER	-	expression tag	UNP P38484
E	248	ALA	-	expression tag	UNP P38484
E	249	ALA	-	expression tag	UNP P38484
E	250	ALA	-	expression tag	UNP P38484
E	251	HIS	-	expression tag	UNP P38484
E	252	HIS	-	expression tag	UNP P38484
E	253	HIS	-	expression tag	UNP P38484
E	254	HIS	-	expression tag	UNP P38484
E	255	HIS	-	expression tag	UNP P38484
E	256	HIS	-	expression tag	UNP P38484
E	257	HIS	-	expression tag	UNP P38484
E	258	HIS	-	expression tag	UNP P38484
I	26	GLY	-	expression tag	UNP P38484
I	27	SER	-	expression tag	UNP P38484
I	248	ALA	-	expression tag	UNP P38484
I	249	ALA	-	expression tag	UNP P38484

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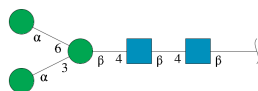
Chain	Residue	Modelled	Actual	Comment	Reference
I	250	ALA	-	expression tag	UNP P38484
I	251	HIS	-	expression tag	UNP P38484
I	252	HIS	-	expression tag	UNP P38484
I	253	HIS	-	expression tag	UNP P38484
I	254	HIS	-	expression tag	UNP P38484
I	255	HIS	-	expression tag	UNP P38484
I	256	HIS	-	expression tag	UNP P38484
I	257	HIS	-	expression tag	UNP P38484
I	258	HIS	-	expression tag	UNP P38484

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



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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



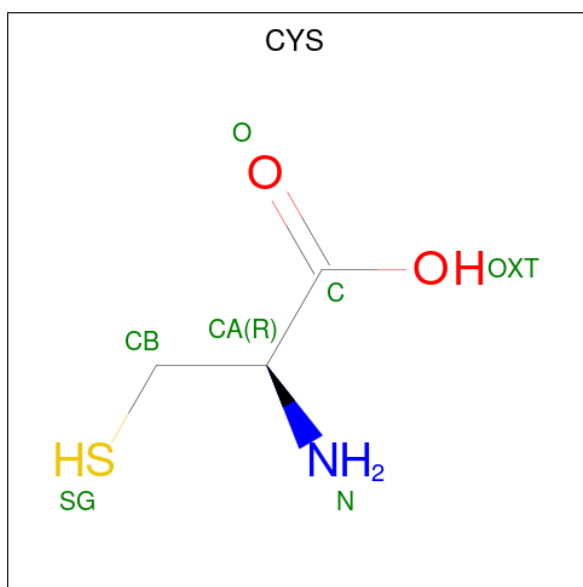
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
8	I	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

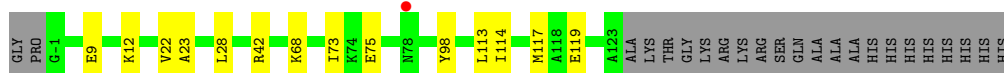
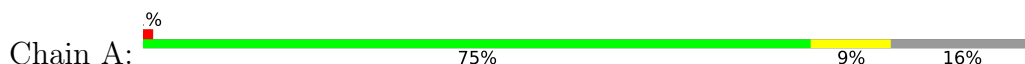
- Molecule 9 is water.

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

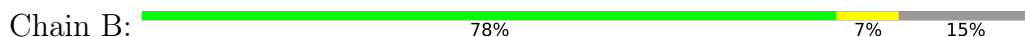
3 Residue-property plots [i](#)

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.

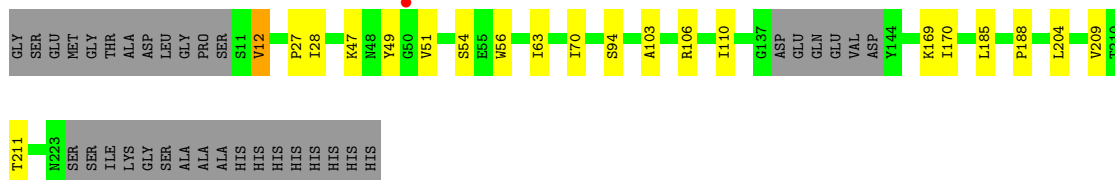
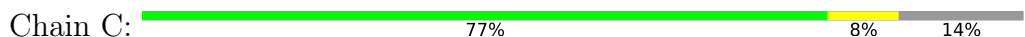
- Molecule 1: Interferon gamma



