



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:50 AM UTC

PDB ID : 5UG0 / pdb_00005ug0
Title : Human antibody H2897 in complex with influenza hemagglutinin H1 Solomon Islands/03/2006
Authors : Raymond, D.D.; Caradonna, T.; Schmidt, A.G.; Harrison, S.C.
Deposited on : 2017-01-06
Resolution : 3.40 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

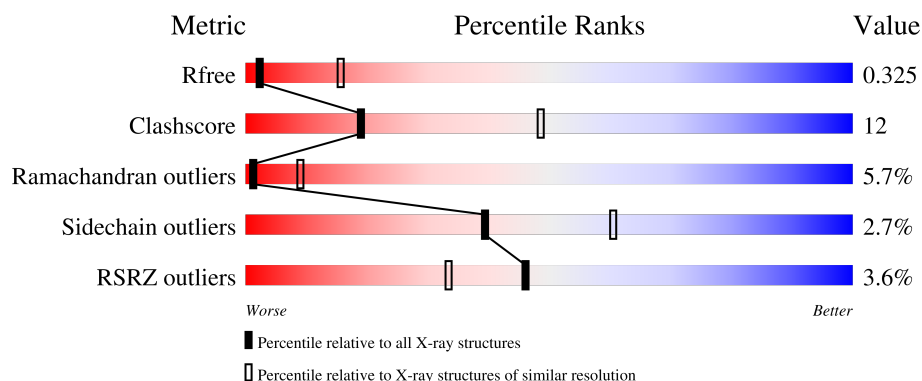
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	327	0% 69% 27% .
2	B	182	2% 71% 18% 7%
3	C	216	5% 62% 32% ..
4	D	232	7% 65% 30% ...
5	E	3	100%

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Mol	Chain	Length	Quality of chain
5	G	3	 100%
6	F	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7416 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2558	1611	445	491	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	expression tag	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1371	857	235	272	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP A7UPX0
B	178	SER	-	expression tag	UNP A7UPX0
B	179	LEU	-	expression tag	UNP A7UPX0
B	180	VAL	-	expression tag	UNP A7UPX0
B	181	PRO	-	expression tag	UNP A7UPX0
B	182	ARG	-	expression tag	UNP A7UPX0

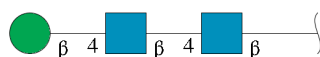
- Molecule 3 is a protein called 2897 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	0	0
			1625	1023	270	328	4			

- Molecule 4 is a protein called 2897 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	227	Total	C	N	O	S	0	0	0
			1686	1061	285	333	7			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



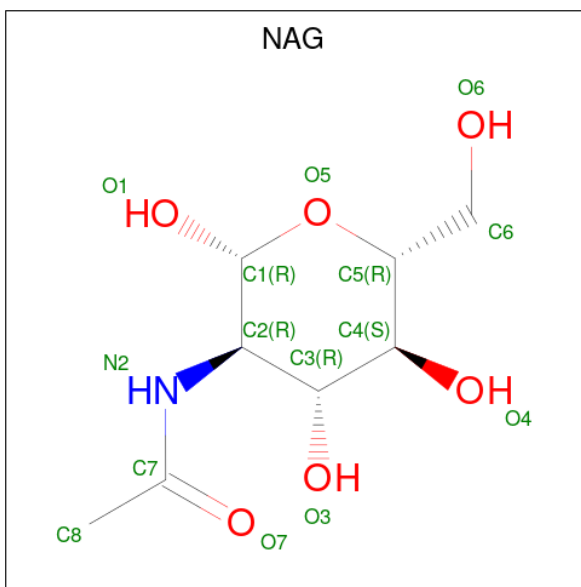
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

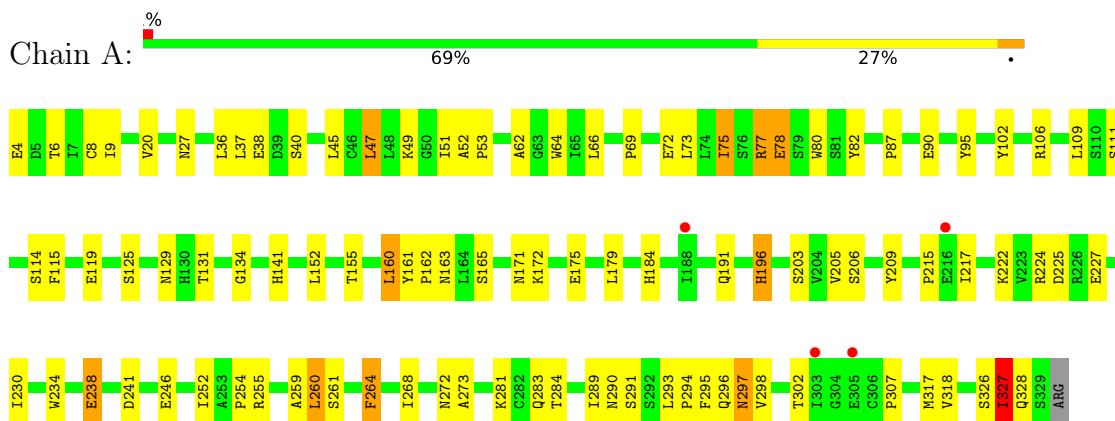


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

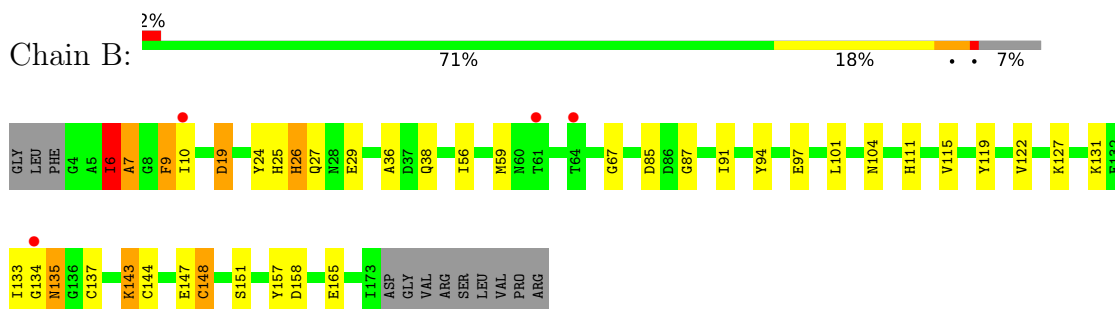
3 Residue-property plots [i](#)

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.

