WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2020 – 01:50 PM BST

PDB ID	:	4GT7
Title	:	An engineered disulfide bond reversibly traps the IgE-Fc3-4 in a closed, non-receptor binding conformation
Authors	:	Wurzburg, B.A.; Kim, B.K.; Jardetzky, T.S.
Deposited on	:	2012-08-28
Resolution	:	2.61 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 (i) symbol.

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

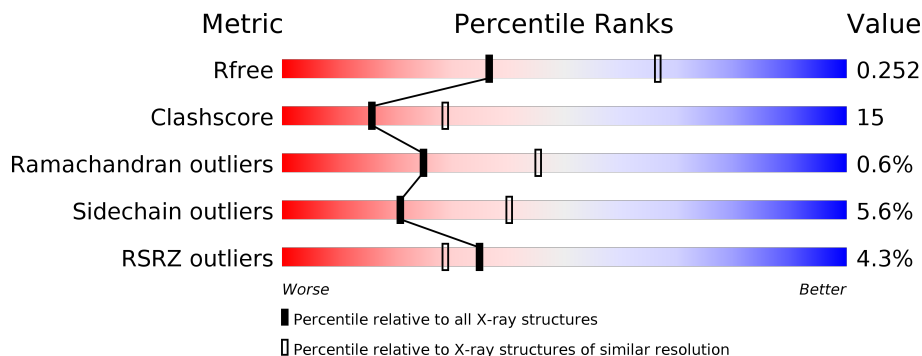|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		15
Ramachandran outliers		0.6%
Sidechain outliers		5.6%
RSRZ outliers		4.3%

Worse　　　　　　　　　　　　　　　　　Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	221	4% 68% 26% · ·
1	B	221	4% 70% 27% ·
1	C	221	7% 65% 30% · ·
1	D	221	2% 67% 27% · ·
2	E	5	60% 40%
2	F	5	60% 40%

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Mol	Chain	Length	Quality of chain
2	G	5	40%　　　　　40%　　　　　20%
3	H	4	75%　　　　　25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7082 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total 1678	C 1049	N 311	O 311	S 7	0	0	0
1	B	213	Total 1673	C 1048	N 306	O 312	S 7	0	0	0
1	C	214	Total 1687	C 1055	N 311	O 314	S 7	0	0	0
1	D	213	Total 1685	C 1054	N 312	O 312	S 7	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	expression tag	UNP P01854
A	326	ASP	-	expression tag	UNP P01854
A	327	PRO	-	expression tag	UNP P01854
A	328	ALA	-	expression tag	UNP P01854
A	335	CYS	GLY	engineered mutation	UNP P01854
B	325	ALA	-	expression tag	UNP P01854
B	326	ASP	-	expression tag	UNP P01854
B	327	PRO	-	expression tag	UNP P01854
B	328	ALA	-	expression tag	UNP P01854
B	335	CYS	GLY	engineered mutation	UNP P01854
C	325	ALA	-	expression tag	UNP P01854
C	326	ASP	-	expression tag	UNP P01854
C	327	PRO	-	expression tag	UNP P01854
C	328	ALA	-	expression tag	UNP P01854
C	335	CYS	GLY	engineered mutation	UNP P01854
D	325	ALA	-	expression tag	UNP P01854
D	326	ASP	-	expression tag	UNP P01854
D	327	PRO	-	expression tag	UNP P01854
D	328	ALA	-	expression tag	UNP P01854
D	335	CYS	GLY	engineered mutation	UNP P01854

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
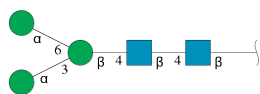
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total 61	C 34	N 2	O 25	0	0	0
2	F	5	Total 61	C 34	N 2	O 25	0	0	0
2	G	5	Total 61	C 34	N 2	O 25	0	0	0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.
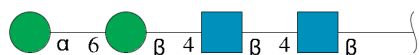
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	4	Total 50	C 28	N 2	O 20	0	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total 34	O 34	0	0
4	B	24	Total 24	O 24	0	0
4	C	25	Total 25	O 25	0	0
4	D	43	Total 43	O 43	0	0