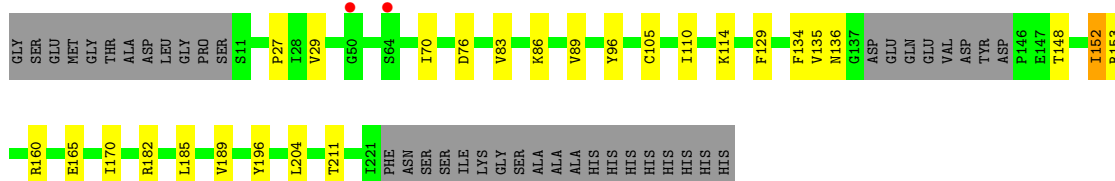
- Molecule 1: Interferon gamma



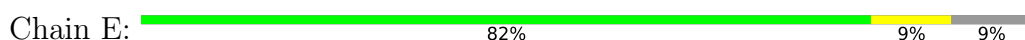
- Molecule 2: Interferon gamma receptor 1



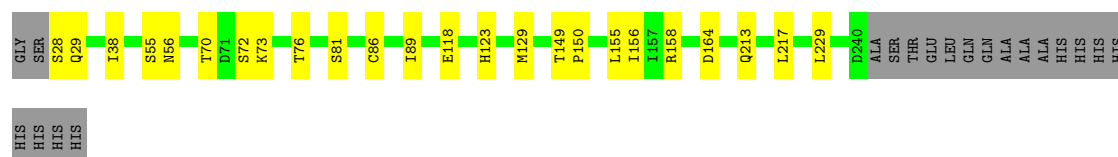
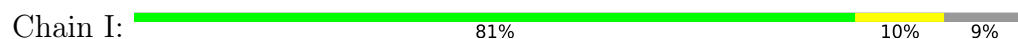
- Molecule 2: Interferon gamma receptor 1



- Molecule 3: Interferon gamma receptor 2



- Molecule 3: Interferon gamma receptor 2



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



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.28Å 151.46Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.19 – 3.25 37.19 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.19-3.25) 88.9 (37.19-3.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.190 , 0.232 0.193 , 0.232	Depositor DCC
R_{free} test set	1783 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	111.2	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 128.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8966	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, EDO, NAG, MAN

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	0.16	0/1045	0.31	0/1399
1	B	0.14	0/1038	0.30	0/1394
2	C	0.17	0/1687	0.35	0/2296
2	D	0.14	0/1613	0.32	0/2201
3	E	0.13	0/1743	0.34	0/2381
3	I	0.20	0/1749	0.43	0/2388
All	All	0.16	0/8875	0.35	0/12059

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1027	0	1021	13	0
1	B	1020	0	993	9	0
2	C	1649	0	1596	14	0
2	D	1577	0	1489	13	0
3	E	1692	0	1624	12	0
3	I	1698	0	1633	15	0
4	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	61	0	52	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	28	0	26	1	0
6	D	28	0	26	0	0
6	E	42	0	39	1	0
6	I	42	0	39	0	0
7	B	4	0	6	0	0
7	C	8	0	12	0	0
7	D	4	0	6	0	0
7	I	8	0	12	1	0
8	E	7	0	3	0	0
8	I	7	0	3	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	I	6	0	0	1	0
All	All	8966	0	8631	63	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 4.