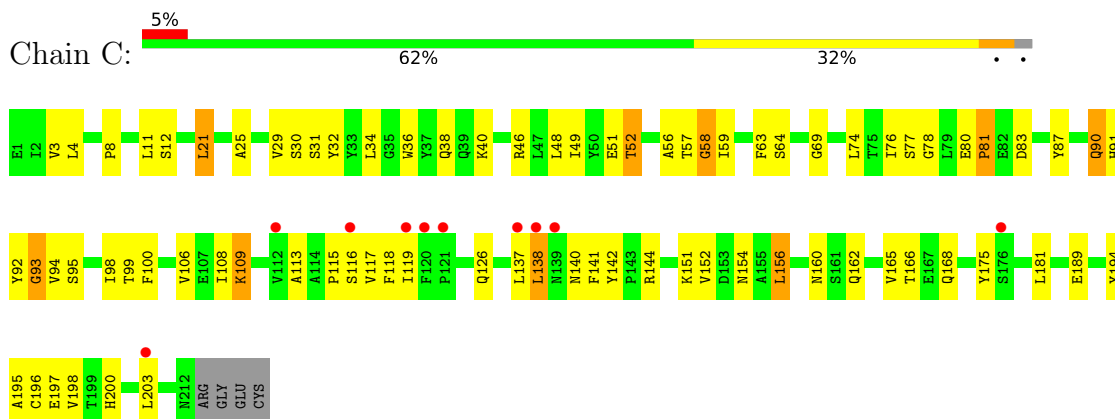
• Molecule 1: Hemagglutinin HA1



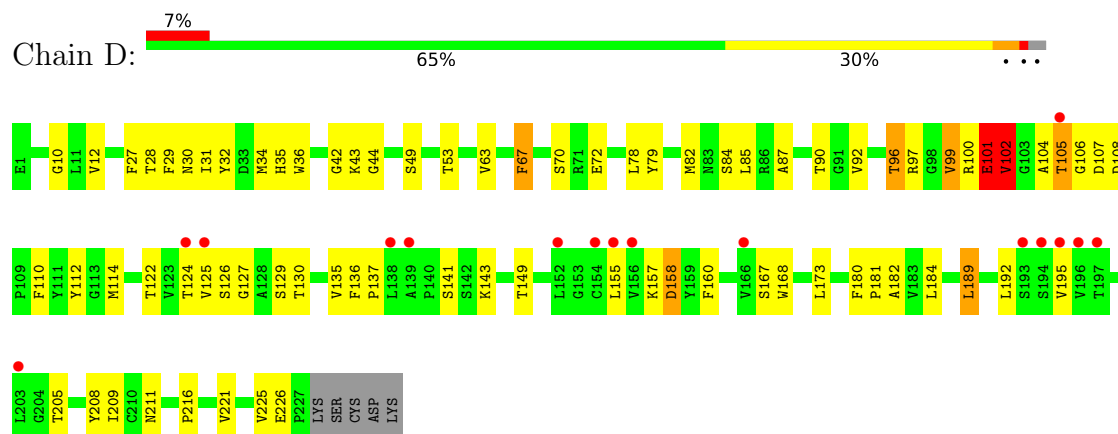
• Molecule 2: Hemagglutinin HA2



• Molecule 3: 2897 light chain



- Molecule 4: 2897 heavy chain



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 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 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.20Å 142.20Å 200.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.41 – 3.40 46.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.41-3.40) 98.8 (46.41-3.40)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.240 , 0.278 0.288 , 0.325	Depositor DCC
R_{free} test set	1621 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	121.4	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 134.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.096 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7416	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.86	1/2624 (0.0%)	1.41	23/3571 (0.6%)
2	B	0.82	1/1397 (0.1%)	1.47	12/1877 (0.6%)
3	C	0.93	0/1662	1.43	19/2259 (0.8%)
4	D	0.84	0/1728	1.34	14/2356 (0.6%)
All	All	0.86	2/7411 (0.0%)	1.41	68/10063 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	ILE	CG1-CD1	-7.21	1.23	1.51
2	B	6	ILE	CG1-CD1	-5.52	1.30	1.51