3 Residue-property plots ⓘ

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: Ig epsilon chain C region
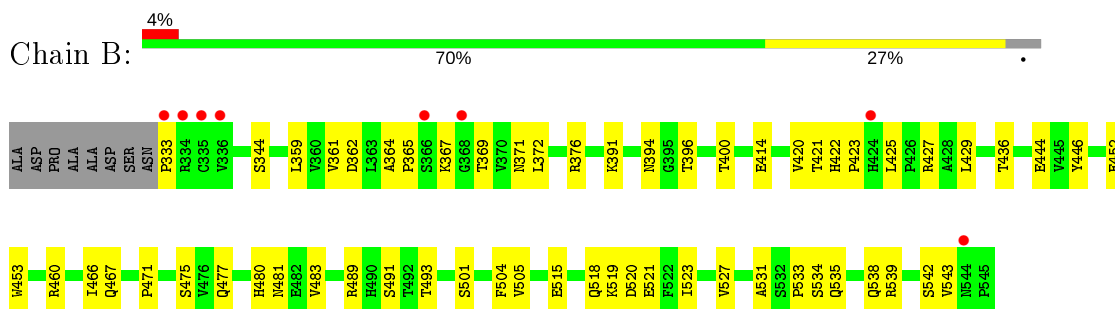
- Molecule 1: Ig epsilon chain C region

- Molecule 1: Ig epsilon chain C region
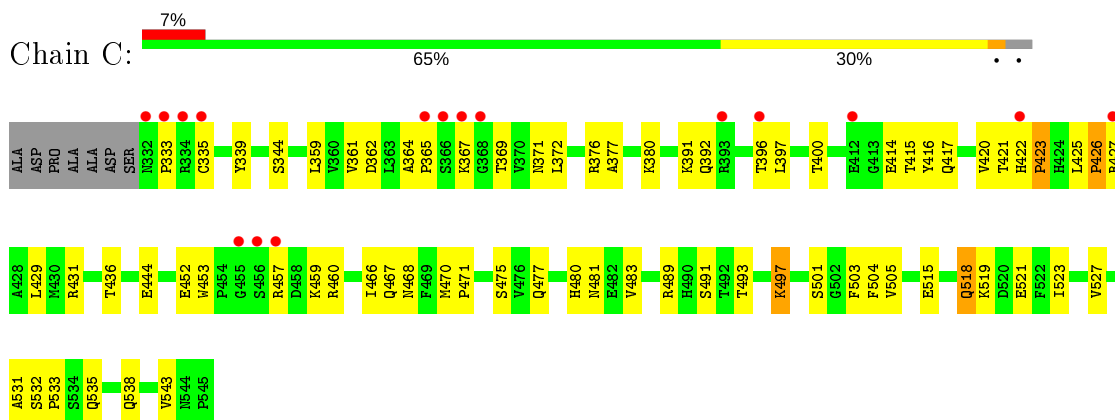
- Molecule 1: Ig epsilon chain C region

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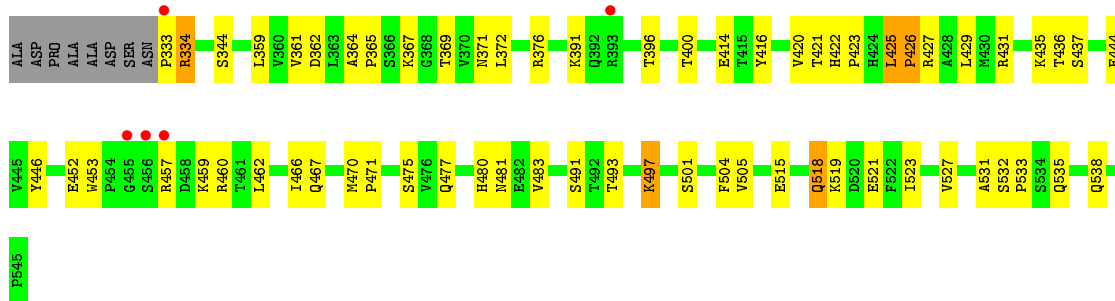
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 2: 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