All (63) 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:C:12:VAL:HG22	2:C:94:SER:HB3	1.68	0.75
3:I:158:ARG:NH1	9:I:401:HOH:O	2.23	0.72
3:I:38:ILE:HG13	3:I:129:MET:HE2	1.80	0.63
1:A:75:GLU:OE1	3:I:70:THR:HG22	2.03	0.59
2:C:110:ILE:HB	2:C:211:THR:HG22	1.86	0.58
3:E:189:LYS:NZ	3:E:198:SER:O	2.37	0.57
3:I:86:CYS:HA	3:I:89:ILE:HD13	1.88	0.56
2:C:169:LYS:NZ	3:I:164:ASP:OD1	2.33	0.56
3:E:150:PRO:HA	3:E:155:LEU:HD23	1.88	0.55
3:E:132:PHE:HB3	6:E:302:NAG:H82	1.90	0.53
1:A:119:GLU:HB3	1:B:42:ARG:HH12	1.73	0.53
1:B:9:GLU:HA	1:B:12:LYS:HB2	1.90	0.53
2:C:28:ILE:HD11	6:C:301:NAG:H82	1.91	0.52
2:D:110:ILE:HD12	2:D:204:LEU:HD11	1.91	0.52
3:I:118:GLU:HA	3:I:123:HIS:HA	1.93	0.50
2:D:27:PRO:HG2	2:D:70:ILE:HG13	1.93	0.50
1:A:42:ARG:HH12	1:B:119:GLU:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:38:ILE:HG13	3:E:129:MET:HE2	1.94	0.49
1:A:113:LEU:HD21	1:B:73:ILE:HD13	1.94	0.49
3:E:51:PRO:HB3	3:E:92:THR:HG21	1.95	0.49
2:C:27:PRO:HG2	2:C:70:ILE:HG13	1.94	0.49
2:D:29:VAL:HG21	2:D:83:VAL:HG11	1.95	0.48
1:A:9:GLU:HG2	1:A:12:LYS:HD3	1.95	0.48
2:C:51:VAL:O	2:C:54:SER:OG	2.30	0.47
2:C:204:LEU:HD22	2:C:209:VAL:HB	1.96	0.47
2:D:134:PHE:CE2	2:D:152:ILE:HD11	2.49	0.47
1:A:73:ILE:HD13	1:B:113:LEU:HD21	1.96	0.47
1:A:28:LEU:HB3	1:B:98:TYR:CE2	2.50	0.47
2:D:105:CYS:SG	2:D:204:LEU:HD23	2.55	0.47
2:D:170:ILE:HD11	2:D:185:LEU:HD13	1.97	0.46
1:A:98:TYR:CE2	1:B:28:LEU:HB3	2.50	0.46
3:E:79:ILE:HD12	3:E:79:ILE:H	1.80	0.46
3:I:118:GLU:HB3	3:I:123:HIS:HB3	1.97	0.46
2:C:188:PRO:HB2	3:I:156:ILE:HD12	1.98	0.46
1:A:68:LYS:HE3	3:I:81:SER:O	2.16	0.46
3:I:56:ASN:ND2	7:I:310:EDO:O2	2.49	0.45
2:D:76:ASP:OD1	2:D:148:THR:OG1	2.31	0.45
1:A:114:ILE:H	1:A:114:ILE:HD12	1.82	0.45
2:D:114:LYS:HB2	2:D:129:PHE:HB2	1.99	0.45
1:B:117:MET:HE3	1:B:117:MET:HB3	1.90	0.44
1:A:22:VAL:HG12	2:C:49:TYR:HE2	1.82	0.44
3:I:72:SER:OG	3:I:73:LYS:N	2.50	0.44
2:D:110:ILE:HB	2:D:211:THR:HG22	1.99	0.44
1:A:117:MET:HE3	1:A:117:MET:HB3	1.83	0.44
3:E:86:CYS:SG	3:E:94:CYS:HB2	2.56	0.44
2:D:86:LYS:HD3	2:D:96:TYR:CZ	2.53	0.44
3:E:64:GLN:NE2	3:E:118:GLU:OE2	2.51	0.43
3:E:65:VAL:HG22	3:E:115:LEU:HD13	2.01	0.43
2:D:153:ARG:NH2	3:E:167:ASP:HA	2.34	0.43
2:D:160:ARG:HA	2:D:165:GLU:HA	1.99	0.43
1:B:114:ILE:H	1:B:114:ILE:HD12	1.84	0.42
2:D:189:VAL:HG12	2:D:196:TYR:CZ	2.54	0.42
2:C:170:ILE:HD11	2:C:185:LEU:HD13	2.02	0.42
3:I:150:PRO:HA	3:I:155:LEU:HD23	2.02	0.42
3:E:218:TRP:CZ2	3:E:220:LYS:HD2	2.54	0.42
3:E:209:CYS:HA	3:E:234:CYS:HA	2.01	0.41
2:C:103:ALA:HB3	2:C:106:ARG:HB3	2.02	0.41
3:I:149:THR:HA	3:I:150:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:63:ILE:HD12	2:C:63:ILE:HA	1.94	0.40
1:A:23:ALA:HA	2:C:49:TYR:CD2	2.57	0.40
3:I:28:SER:OG	3:I:29:GLN:N	2.55	0.40
3:I:213:GLN:HB2	3:I:229:LEU:HG	2.02	0.40
2:C:47:LYS:HB2	2:C:56:TRP:CE3	2.56	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	123/148 (83%)	121 (98%)	2 (2%)	0	100	100
1	B	124/148 (84%)	123 (99%)	1 (1%)	0	100	100
2	C	203/242 (84%)	197 (97%)	6 (3%)	0	100	100
2	D	199/242 (82%)	194 (98%)	5 (2%)	0	100	100
3	E	211/233 (91%)	203 (96%)	8 (4%)	0	100	100
3	I	211/233 (91%)	205 (97%)	6 (3%)	0	100	100
All	All	1071/1246 (86%)	1043 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/132 (87%)	115 (100%)	0	100	100
1	B	112/132 (85%)	112 (100%)	0	100	100
2	C	188/218 (86%)	187 (100%)	1 (0%)	81	82
2	D	175/218 (80%)	170 (97%)	5 (3%)	37	60
3	E	187/203 (92%)	186 (100%)	1 (0%)	81	82
3	I	188/203 (93%)	185 (98%)	3 (2%)	55	70
All	All	965/1106 (87%)	955 (99%)	10 (1%)	68	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	12	VAL
2	D	89	VAL
2	D	135	VAL
2	D	136	ASN
2	D	152	ILE
2	D	182	ARG
3	E	76	THR
3	I	55	SER
3	I	76	THR
3	I	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	46	GLN
1	A	78	ASN
1	A	83	ASN
1	A	104	ASN
1	B	46	GLN
1	B	78	ASN
1	B	115	GLN
2	C	26	ASN
2	C	48	ASN
2	C	195	GLN
2	D	123	GLN
3	E	34	GLN
3	E	187	GLN
3	I	29	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