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLU	N-CA-C	-8.09	104.56	114.75
3	C	138	LEU	CD1-CG-CD2	-7.97	93.27	110.80
3	C	51	GLU	CA-C-N	7.94	136.71	121.54
3	C	51	GLU	C-N-CA	7.94	136.71	121.54
1	A	160	LEU	CD1-CG-CD2	-7.85	93.52	110.80
4	D	67	PHE	CA-CB-CG	7.74	121.54	113.80
1	A	272	ASN	CA-CB-CG	7.31	119.91	112.60
1	A	27	ASN	CA-CB-CG	7.11	119.71	112.60
3	C	189	GLU	CA-C-N	6.99	129.95	120.38
3	C	189	GLU	C-N-CA	6.99	129.95	120.38
4	D	107	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	281	LYS	N-CA-C	-6.85	105.48	114.31
3	C	21	LEU	CD1-CG-CD2	-6.75	95.95	110.80
4	D	101	GLU	CA-C-N	6.65	133.94	121.97
4	D	101	GLU	C-N-CA	6.65	133.94	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	CA-CB-CG	6.56	119.16	112.60
3	C	93	GLY	N-CA-C	6.46	118.84	110.45
1	A	77	ARG	CA-C-N	6.44	132.73	121.52
1	A	77	ARG	C-N-CA	6.44	132.73	121.52
1	A	272	ASN	CA-C-N	6.42	129.81	120.51
1	A	272	ASN	C-N-CA	6.42	129.81	120.51
3	C	30	SER	CA-C-N	6.30	133.57	121.54
3	C	30	SER	C-N-CA	6.30	133.57	121.54
4	D	29	PHE	CA-C-N	6.06	130.39	120.63
4	D	29	PHE	C-N-CA	6.06	130.39	120.63
2	B	9	PHE	CA-CB-CG	5.87	119.67	113.80
2	B	104	ASN	N-CA-C	-5.83	105.00	111.36
2	B	158	ASP	CA-C-N	5.72	127.24	120.09
2	B	158	ASP	C-N-CA	5.72	127.24	120.09
3	C	34	LEU	N-CA-C	5.59	117.81	109.59
2	B	144	CYS	CA-C-N	5.49	129.55	120.94
2	B	144	CYS	C-N-CA	5.49	129.55	120.94
4	D	102	VAL	N-CA-C	-5.47	97.95	109.34
4	D	126	SER	N-CA-C	5.47	116.97	110.19
1	A	205	VAL	CA-C-N	5.44	131.29	122.53
1	A	205	VAL	C-N-CA	5.44	131.29	122.53
1	A	259	ALA	CA-C-N	5.42	130.83	120.97
1	A	259	ALA	C-N-CA	5.42	130.83	120.97
3	C	162	GLN	CA-C-N	5.39	128.76	121.05
3	C	162	GLN	C-N-CA	5.39	128.76	121.05
2	B	29	GLU	N-CA-C	-5.35	106.75	113.28
1	A	290	ASN	CA-C-N	5.32	131.71	121.54
1	A	290	ASN	C-N-CA	5.32	131.71	121.54
3	C	81	PRO	CA-C-N	5.32	127.41	120.28
3	C	81	PRO	C-N-CA	5.32	127.41	120.28
3	C	77	SER	CA-C-N	5.32	125.73	119.94
3	C	77	SER	C-N-CA	5.32	125.73	119.94
2	B	147	GLU	CB-CG-CD	5.31	121.63	112.60
4	D	184	LEU	CD1-CG-CD2	-5.29	99.17	110.80
1	A	273	ALA	N-CA-C	5.27	115.66	109.60
2	B	165	GLU	CA-C-N	5.27	127.34	120.28
2	B	165	GLU	C-N-CA	5.27	127.34	120.28
4	D	96	THR	N-CA-C	5.21	117.11	109.24
1	A	95	TYR	N-CA-C	-5.21	103.09	109.65
1	A	163	ASN	CA-CB-CG	5.20	117.80	112.60
3	C	52	THR	N-CA-CB	5.18	119.24	110.49
1	A	160	LEU	CA-C-N	5.17	134.43	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	LEU	C-N-CA	5.17	134.43	121.80
1	A	171	ASN	CA-C-N	5.17	131.42	121.54
1	A	171	ASN	C-N-CA	5.17	131.42	121.54
3	C	78	GLY	CA-C-N	5.17	129.70	122.36
3	C	78	GLY	C-N-CA	5.17	129.70	122.36
2	B	94	TYR	CA-C-N	5.14	127.42	120.38
2	B	94	TYR	C-N-CA	5.14	127.42	120.38
4	D	28	THR	CA-C-N	5.12	127.90	120.79
4	D	28	THR	C-N-CA	5.12	127.90	120.79
4	D	129	SER	CA-C-N	5.09	131.26	121.54
4	D	129	SER	C-N-CA	5.09	131.26	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2558	0	2463	61	0
2	B	1371	0	1299	20	0
3	C	1625	0	1583	55	0
4	D	1686	0	1636	54	0
5	E	39	0	34	1	0
5	G	39	0	34	0	0
6	F	28	0	25	0	0
7	A	56	0	52	0	0
7	B	14	0	13	0	0
All	All	7416	0	7139	172	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 12.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:VAL:HG22	4:D:122:THR:HG22	1.28	1.12
1:A:37:LEU:HD11	1:A:297:ASN:HB3	1.39	1.03
1:A:80:TRP:CH2	1:A:115:PHE:HE2	1.80	1.00
1:A:80:TRP:HH2	1:A:115:PHE:HE2	1.05	0.92
1:A:80:TRP:CH2	1:A:115:PHE:CE2	2.64	0.86
1:A:64:TRP:CD1	1:A:73:LEU:HD11	2.15	0.82
4:D:96:THR:CG2	4:D:114:MET:HB3	2.11	0.81
3:C:152:VAL:HG21	3:C:156:LEU:HD12	1.63	0.81
3:C:46:ARG:HH21	3:C:59:ILE:CD1	1.93	0.80
2:B:10:ILE:HB	2:B:135:ASN:HB3	1.65	0.79
4:D:96:THR:HG21	4:D:114:MET:HB3	1.62	0.79
4:D:160:PHE:HB2	4:D:189:LEU:HD23	1.68	0.76
4:D:92:VAL:HG22	4:D:122:THR:CG2	2.16	0.73
4:D:72:GLU:HG2	4:D:79:TYR:HE2	1.53	0.72
4:D:12:VAL:HG21	4:D:85:LEU:HD13	1.73	0.70
4:D:53:THR:HG21	4:D:101:GLU:HG2	1.73	0.70
4:D:34:MET:HB3	4:D:78:LEU:HD22	1.74	0.70
1:A:80:TRP:HH2	1:A:115:PHE:CE2	1.97	0.69
3:C:56:ALA:HB3	3:C:59:ILE:CG1	2.23	0.68
4:D:155:LEU:CD2	4:D:157:LYS:HB2	2.25	0.67
3:C:46:ARG:HH21	3:C:59:ILE:HD12	1.61	0.65
3:C:151:LYS:HB2	3:C:195:ALA:HB3	1.79	0.65
3:C:90:GLN:NE2	3:C:92:TYR:HB2	2.12	0.64
3:C:21:LEU:CD1	3:C:36:TRP:CZ3	2.81	0.64
3:C:3:VAL:O	3:C:25:ALA:HA	1.99	0.63
3:C:36:TRP:HB2	3:C:49:ILE:HD13	1.79	0.63
2:B:6:ILE:HG22	2:B:7:ALA:N	2.13	0.62
3:C:80:GLU:HB3	3:C:81:PRO:HD2	1.80	0.62
1:A:295:PHE:HE1	2:B:59:MET:HE2	1.65	0.62
4:D:31:ILE:HA	4:D:101:GLU:HG3	1.82	0.62
3:C:56:ALA:HB3	3:C:59:ILE:HG12	1.81	0.62
1:A:106:ARG:HH21	1:A:268:ILE:HG21	1.65	0.62
3:C:160:ASN:HA	3:C:181:LEU:HD12	1.82	0.61
1:A:294:PRO:HG3	2:B:56:ILE:HG12	1.82	0.61
1:A:62:ALA:HB2	1:A:102:TYR:CE1	2.36	0.61
2:B:19:ASP:HB2	2:B:36:ALA:HB3	1.83	0.61
3:C:48:LEU:HB2	3:C:49:ILE:HD12	1.83	0.61
1:A:160:LEU:HG	1:A:196:HIS:HB2	1.83	0.61
1:A:191:GLN:HB2	1:A:217:ILE:HD11	1.83	0.60
1:A:9:ILE:HD13	2:B:119:TYR:HA	1.83	0.60
1:A:295:PHE:CE1	2:B:59:MET:HE2	2.37	0.59
4:D:180:PHE:HE1	4:D:195:VAL:HG12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:OE2	1:A:40:SER:HB3	2.01	0.59
3:C:38:GLN:OE1	3:C:46:ARG:HD3	2.02	0.59
2:B:6:ILE:HG22	2:B:7:ALA:H	1.68	0.59
4:D:99:VAL:HG21	4:D:112:TYR:CE1	2.38	0.59
1:A:4:GLU:HA	2:B:143:LYS:HE2	1.85	0.58
3:C:113:ALA:HB3	3:C:142:TYR:H	1.67	0.58
4:D:34:MET:CB	4:D:78:LEU:HD22	2.34	0.58
1:A:6:THR:OG1	2:B:27:GLN:HB3	2.05	0.56
4:D:63:VAL:HG12	4:D:67:PHE:HB2	1.86	0.56
3:C:12:SER:HB2	3:C:109:LYS:HB2	1.88	0.56
4:D:167:SER:HB3	4:D:211:ASN:HB2	1.88	0.56