Chain F:

• Molecule 2: 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

Chain G:
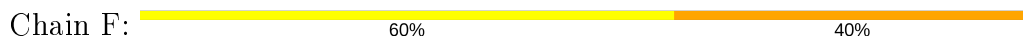
• Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:
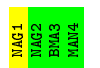
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.75Å 104.81Å 45.90Å 90.00° 94.51° 90.00°	Depositor
Resolution (Å)	29.20 – 2.61 29.38 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.20-2.61) 97.2 (29.38-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	2.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.190 , 0.253 0.191 , 0.252	Depositor DCC
R_{free} test set	1395 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.9	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7082	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]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: BMA, 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	0.46	0/1721	0.59	0/2343
1	B	0.45	0/1717	0.59	0/2340
1	C	0.44	0/1731	0.58	0/2359
1	D	0.46	0/1729	0.59	0/2354
All	All	0.45	0/6898	0.59	0/9396

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	1678	0	1661	56	0
1	B	1673	0	1647	50	0
1	C	1687	0	1663	65	0
1	D	1685	0	1669	51	0
2	E	61	0	52	1	0
2	F	61	0	52	1	0
2	G	61	0	52	1	0
3	H	50	0	43	0	0
4	A	34	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	1	0
4	C	25	0	0	2	0
4	D	43	0	0	1	0
All	All	7082	0	6839	202	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 15.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:HIS:HB3	1:C:425:LEU:HB2	1.38	1.01
1:A:422:HIS:HD2	1:A:423:PRO:HD2	1.33	0.93
1:C:429:LEU:HD21	1:D:333:PRO:HG3	1.54	0.87
1:C:422:HIS:CG	1:C:423:PRO:HD2	2.09	0.86
1:D:481:ASN:HD21	1:D:519:LYS:HG2	1.44	0.82
1:D:481:ASN:ND2	1:D:519:LYS:HG2	1.94	0.82
1:C:422:HIS:ND1	1:C:423:PRO:HD2	1.95	0.81
1:C:481:ASN:ND2	1:C:519:LYS:HG2	1.96	0.81
1:C:481:ASN:HD21	1:C:519:LYS:HG2	1.46	0.80
1:D:422:HIS:CD2	1:D:423:PRO:HD2	2.17	0.79
1:B:422:HIS:ND1	1:B:423:PRO:HD2	1.95	0.79
1:C:425:LEU:HD12	1:C:426:PRO:HD2	1.64	0.79
1:A:481:ASN:HD21	1:A:519:LYS:HG2	1.47	0.78
1:A:481:ASN:ND2	1:A:519:LYS:HG2	1.98	0.78
1:B:371:ASN:HB2	1:B:421:THR:HB	1.65	0.77