7 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	F	1	4,3	14,14,15	0.51	0	17,19,21	0.58	0
4	NAG	F	2	4	14,14,15	0.25	0	17,19,21	0.37	0
5	NAG	G	1	5,3	14,14,15	0.28	0	17,19,21	0.47	0
5	NAG	G	2	5	14,14,15	0.20	0	17,19,21	0.45	0
5	BMA	G	3	5	11,11,12	0.59	0	15,15,17	0.84	0
5	MAN	G	4	5	11,11,12	0.66	0	15,15,17	0.96	1 (6%)
5	MAN	G	5	5	11,11,12	0.88	0	15,15,17	1.06	2 (13%)

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	F	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
5	NAG	G	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4	MAN	C1-O5-C5	2.65	115.74	112.19
5	G	5	MAN	C1-O5-C5	2.29	115.25	112.19
5	G	5	MAN	O2-C2-C3	-2.09	105.82	110.15

There are no chirality outliers.

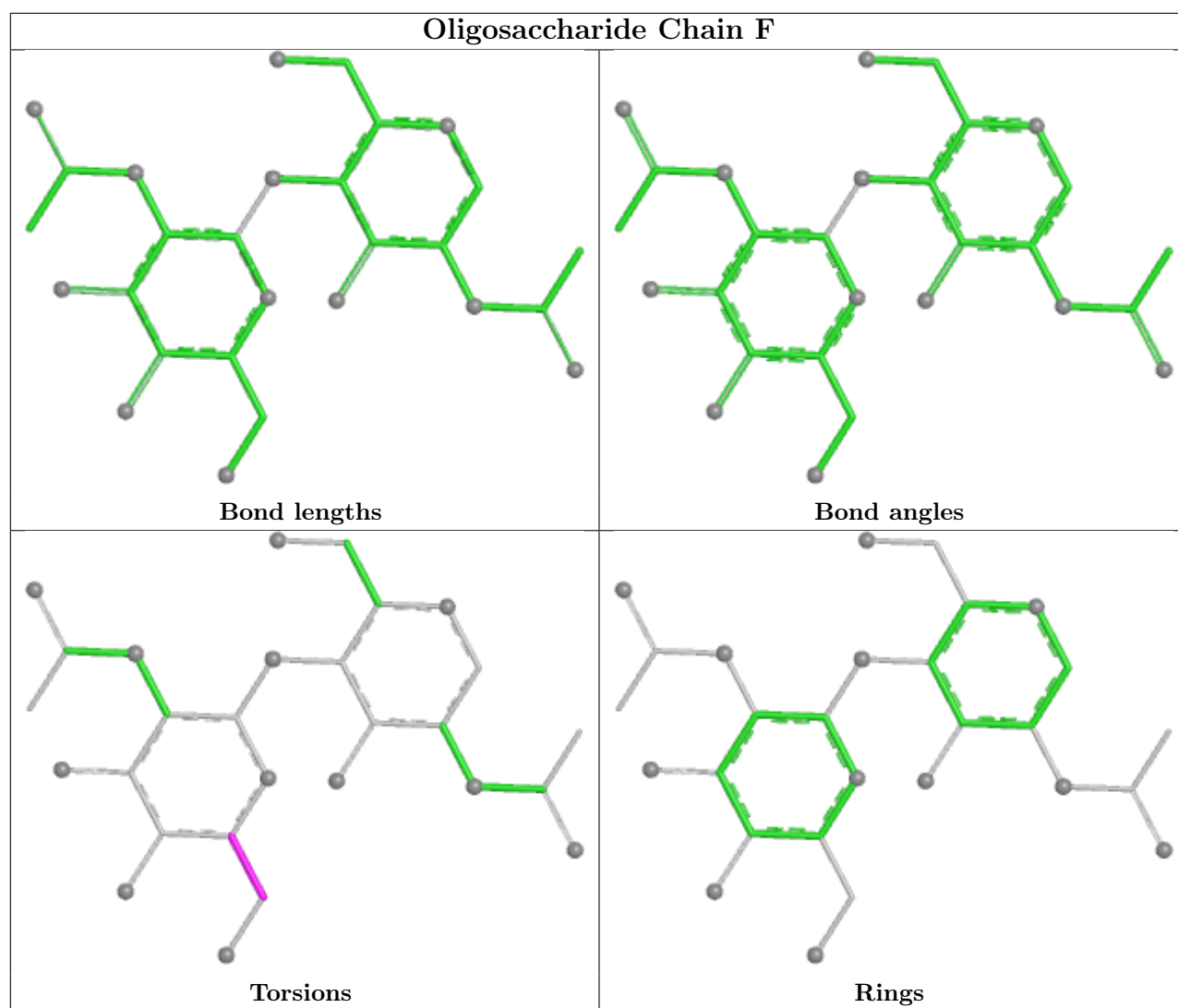
All (3) torsion outliers are listed below:

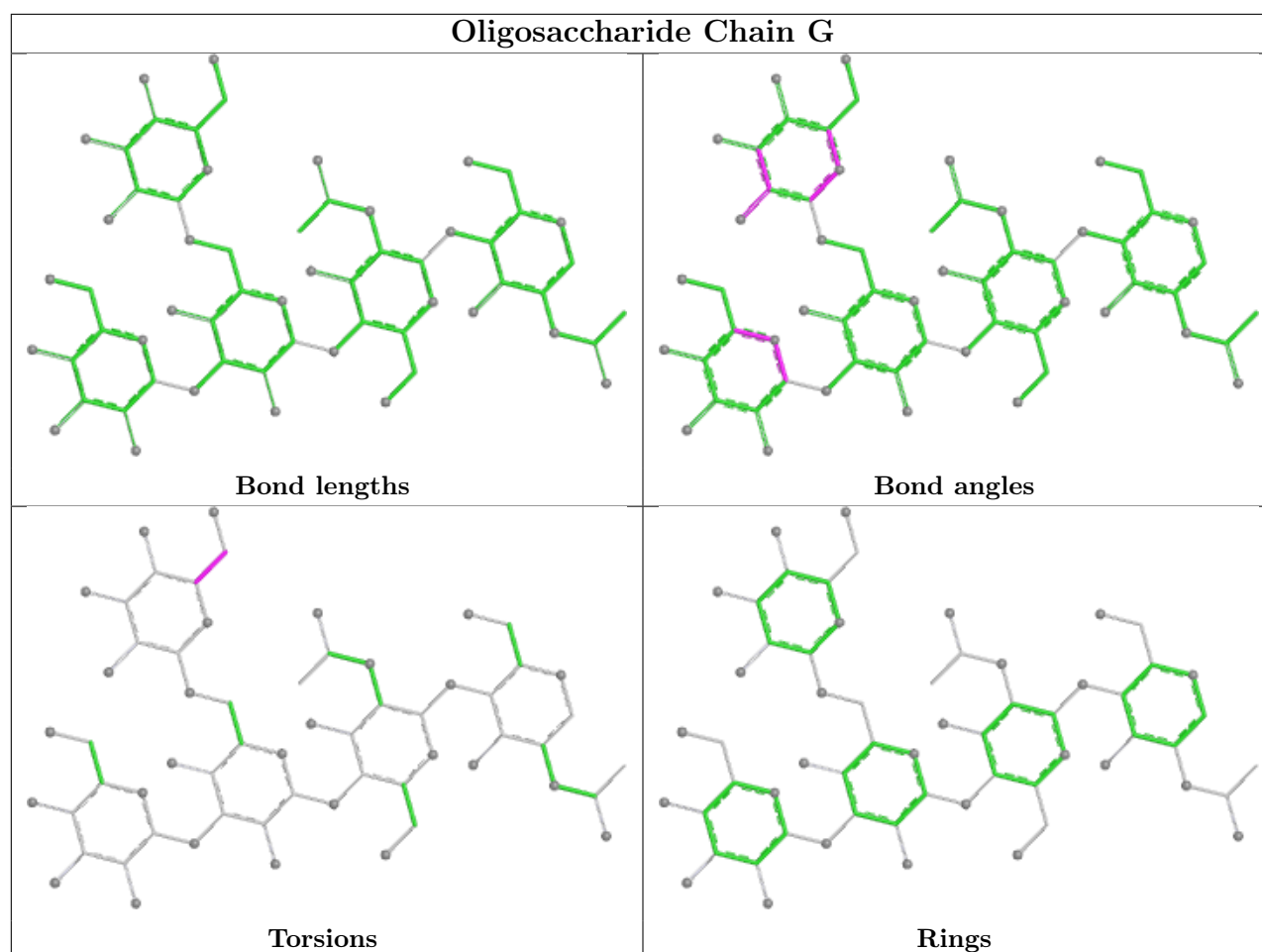
Mol	Chain	Res	Type	Atoms
5	G	5	MAN	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	D	303	-	3,3,3	0.44	0	2,2,2	0.42	0
6	NAG	I	301	3	14,14,15	0.26	0	17,19,21	0.50	0
8	CYS	I	309	3	5,6,6	1.07	1 (20%)	3,7,7	1.62	1 (33%)
6	NAG	B	301	1	14,14,15	0.22	0	17,19,21	0.48	0
6	NAG	C	302	2	14,14,15	0.24	0	17,19,21	0.44	0
8	CYS	E	306	3	5,6,6	1.24	1 (20%)	3,7,7	1.81	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	301	2	14,14,15	0.42	0	17,19,21	0.50	0
6	NAG	E	302	3	14,14,15	0.22	0	17,19,21	0.40	0
7	EDO	C	303	-	3,3,3	0.43	0	2,2,2	0.47	0
7	EDO	I	311	-	3,3,3	0.46	0	2,2,2	0.30	0
6	NAG	D	302	2	14,14,15	0.31	0	17,19,21	0.53	0
6	NAG	E	301	3	14,14,15	0.20	0	17,19,21	0.51	0
6	NAG	I	308	3	14,14,15	0.30	0	17,19,21	0.51	0
6	NAG	E	305	3	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	A	301	1	14,14,15	0.25	0	17,19,21	0.46	0
7	EDO	B	302	-	3,3,3	0.43	0	2,2,2	0.40	0
6	NAG	I	307	3	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	D	301	2	14,14,15	0.22	0	17,19,21	0.45	0
7	EDO	C	304	-	3,3,3	0.48	0	2,2,2	0.21	0
7	EDO	I	310	-	3,3,3	0.46	0	2,2,2	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	D	303	-	-	0/1/1/1	-
6	NAG	I	301	3	-	2/6/23/26	0/1/1/1
8	CYS	I	309	3	-	1/6/6/6	-
6	NAG	B	301	1	-	1/6/23/26	0/1/1/1
6	NAG	C	302	2	-	2/6/23/26	0/1/1/1
8	CYS	E	306	3	-	1/6/6/6	-
6	NAG	C	301	2	-	2/6/23/26	0/1/1/1
6	NAG	E	302	3	-	2/6/23/26	0/1/1/1
7	EDO	C	303	-	-	0/1/1/1	-
7	EDO	I	311	-	-	1/1/1/1	-
6	NAG	D	302	2	-	1/6/23/26	0/1/1/1
6	NAG	E	301	3	-	2/6/23/26	0/1/1/1
6	NAG	I	308	3	-	1/6/23/26	0/1/1/1
6	NAG	E	305	3	-	2/6/23/26	0/1/1/1
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
7	EDO	B	302	-	-	1/1/1/1	-
6	NAG	I	307	3	-	2/6/23/26	0/1/1/1
6	NAG	D	301	2	-	2/6/23/26	0/1/1/1
7	EDO	C	304	-	-	0/1/1/1	-
7	EDO	I	310	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	306	CYS	OXT-C	-2.20	1.23	1.30
8	I	309	CYS	OXT-C	-2.09	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	306	CYS	OXT-C-O	-3.01	117.25	124.08
8	I	309	CYS	OXT-C-O	-2.76	117.83	124.08