3:C:126:GLN:HB3	4:D:136:PHE:CZ	2.42	0.55
2:B:7:ALA:HA	2:B:137:CYS:SG	2.46	0.55
3:C:21:LEU:HD12	3:C:36:TRP:CZ3	2.42	0.55
3:C:93:GLY:HA2	4:D:112:TYR:CE1	2.42	0.55
1:A:296:GLN:HE21	1:A:298:VAL:HB	1.72	0.55
4:D:90:THR:HG22	4:D:124:THR:HA	1.88	0.55
4:D:182:ALA:HA	4:D:192:LEU:HB3	1.89	0.55
3:C:144:ARG:HE	3:C:165:VAL:HG11	1.72	0.54
4:D:136:PHE:CZ	4:D:155:LEU:HD22	2.43	0.54
1:A:75:ILE:C	1:A:77:ARG:H	2.16	0.54
4:D:101:GLU:O	4:D:102:VAL:HG23	2.08	0.53
2:B:111:HIS:O	2:B:115:VAL:HG23	2.08	0.53
3:C:152:VAL:HG13	3:C:194:TYR:HE2	1.73	0.53
4:D:31:ILE:HD12	4:D:100:ARG:HG3	1.90	0.53
1:A:8:CYS:O	2:B:24:TYR:HA	2.09	0.53
1:A:224:ARG:HH12	5:E:1:NAG:C7	2.22	0.53
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.91	0.52
3:C:166:THR:HG22	4:D:181:PRO:HD3	1.90	0.52
1:A:78:GLU:O	1:A:114:SER:HA	2.10	0.52
1:A:230:ILE:HG21	1:A:252:ILE:HG13	1.91	0.52
3:C:8:PRO:HG3	3:C:11:LEU:HD13	1.91	0.52
3:C:152:VAL:HG22	3:C:194:TYR:HD2	1.75	0.51
1:A:20:VAL:HG21	1:A:318:VAL:HB	1.93	0.51
1:A:64:TRP:HD1	1:A:73:LEU:HD11	1.68	0.51
1:A:69:PRO:HB2	1:A:141:HIS:HB2	1.93	0.51
1:A:179:LEU:O	1:A:254:PRO:HB3	2.10	0.50
3:C:117:VAL:HG22	3:C:198:VAL:HG21	1.92	0.50
1:A:62:ALA:HB2	1:A:102:TYR:HE1	1.76	0.50
4:D:63:VAL:HG12	4:D:63:VAL:O	2.11	0.50
3:C:49:ILE:HD12	3:C:49:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:TRP:CB	4:D:173:LEU:HD12	2.42	0.50
1:A:160:LEU:HD23	1:A:161:TYR:O	2.11	0.50
4:D:70:SER:O	4:D:78:LEU:HD12	2.11	0.49
3:C:92:TYR:HE2	4:D:99:VAL:HG23	1.77	0.49
4:D:158:ASP:HB3	4:D:189:LEU:HD13	1.94	0.49
1:A:9:ILE:CD1	2:B:119:TYR:HA	2.43	0.49
3:C:118:PHE:HB2	3:C:137:LEU:HB2	1.95	0.48
3:C:11:LEU:HB3	3:C:106:VAL:HG22	1.94	0.48
4:D:97:ARG:HG2	4:D:97:ARG:HH11	1.78	0.48
4:D:168:TRP:HB3	4:D:173:LEU:HD12	1.96	0.48
1:A:8:CYS:HB2	2:B:25:HIS:HB3	1.96	0.48
1:A:36:LEU:HD11	1:A:317:MET:HB2	1.96	0.48
4:D:63:VAL:HG11	4:D:67:PHE:CD1	2.49	0.48
3:C:138:LEU:HD12	3:C:141:PHE:CE1	2.49	0.47
1:A:227:GLU:H	4:D:105:THR:HG23	1.79	0.47
1:A:179:LEU:HD23	1:A:234:TRP:CB	2.44	0.47
4:D:32:TYR:CG	4:D:97:ARG:HD2	2.49	0.47
3:C:144:ARG:HH21	3:C:165:VAL:HG12	1.80	0.47
3:C:90:GLN:NE2	4:D:114:MET:HE2	2.29	0.46
4:D:135:VAL:HB	4:D:221:VAL:HG11	1.97	0.46
1:A:179:LEU:CD2	1:A:234:TRP:HB3	2.45	0.46
4:D:209:ILE:HD12	4:D:211:ASN:HD21	1.80	0.46
1:A:9:ILE:HD11	2:B:122:VAL:HG21	1.95	0.46
1:A:38:GLU:HG2	1:A:289:ILE:HG23	1.98	0.46
3:C:116:SER:O	3:C:138:LEU:HA	2.14	0.46
1:A:184:HIS:CD2	1:A:215:PRO:HA	2.51	0.46
1:A:203:SER:HB3	1:A:246:GLU:HB2	1.97	0.46
3:C:48:LEU:HD22	3:C:59:ILE:HG21	1.96	0.46
3:C:152:VAL:HG13	3:C:194:TYR:CE2	2.49	0.46
3:C:56:ALA:C	3:C:58:GLY:H	2.24	0.46
1:A:152:LEU:HB2	1:A:255:ARG:HB2	1.98	0.46
3:C:115:PRO:HD3	3:C:200:HIS:ND1	2.32	0.45
1:A:293:LEU:O	1:A:307:PRO:HB3	2.16	0.45
1:A:45:LEU:HD23	1:A:283:GLN:NE2	2.32	0.45
1:A:131:THR:HG23	1:A:155:THR:OG1	2.17	0.45
4:D:96:THR:HG22	4:D:97:ARG:N	2.31	0.45
4:D:100:ARG:HE	4:D:104:ALA:HB3	1.82	0.45
1:A:327:ILE:HG22	1:A:328:GLN:N	2.32	0.45
3:C:64:SER:O	3:C:74:LEU:HD12	2.16	0.45
1:A:238:GLU:HG2	1:A:241:ASP:HB2	1.97	0.45
4:D:155:LEU:HD23	4:D:157:LYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:ILE:HD12	3:C:196:CYS:HB2	1.98	0.44
1:A:206:SER:HB2	1:A:209:TYR:HB3	1.99	0.44
3:C:92:TYR:CD1	3:C:98:ILE:HD12	2.51	0.44
1:A:53:PRO:HG3	1:A:82:TYR:CZ	2.52	0.44
3:C:29:VAL:HG13	3:C:91:HIS:CD2	2.52	0.44
2:B:131:LYS:HG3	2:B:133:ILE:HG23	1.98	0.44
3:C:63:PHE:CD1	3:C:76:ILE:HG12	2.53	0.44
4:D:100:ARG:NH2	4:D:110:PHE:HB2	2.32	0.44
3:C:90:GLN:HE21	4:D:114:MET:HE2	1.83	0.43
4:D:82:MET:HB3	4:D:85:LEU:HD21	2.00	0.43
4:D:27:PHE:CE1	4:D:97:ARG:HD3	2.54	0.43
4:D:43:LYS:HG2	4:D:44:GLY:H	1.82	0.43
4:D:182:ALA:HB2	4:D:192:LEU:HD23	2.00	0.43
1:A:49:LYS:HB2	1:A:51:ILE:HD12	2.00	0.43
3:C:90:GLN:CD	3:C:92:TYR:HB2	2.43	0.43
2:B:87:GLY:O	2:B:91:ILE:HG12	2.18	0.43
4:D:63:VAL:CG1	4:D:67:PHE:HB2	2.48	0.43
4:D:32:TYR:OH	4:D:108:ASP:HB3	2.19	0.42
1:A:111:SER:HB3	1:A:264:PHE:CE2	2.54	0.42
1:A:222:LYS:HG3	1:A:227:GLU:HG3	2.01	0.42
2:B:148:CYS:O	2:B:151:SER:HB2	2.19	0.42
3:C:151:LYS:HE2	3:C:197:GLU:HB2	2.01	0.42
1:A:66:LEU:HD23	1:A:179:LEU:HD13	2.00	0.42
1:A:73:LEU:O	1:A:77:ARG:HB2	2.19	0.42
4:D:63:VAL:CG1	4:D:67:PHE:CG	3.03	0.42
3:C:92:TYR:HD1	3:C:98:ILE:HD12	1.83	0.42
3:C:4:LEU:HD12	3:C:25:ALA:HB2	2.02	0.42
1:A:36:LEU:HA	1:A:293:LEU:HD22	2.00	0.41
1:A:160:LEU:O	1:A:162:PRO:HD3	2.20	0.41
3:C:115:PRO:HD2	3:C:203:LEU:HG	2.02	0.41
4:D:208:TYR:CE1	4:D:225:VAL:HB	2.54	0.41
3:C:40:LYS:HE3	3:C:46:ARG:HH11	1.85	0.41
3:C:49:ILE:HD11	3:C:74:LEU:HD13	2.03	0.41
1:A:134:GLY:HA2	4:D:102:VAL:HG21	2.02	0.41
1:A:260:LEU:H	1:A:260:LEU:HD23	1.86	0.41
1:A:47:LEU:HB3	1:A:52:ALA:HA	2.02	0.41
1:A:73:LEU:C	1:A:75:ILE:H	2.28	0.41
3:C:11:LEU:O	3:C:106:VAL:HA	2.21	0.41
3:C:168:GLN:HG3	3:C:175:TYR:CZ	2.56	0.41
4:D:87:ALA:HA	4:D:125:VAL:HG21	2.03	0.41
1:A:75:ILE:C	1:A:77:ARG:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:LYS:NZ	4:D:149:THR:HG21	2.35	0.40
3:C:56:ALA:HB3	3:C:59:ILE:HB	2.03	0.40
4:D:36:TRP:HD1	4:D:49:SER:OG	2.04	0.40
3:C:138:LEU:CD1	3:C:141:PHE:CE1	3.05	0.40
1:A:222:LYS:HE3	1:A:227:GLU:HG3	2.02	0.40
2:B:97:GLU:O	2:B:101:LEU:HD13	2.21	0.40
3:C:38:GLN:HB2	3:C:48:LEU:HD11	2.04	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	324/327 (99%)	278 (86%)	37 (11%)	9 (3%)	4	19
2	B	168/182 (92%)	144 (86%)	14 (8%)	10 (6%)	1	7
3	C	210/216 (97%)	168 (80%)	26 (12%)	16 (8%)	1	5
4	D	225/232 (97%)	184 (82%)	23 (10%)	18 (8%)	1	4
All	All	927/957 (97%)	774 (84%)	100 (11%)	53 (6%)	1	9