1:D:371:ASN:HB2	1:D:421:THR:HB	1.67	0.77
1:A:371:ASN:HB2	1:A:421:THR:HB	1.67	0.76
1:C:371:ASN:HB2	1:C:421:THR:HB	1.68	0.76
1:C:431:ARG:HH22	1:D:333:PRO:HD3	1.52	0.73
1:B:481:ASN:ND2	1:B:519:LYS:HG2	2.05	0.70
1:A:362:ASP:HA	1:A:396:THR:HG23	1.73	0.69
1:B:481:ASN:HD21	1:B:519:LYS:HG2	1.56	0.69
1:A:453:TRP:CE2	1:B:444:GLU:HG2	2.31	0.66
1:C:521:GLU:HA	1:C:521:GLU:OE1	1.97	0.65
1:C:431:ARG:NH2	1:D:333:PRO:HD3	2.12	0.65
1:B:460:ARG:HG3	1:B:543:VAL:HG13	1.79	0.65
1:B:533:PRO:HG3	1:C:415:THR:HG21	1.78	0.64
1:D:422:HIS:HB3	1:D:425:LEU:HG	1.79	0.64
1:B:521:GLU:HA	1:B:521:GLU:OE1	1.98	0.63
1:A:422:HIS:CD2	1:A:423:PRO:HD2	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:VAL:HB	1:D:429:LEU:HB2	1.81	0.63
1:C:489:ARG:NH1	4:C:719:HOH:O	2.32	0.62
1:B:422:HIS:HB3	1:B:425:LEU:HD12	1.81	0.62
1:B:420:VAL:HB	1:B:429:LEU:HB2	1.80	0.62
1:D:521:GLU:HA	1:D:521:GLU:OE1	1.98	0.62
1:B:475:SER:HB2	1:B:527:VAL:HB	1.83	0.61
1:C:362:ASP:HA	1:C:396:THR:HG23	1.84	0.60
1:A:521:GLU:HA	1:A:521:GLU:OE1	2.01	0.60
1:C:376:ARG:O	4:C:723:HOH:O	2.16	0.60
1:A:420:VAL:HB	1:A:429:LEU:HB2	1.83	0.60
1:B:520:ASP:CG	1:B:542:SER:HB2	2.22	0.59
1:B:376:ARG:HD2	1:B:414:GLU:OE2	2.03	0.59
1:D:372:LEU:CD2	1:D:420:VAL:HG22	2.34	0.58
1:D:435:LYS:O	4:D:720:HOH:O	2.16	0.58
1:C:333:PRO:HD3	1:D:431:ARG:NH2	2.19	0.58
1:C:444:GLU:HG2	1:D:453:TRP:CE2	2.39	0.58
1:B:520:ASP:O	1:B:542:SER:HB3	2.04	0.57
1:C:372:LEU:CD2	1:C:420:VAL:HG22	2.34	0.57
1:C:376:ARG:HD2	1:C:414:GLU:OE2	2.04	0.57
1:C:420:VAL:HB	1:C:429:LEU:HB2	1.86	0.56
1:C:453:TRP:CE2	1:D:444:GLU:HG2	2.40	0.56
1:C:422:HIS:CE1	1:C:423:PRO:HD2	2.40	0.56
1:A:422:HIS:HD2	1:A:423:PRO:CD	2.14	0.56
1:A:475:SER:HB2	1:A:527:VAL:HB	1.87	0.56
1:A:372:LEU:CD2	1:A:420:VAL:HG22	2.35	0.55
1:A:376:ARG:HD2	1:A:414:GLU:OE2	2.06	0.55
1:A:444:GLU:O	1:A:466:ILE:HA	2.06	0.55
1:C:365:PRO:HB3	1:C:391:LYS:HE2	1.88	0.55
1:A:460:ARG:HG3	1:A:543:VAL:HG11	1.89	0.55
1:A:454:PRO:HA	1:A:457:ARG:CZ	2.37	0.55
1:C:444:GLU:O	1:C:466:ILE:HA	2.06	0.54
1:C:475:SER:HB2	1:C:527:VAL:HB	1.89	0.54
1:B:364:ALA:HB3	1:B:367:LYS:HG3	1.90	0.54
1:C:364:ALA:HB3	1:C:367:LYS:HG3	1.88	0.54
1:D:334:ARG:HH12	1:D:364:ALA:HB2	1.72	0.54