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	309	CYS	C-CA-CB-SG
6	C	301	NAG	O5-C5-C6-O6
6	E	301	NAG	O5-C5-C6-O6
6	I	301	NAG	O5-C5-C6-O6
6	E	305	NAG	C4-C5-C6-O6
6	I	301	NAG	C4-C5-C6-O6
6	C	301	NAG	C4-C5-C6-O6
6	E	301	NAG	C4-C5-C6-O6
6	E	305	NAG	O5-C5-C6-O6
6	I	307	NAG	C4-C5-C6-O6
6	I	307	NAG	O5-C5-C6-O6
6	D	301	NAG	O5-C5-C6-O6
6	C	302	NAG	O5-C5-C6-O6
6	D	301	NAG	C4-C5-C6-O6
6	C	302	NAG	C4-C5-C6-O6
6	A	301	NAG	O5-C5-C6-O6
6	E	302	NAG	C4-C5-C6-O6
6	E	302	NAG	O5-C5-C6-O6
6	B	301	NAG	O5-C5-C6-O6
6	I	308	NAG	O5-C5-C6-O6
7	B	302	EDO	O1-C1-C2-O2
7	I	311	EDO	O1-C1-C2-O2
6	D	302	NAG	O5-C5-C6-O6
6	A	301	NAG	C4-C5-C6-O6
8	E	306	CYS	C-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	NAG	1	0
6	E	302	NAG	1	0
7	I	310	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	125/148 (84%)	-0.35	1 (0%) 82 68	95, 125, 166, 216	0
1	B	126/148 (85%)	-0.40	0 100 100	97, 143, 187, 246	0
2	C	207/242 (85%)	-0.25	1 (0%) 87 76	102, 140, 197, 265	0
2	D	203/242 (83%)	-0.12	2 (0%) 79 62	105, 172, 245, 284	0
3	E	213/233 (91%)	-0.17	0 100 100	179, 244, 297, 339	0
3	I	213/233 (91%)	-0.37	0 100 100	81, 114, 182, 241	0
All	All	1087/1246 (87%)	-0.26	4 (0%) 88 78	81, 149, 270, 339	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	50	GLY	5.2
2	D	64	SER	3.6
1	A	78	ASN	2.2
2	C	50	GLY	2.1