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ILE
2	B	135	ASN
3	C	31	SER
3	C	32	TYR
3	C	140	ASN
4	D	99	VAL
4	D	102	VAL
4	D	205	THR

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Mol	Chain	Res	Type
1	A	75	ILE
1	A	172	LYS
1	A	196	HIS
1	A	291	SER
2	B	67	GLY
2	B	134	GLY
3	C	87	TYR
3	C	108	ILE
4	D	101	GLU
4	D	127	GLY
4	D	130	THR
1	A	119	GLU
1	A	125	SER
2	B	7	ALA
2	B	9	PHE
3	C	58	GLY
3	C	94	VAL
3	C	95	SER
3	C	109	LYS
4	D	84	SER
4	D	137	PRO
4	D	189	LEU
4	D	226	GLU
1	A	87	PRO
2	B	6	ILE
2	B	26	HIS
2	B	127	LYS
2	B	143	LYS
2	B	157	TYR
3	C	57	THR
3	C	156	LEU
4	D	105	THR
4	D	106	GLY
3	C	83	ASP
3	C	99	THR
3	C	154	ASN
4	D	141	SER
4	D	158	ASP
1	A	326	SER
3	C	52	THR
4	D	30	ASN
4	D	10	GLY

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Mol	Chain	Res	Type
4	D	42	GLY
4	D	216	PRO
3	C	69	GLY

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	286/287 (100%)	272 (95%)	14 (5%)	22	49
2	B	147/157 (94%)	142 (97%)	5 (3%)	32	57
3	C	184/187 (98%)	182 (99%)	2 (1%)	65	74
4	D	186/191 (97%)	185 (100%)	1 (0%)	81	81
All	All	803/822 (98%)	781 (97%)	22 (3%)	39	60

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	72	GLU
1	A	90	GLU
1	A	109	LEU
1	A	129	ASN
1	A	165	SER
1	A	175	GLU
1	A	238	GLU
1	A	260	LEU
1	A	261	SER
1	A	264	PHE
1	A	284	THR
1	A	297	ASN
1	A	302	THR
2	B	19	ASP
2	B	26	HIS
2	B	38	GLN
2	B	85	ASP

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Mol	Chain	Res	Type
2	B	148	CYS
3	C	90	GLN
3	C	100	PHE
4	D	35	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	55	GLN
1	A	184	HIS
1	A	187	ASN
1	A	270	ASN
1	A	290	ASN
1	A	296	GLN
2	B	43	ASN
2	B	46	ASN
2	B	60	ASN
2	B	169	ASN
3	C	39	GLN
3	C	43	GLN
3	C	90	GLN
3	C	91	HIS
3	C	160	ASN
4	D	76	ASN
4	D	185	GLN
4	D	211	ASN

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](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	E	1	1,5	14,14,15	0.34	0	17,19,21	0.74	0
5	NAG	E	2	5	14,14,15	0.35	0	17,19,21	1.33	3 (17%)
5	BMA	E	3	5	11,11,12	0.37	0	15,15,17	0.83	1 (6%)
6	NAG	F	1	6,1	14,14,15	0.38	0	17,19,21	0.89	1 (5%)
6	NAG	F	2	6	14,14,15	0.37	0	17,19,21	0.88	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.36	0	17,19,21	1.05	2 (11%)
5	NAG	G	2	5	14,14,15	0.35	0	17,19,21	0.97	2 (11%)
5	BMA	G	3	5	11,11,12	0.41	0	15,15,17	0.93	1 (6%)

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	NAG	O5-C1-C2	-3.81	105.39	111.29
6	F	2	NAG	C1-O5-C5	3.14	116.39	112.19
5	G	3	BMA	C1-O5-C5	3.10	116.34	112.19
5	G	2	NAG	O5-C1-C2	-2.86	106.87	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C1-O5-C5	2.84	116.00	112.19
5	E	3	BMA	C1-O5-C5	2.75	115.87	112.19
5	E	2	NAG	C1-C2-N2	2.60	114.53	110.43
5	G	1	NAG	O5-C1-C2	-2.49	107.44	111.29
5	G	2	NAG	C1-O5-C5	2.36	115.35	112.19
6	F	1	NAG	O5-C1-C2	-2.29	107.75	111.29
5	E	2	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