1:D:376:ARG:HD2	1:D:414:GLU:OE2	2.08	0.54
1:D:475:SER:HB2	1:D:527:VAL:HB	1.89	0.54
1:B:444:GLU:O	1:B:466:ILE:HA	2.07	0.53
1:A:364:ALA:HB3	1:A:367:LYS:HG3	1.91	0.53
1:C:425:LEU:CD1	1:C:426:PRO:HD2	2.35	0.53
1:B:534:SER:HB3	1:C:377:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ARG:HG3	1:B:543:VAL:CG1	2.39	0.52
1:D:444:GLU:O	1:D:466:ILE:HA	2.10	0.52
1:A:365:PRO:HB3	1:A:391:LYS:HE2	1.91	0.52
1:A:452:GLU:OE2	1:A:457:ARG:HD3	2.09	0.52
1:A:429:LEU:HD21	1:B:333:PRO:HG3	1.90	0.52
1:D:364:ALA:HB3	1:D:367:LYS:HG3	1.91	0.52
1:B:372:LEU:CD2	1:B:420:VAL:HG22	2.39	0.51
1:C:361:VAL:HG12	1:C:362:ASP:N	2.26	0.51
1:C:429:LEU:CD2	1:D:333:PRO:HG3	2.36	0.51
1:C:392:GLN:HB2	1:C:396:THR:HB	1.91	0.51
1:A:392:GLN:HB2	1:A:396:THR:HB	1.92	0.50
1:C:359:LEU:HD13	1:C:400:THR:HG22	1.94	0.50
1:C:493:THR:HG21	1:D:493:THR:HG21	1.93	0.50
1:B:361:VAL:HG12	1:B:362:ASP:N	2.26	0.50
1:C:372:LEU:HD22	1:C:420:VAL:HG22	1.93	0.50
1:B:489:ARG:NH1	4:B:702:HOH:O	2.42	0.50
1:A:454:PRO:HA	1:A:457:ARG:NH2	2.26	0.49
1:C:396:THR:HG22	1:C:397:LEU:N	2.27	0.49
1:D:365:PRO:HB3	1:D:391:LYS:HE2	1.93	0.49
1:D:422:HIS:HB3	1:D:425:LEU:CG	2.42	0.49
1:B:365:PRO:HB3	1:B:391:LYS:HE2	1.94	0.49
1:C:452:GLU:CD	1:C:457:ARG:HB2	2.34	0.48
1:D:359:LEU:HD13	1:D:400:THR:HG22	1.94	0.48
1:C:519:LYS:NZ	1:C:521:GLU:HB2	2.28	0.48
1:D:467:GLN:HA	1:D:504:PHE:HA	1.96	0.48
1:C:422:HIS:HB3	1:C:425:LEU:CB	2.27	0.48
1:B:359:LEU:HD13	1:B:400:THR:HG22	1.95	0.47
1:C:481:ASN:HD21	1:C:519:LYS:CG	2.22	0.47
1:D:361:VAL:HG12	1:D:362:ASP:N	2.28	0.47
1:A:493:THR:HG21	1:B:493:THR:HG21	1.95	0.47
1:C:452:GLU:HB2	1:C:460:ARG:NH2	2.29	0.47
1:D:459:LYS:O	1:D:460:ARG:HD3	2.14	0.47
1:B:515:GLU:O	1:B:518:GLN:HG3	2.14	0.47
1:B:436:THR:HG23	1:B:471:PRO:HG3	1.96	0.47
1:D:372:LEU:HD22	1:D:420:VAL:HG22	1.95	0.47
1:D:334:ARG:NE	1:D:362:ASP:O	2.48	0.47
1:A:539:ARG:HH22	1:B:453:TRP:HZ3	1.63	0.47
1:B:359:LEU:CD1	1:B:400:THR:HG22	2.45	0.46
1:B:531:ALA:O	1:B:535:GLN:HA	2.15	0.46
1:A:460:ARG:HG3	1:A:543:VAL:CG1	2.45	0.46
1:A:453:TRP:HB2	1:B:446:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:HIS:HD2	1:B:521:GLU:O	1.98	0.46
1:A:372:LEU:HD22	1:A:420:VAL:HG22	1.98	0.46