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

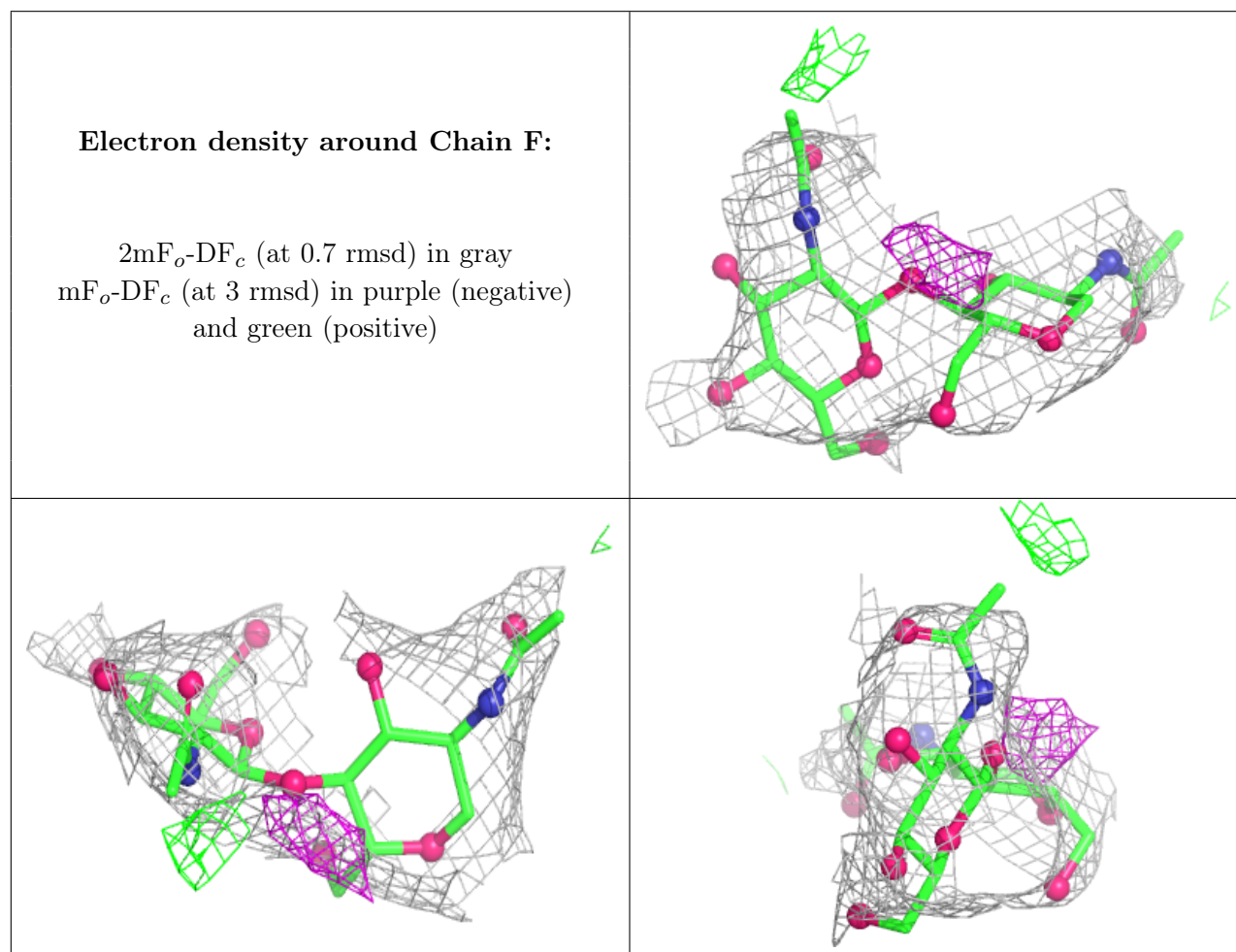
There are no non-standard protein/DNA/RNA residues in this entry.