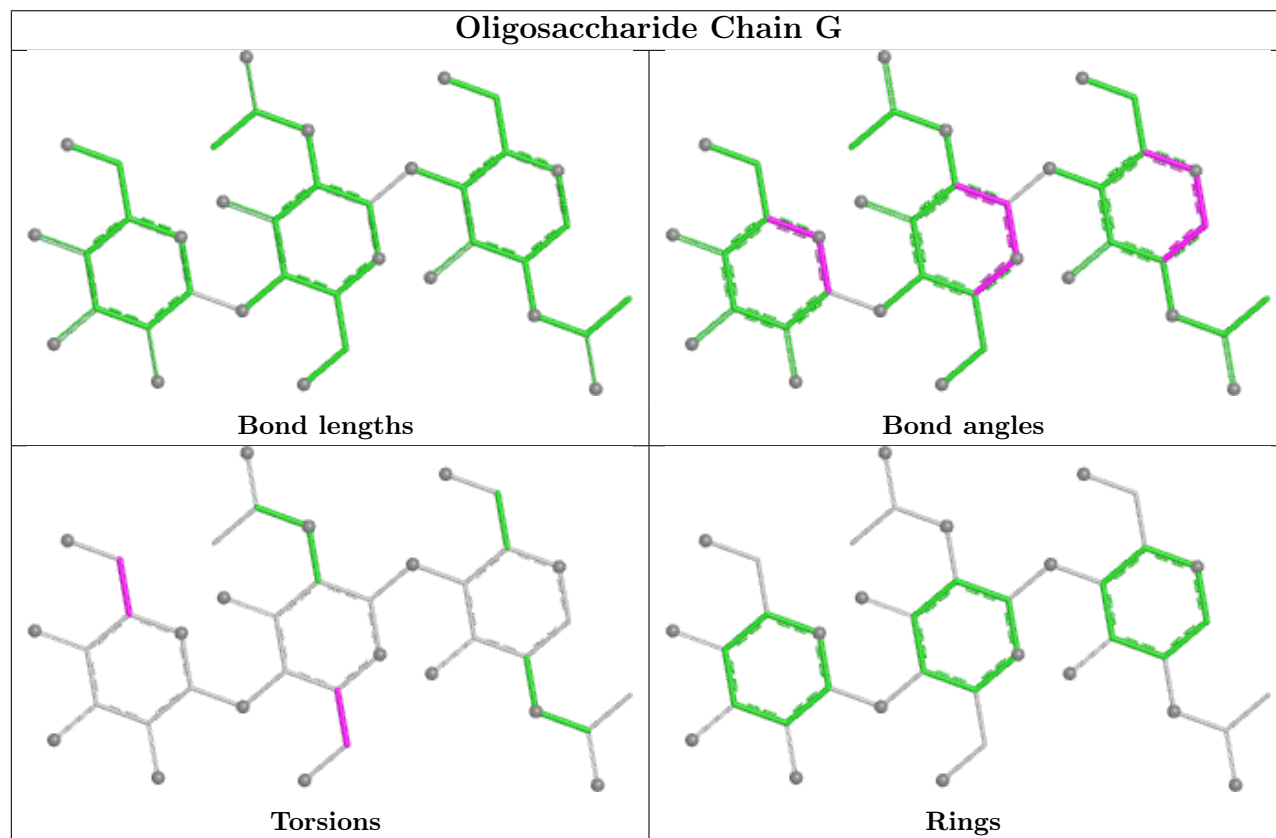
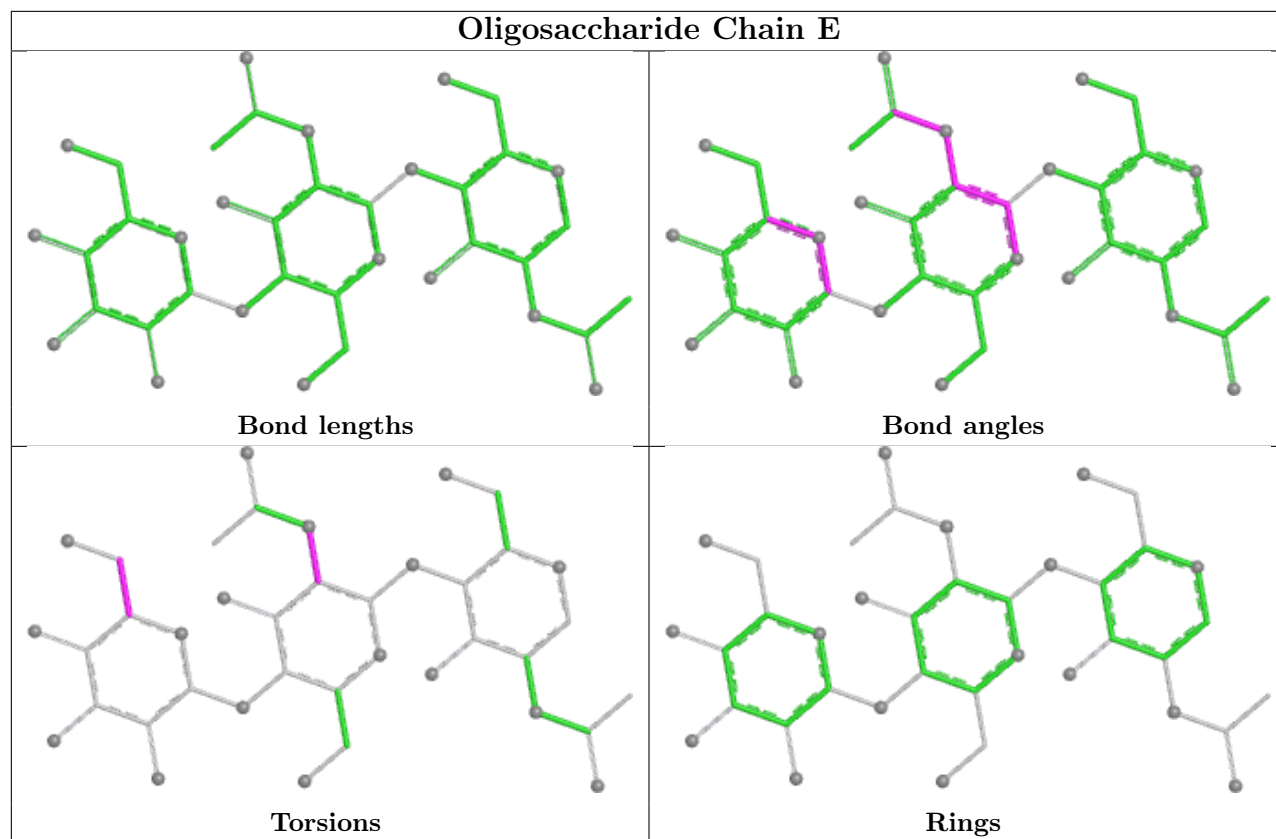
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C1-C2-N2-C7
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6