1:A:467:GLN:HA	1:A:504:PHE:HA	1.98	0.46
1:B:361:VAL:CG1	1:B:362:ASP:N	2.79	0.45
1:A:444:GLU:HG2	1:B:453:TRP:CE2	2.51	0.45
1:B:436:THR:CG2	1:B:471:PRO:HG3	2.47	0.45
1:D:452:GLU:HB2	1:D:460:ARG:NH2	2.31	0.45
2:F:3:BMA:O2	2:F:4:MAN:H5	2.16	0.45
1:C:523:ILE:CG2	1:C:538:GLN:HB2	2.47	0.45
1:A:486:PRO:HD3	4:A:709:HOH:O	2.16	0.45
1:B:452:GLU:HB2	1:B:460:ARG:NH2	2.31	0.45
1:B:467:GLN:HA	1:B:504:PHE:HA	1.98	0.45
1:A:429:LEU:CD2	1:B:333:PRO:HD3	2.47	0.45
1:C:422:HIS:CG	1:C:423:PRO:CD	2.92	0.45
1:A:425:LEU:HG	1:A:426:PRO:HD2	1.98	0.45
1:D:515:GLU:O	1:D:518:GLN:HG3	2.17	0.44
1:D:519:LYS:NZ	1:D:521:GLU:HB2	2.32	0.44
1:C:470:MET:HA	1:C:471:PRO:C	2.36	0.44
1:D:481:ASN:HD21	1:D:519:LYS:CG	2.22	0.44
1:A:361:VAL:HG12	1:A:362:ASP:N	2.32	0.44
2:E:3:BMA:H61	2:E:5:MAN:H3	1.99	0.44
1:C:480:HIS:HD2	1:C:521:GLU:O	2.01	0.44
1:C:532:SER:HA	1:C:533:PRO:HA	1.71	0.44
1:D:519:LYS:HZ3	1:D:521:GLU:HB2	1.83	0.44
1:B:394:ASN:OD1	1:B:396:THR:HB	2.18	0.44
1:C:361:VAL:CG1	1:C:362:ASP:N	2.81	0.44
1:C:467:GLN:HA	1:C:504:PHE:HA	1.99	0.44
1:A:531:ALA:O	1:A:535:GLN:HA	2.18	0.44
1:A:532:SER:HA	1:A:533:PRO:HA	1.71	0.44
1:D:422:HIS:CG	1:D:423:PRO:HD2	2.51	0.43
1:A:497:LYS:HB3	1:A:497:LYS:HE2	1.78	0.43
1:D:426:PRO:HB2	1:D:427:ARG:H	1.54	0.43
1:C:359:LEU:CD1	1:C:400:THR:HG22	2.49	0.43
1:D:452:GLU:CD	1:D:457:ARG:HB2	2.39	0.43
1:A:362:ASP:CA	1:A:396:THR:HG23	2.44	0.43
1:D:523:ILE:CG2	1:D:538:GLN:HB2	2.49	0.43
1:C:459:LYS:O	1:C:460:ARG:HD3	2.18	0.43
1:D:521:GLU:OE1	1:D:521:GLU:CA	2.67	0.43
1:B:372:LEU:HD22	1:B:420:VAL:HG22	2.00	0.43
1:C:376:ARG:NH2	1:C:380:LYS:HB3	2.34	0.43
1:C:515:GLU:O	1:C:518:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:LYS:HE2	1:D:497:LYS:HB3	1.81	0.43
1:A:515:GLU:O	1:A:518:GLN:HG3	2.19	0.43
1:B:523:ILE:CG2	1:B:538:GLN:HB2	2.49	0.43
1:A:523:ILE:CG2	1:A:538:GLN:HB2	2.49	0.43
1:C:519:LYS:HZ3	1:C:521:GLU:HB2	1.83	0.42
1:C:468:ASN:N	1:C:503:PHE:O	2.51	0.42
1:D:362:ASP:HA	1:D:396:THR:HB	2.00	0.42
1:B:519:LYS:NZ	1:B:521:GLU:HB2	2.34	0.42
1:C:376:ARG:HD3	1:C:416:TYR:CE2	2.54	0.42
1:A:519:LYS:NZ	1:A:521:GLU:HB2	2.35	0.42
1:B:422:HIS:CG	1:B:423:PRO:HD2	2.53	0.42
1:A:452:GLU:HB2	1:A:460:ARG:NH2	2.33	0.42