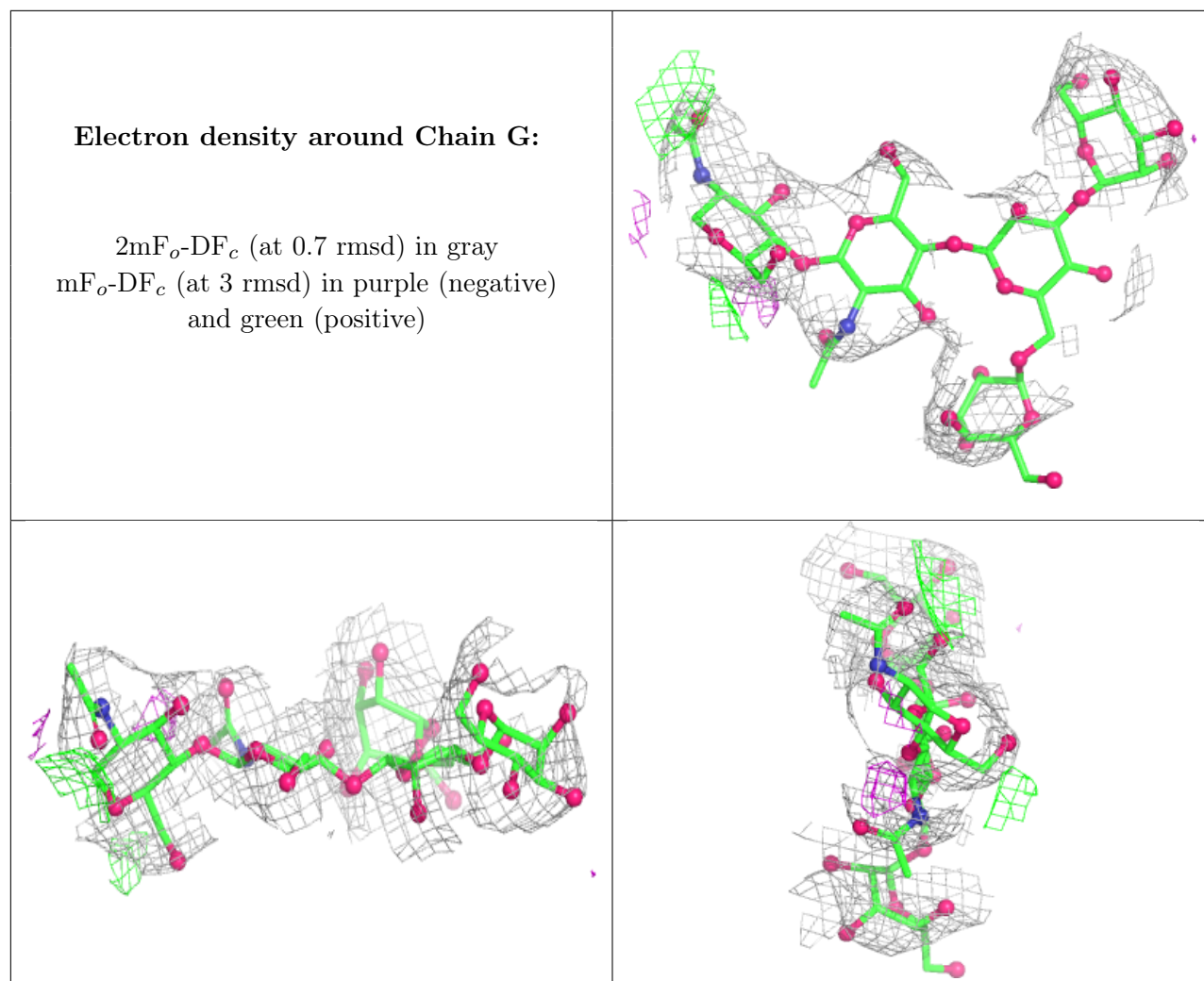
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	1	14/15	-	-	173,226,263,275	0
4	NAG	F	2	14/15	-	-	190,240,263,276	0
5	NAG	G	2	14/15	0.35	0.11	144,168,223,244	0
5	NAG	G	1	14/15	0.73	0.08	105,124,150,150	0
5	BMA	G	3	11/12	-	-	242,252,272,284	0
5	MAN	G	4	11/12	-	-	206,244,270,271	0
5	MAN	G	5	11/12	-	-	251,268,292,296	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	D	303	4/4	0.21	0.22	184,184,184,186	0
7	EDO	C	304	4/4	0.35	0.18	158,158,169,172	0
6	NAG	E	305	14/15	0.37	0.09	208,257,290,291	0
7	EDO	C	303	4/4	0.50	0.17	157,159,174,175	0
7	EDO	I	310	4/4	0.52	0.23	119,133,158,168	0
6	NAG	I	307	14/15	0.60	0.09	180,217,239,252	0
8	CYS	E	306	7/7	0.63	0.08	208,217,245,247	0
6	NAG	B	301	14/15	0.65	0.09	176,210,231,233	0
7	EDO	I	311	4/4	0.69	0.22	144,154,164,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	301	14/15	0.74	0.08	181,225,237,239	0
6	NAG	C	302	14/15	0.76	0.08	149,197,222,231	0
6	NAG	E	301	14/15	0.79	0.09	201,238,244,250	0
8	CYS	I	309	7/7	0.79	0.12	154,180,201,214	0
7	EDO	B	302	4/4	0.81	0.42	148,151,164,166	0
6	NAG	D	301	14/15	0.81	0.07	159,192,217,231	0
6	NAG	I	301	14/15	0.83	0.10	106,140,171,178	0
6	NAG	E	302	14/15	0.84	0.07	185,211,222,224	0
6	NAG	D	302	14/15	0.93	0.07	131,165,219,234	0
6	NAG	C	301	14/15	0.94	0.07	115,152,200,215	0
6	NAG	I	308	14/15	0.96	0.17	116,158,235,267	0

6.5 Other polymers [i](#)

There are no such residues in this entry.