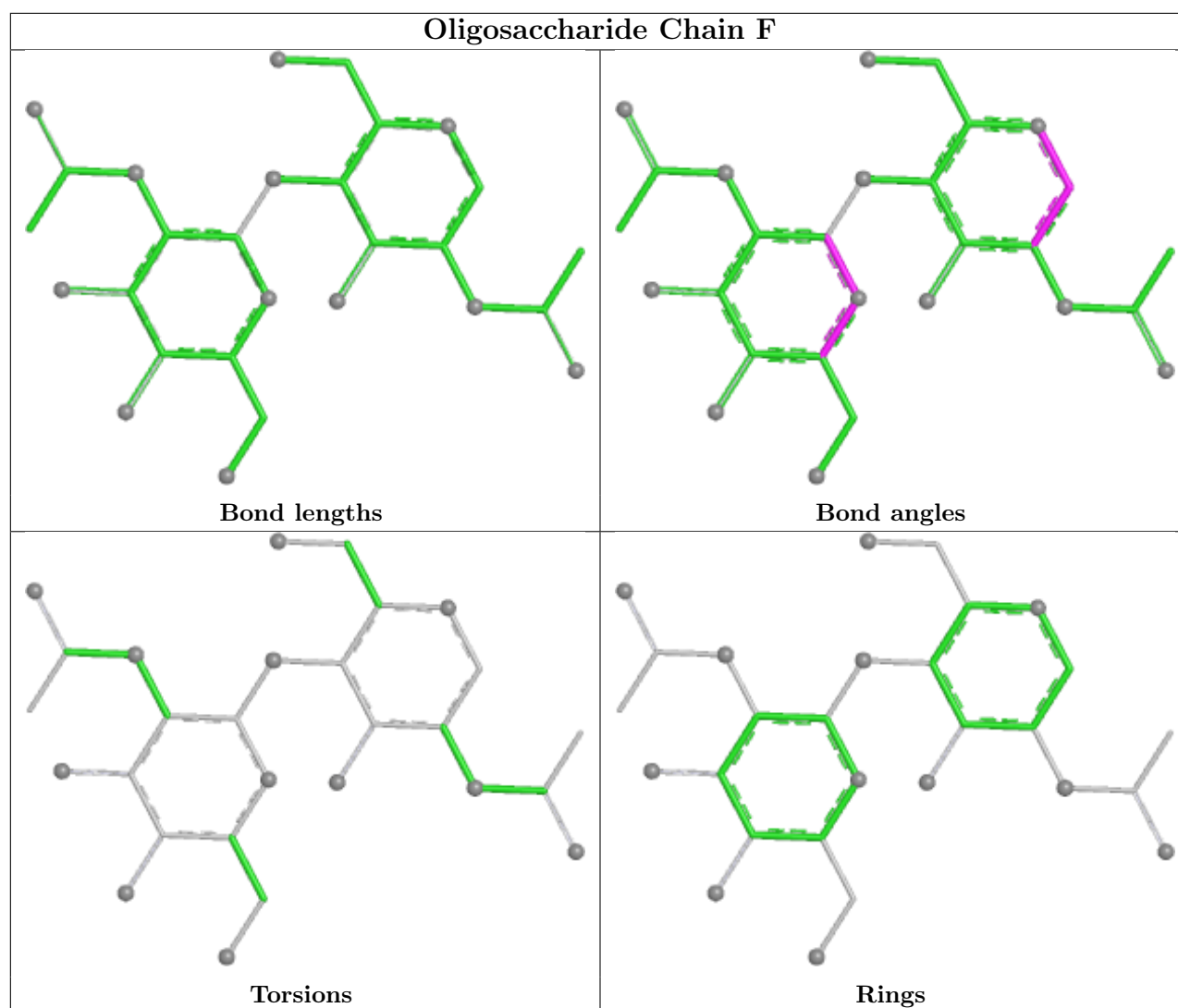
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	406	1	14,14,15	0.38	0	17,19,21	0.41	0
7	NAG	B	201	2	14,14,15	0.36	0	17,19,21	0.52	0
7	NAG	A	407	-	14,14,15	0.32	0	19,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	401	1	14,14,15	0.35	0	17,19,21	0.85	1 (5%)
7	NAG	A	402	1	14,14,15	0.41	0	17,19,21	1.81	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
7	NAG	A	406	1	-	2/6/23/26	0/1/1/1
7	NAG	B	201	2	-	1/6/23/26	0/1/1/1
7	NAG	A	407	-	-	1/6/22/26	0/1/1/1
7	NAG	A	401	1	-	1/6/23/26	0/1/1/1
7	NAG	A	402	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	402	NAG	O5-C1-C2	5.18	119.31	111.29
7	A	402	NAG	C1-O5-C5	4.66	118.43	112.19
7	A	407	NAG	O1-C1-C2	2.43	114.26	109.22
7	A	401	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	406	NAG	O5-C5-C6-O6
7	A	401	NAG	O5-C5-C6-O6
7	B	201	NAG	O5-C5-C6-O6
7	A	402	NAG	C4-C5-C6-O6
7	A	402	NAG	O5-C5-C6-O6
7	A	407	NAG	O5-C5-C6-O6
7	A	406	NAG	C4-C5-C6-O6

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	326/327 (99%)	-0.10	4 (1%)	76 63	112, 136, 159, 178	0
2	B	170/182 (93%)	-0.01	4 (2%)	59 45	102, 142, 175, 188	0
3	C	212/216 (98%)	0.30	10 (4%)	36 27	128, 171, 231, 243	0
4	D	227/232 (97%)	0.42	16 (7%)	22 18	121, 153, 250, 257	0
All	All	935/957 (97%)	0.13	34 (3%)	46 33	102, 146, 235, 257	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	194	SER	8.4
4	D	195	VAL	7.2
4	D	196	VAL	6.1
3	C	138	LEU	5.2
4	D	197	THR	5.1
3	C	137	LEU	4.2
3	C	120	PHE	4.2
4	D	138	LEU	4.2
4	D	193	SER	4.2
2	B	61	THR	4.1
3	C	121	PRO	3.4
4	D	154	CYS	3.1
3	C	119	ILE	3.1
4	D	125	VAL	2.9
3	C	116	SER	2.8
4	D	139	ALA	2.8
2	B	10	ILE	2.7
3	C	176	SER	2.7
4	D	155	LEU	2.6
3	C	112	VAL	2.6
2	B	64	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	188	ILE	2.5
1	A	216	GLU	2.4
1	A	305	GLU	2.4
1	A	303	ILE	2.3
4	D	203	LEU	2.3
4	D	156	VAL	2.2
2	B	134	GLY	2.2
3	C	203	LEU	2.2
4	D	124	THR	2.2
3	C	139	ASN	2.2
4	D	166	VAL	2.1
4	D	152	LEU	2.1
4	D	105	THR	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](#)

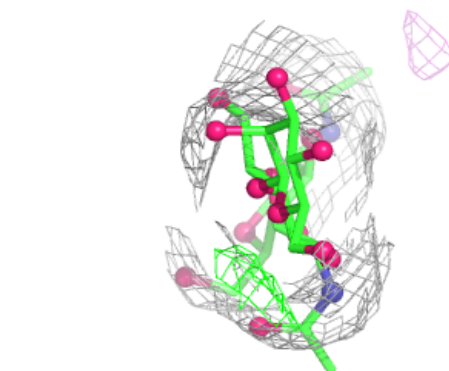
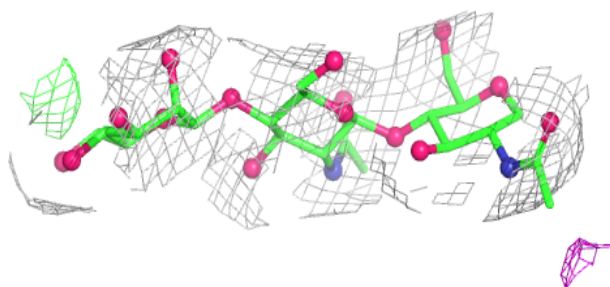
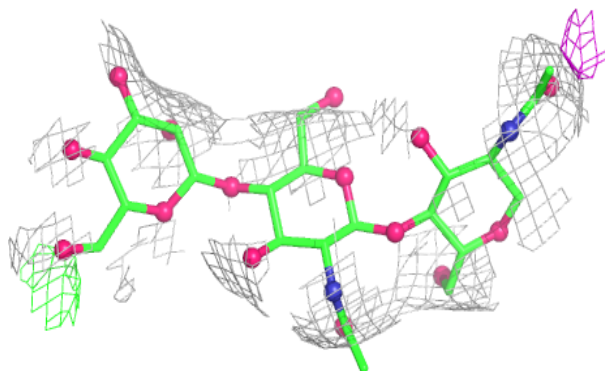
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	E	3	11/12	0.31	0.12	209,214,215,215	0
5	BMA	G	3	11/12	0.54	0.12	224,227,227,228	0
6	NAG	F	1	14/15	0.61	0.16	209,213,215,217	0
6	NAG	F	2	14/15	0.72	0.11	213,219,220,220	0
5	NAG	G	1	14/15	0.76	0.11	208,211,216,219	0
5	NAG	G	2	14/15	0.78	0.12	222,225,226,227	0
5	NAG	E	2	14/15	0.86	0.10	188,192,198,204	0
5	NAG	E	1	14/15	0.94	0.09	156,165,172,180	0

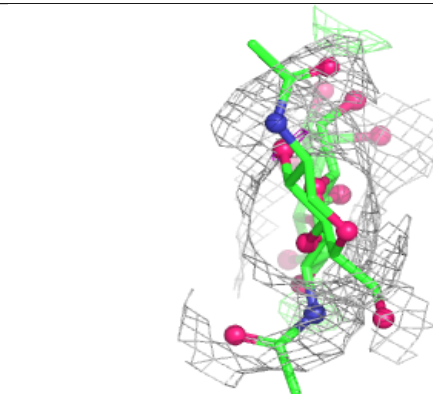
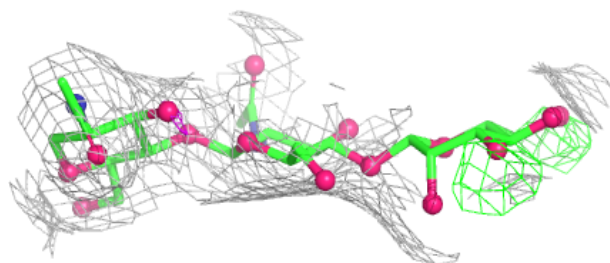
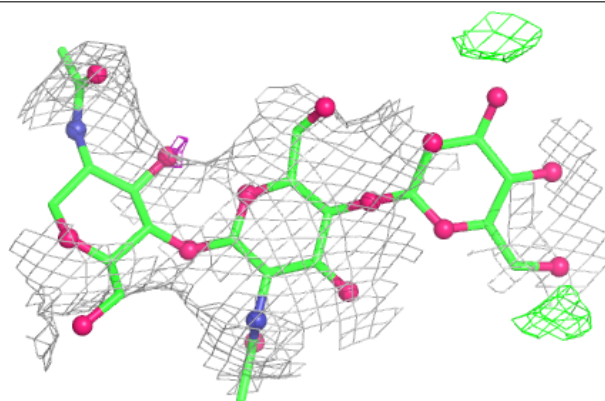
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

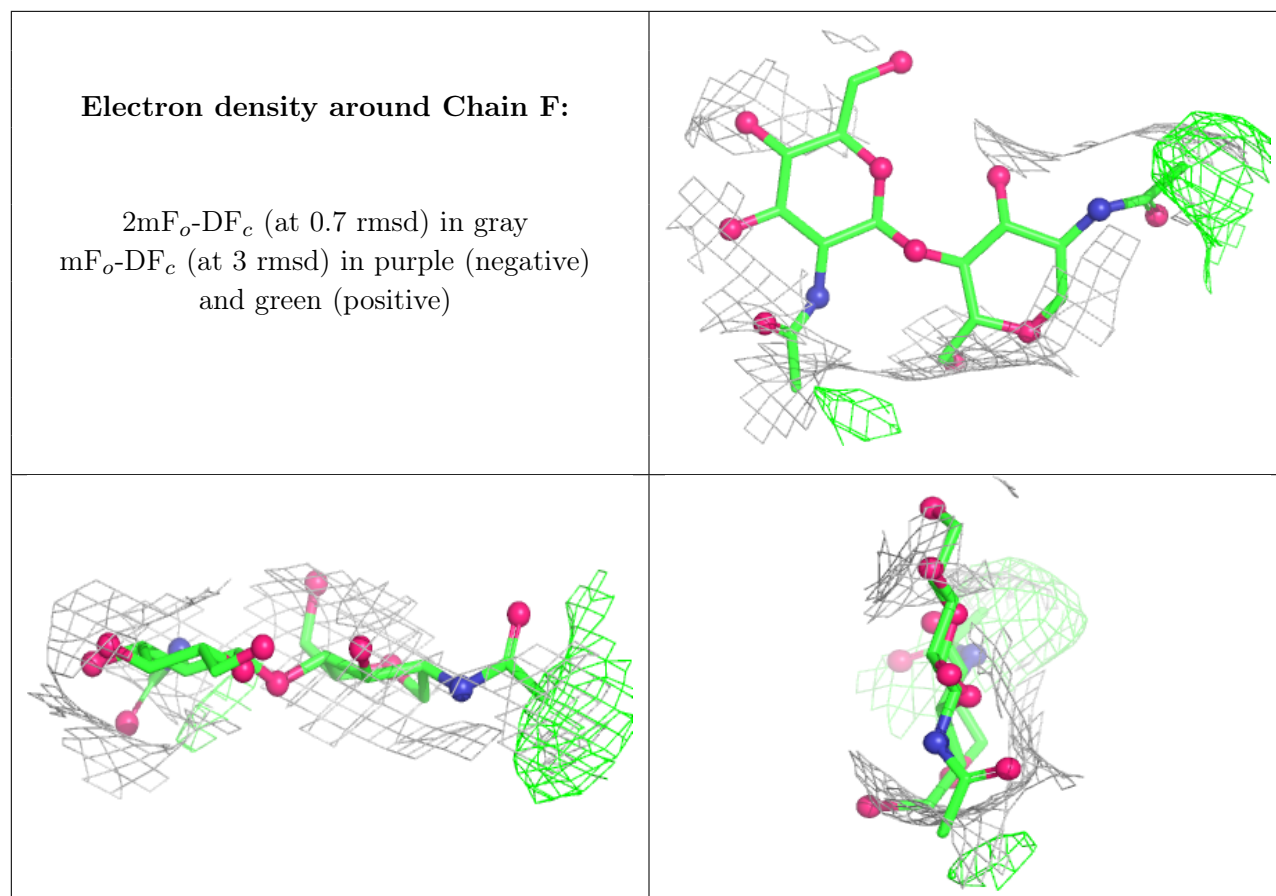
Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain G:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	201	14/15	0.34	0.15	241,244,247,247	0
7	NAG	A	407	14/15	0.57	0.09	199,208,209,209	0
7	NAG	A	402	14/15	0.68	0.10	190,193,195,196	0
7	NAG	A	406	14/15	0.69	0.11	212,214,217,218	0
7	NAG	A	401	14/15	0.91	0.08	181,185,188,188	0

6.5 Other polymers [i](#)

There are no such residues in this entry.