1:C:467:GLN:O	1:C:468:ASN:HB2	2.19	0.42
1:D:361:VAL:CG1	1:D:362:ASP:N	2.83	0.42
1:C:453:TRP:HB2	1:D:446:TYR:OH	2.19	0.42
1:D:422:HIS:O	1:D:425:LEU:HB2	2.20	0.42
1:D:462:LEU:HD23	1:D:462:LEU:N	2.35	0.42
1:A:481:ASN:HD21	1:A:519:LYS:CG	2.24	0.42
1:C:531:ALA:O	1:C:535:GLN:HA	2.20	0.42
1:D:470:MET:HA	1:D:471:PRO:C	2.40	0.42
1:A:359:LEU:HD13	1:A:400:THR:HG22	2.01	0.42
1:A:367:LYS:O	1:A:422:HIS:CE1	2.73	0.42
1:A:480:HIS:HD2	1:A:521:GLU:O	2.03	0.42
1:A:392:GLN:HB2	1:A:394:ASN:OD1	2.20	0.41
1:A:453:TRP:CH2	1:B:444:GLU:HA	2.55	0.41
1:C:339:TYR:CD1	2:G:3:BMA:H3	2.55	0.41
1:C:417:GLN:HG3	1:C:431:ARG:O	2.21	0.41
1:C:470:MET:HA	1:C:471:PRO:O	2.20	0.41
1:D:376:ARG:HD3	1:D:416:TYR:CE2	2.56	0.41
1:A:421:THR:O	1:A:422:HIS:HB2	2.21	0.41
1:A:467:GLN:O	1:A:468:ASN:HB2	2.20	0.41
1:B:427:ARG:HA	1:B:427:ARG:HD3	1.95	0.41
1:D:480:HIS:HD2	1:D:521:GLU:O	2.04	0.41
1:A:453:TRP:CD2	1:B:444:GLU:HG2	2.56	0.41
1:B:539:ARG:HD3	1:C:427:ARG:HH22	1.85	0.41
1:C:497:LYS:HE2	1:C:497:LYS:HB3	1.88	0.41
1:D:531:ALA:O	1:D:535:GLN:HA	2.20	0.41
1:A:470:MET:HA	1:A:471:PRO:C	2.42	0.41
1:A:539:ARG:NH2	1:B:453:TRP:HZ3	2.19	0.41
1:C:362:ASP:CA	1:C:396:THR:HG23	2.50	0.41
1:A:459:LYS:O	1:A:460:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:NH1	1:A:543:VAL:CG1	2.84	0.40
1:A:519:LYS:HZ3	1:A:521:GLU:HB2	1.86	0.40
1:D:532:SER:HA	1:D:533:PRO:HA	1.70	0.40
1:B:520:ASP:O	1:B:542:SER:CB	2.70	0.40
1:C:460:ARG:HG3	1:C:543:VAL:HG13	2.03	0.40
1:A:359:LEU:CD1	1:A:400:THR:HG22	2.51	0.40
1:B:480:HIS:O	1:B:481:ASN:HB2	2.21	0.40
1:C:480:HIS:O	1:C:481:ASN:HB2	2.21	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	210/221 (95%)	200 (95%)	8 (4%)	2 (1%)	15	30
1	B	211/221 (96%)	198 (94%)	13 (6%)	0	100	100
1	C	212/221 (96%)	199 (94%)	11 (5%)	2 (1%)	17	33
1	D	211/221 (96%)	201 (95%)	9 (4%)	1 (0%)	29	50
All	All	844/884 (96%)	798 (94%)	41 (5%)	5 (1%)	25	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	PRO
1	C	423	PRO
1	D	426	PRO
1	C	426	PRO
1	A	454	PRO

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	188/194 (97%)	177 (94%)	11 (6%)	19	37
1	B	187/194 (96%)	180 (96%)	7 (4%)	34	58
1	C	189/194 (97%)	178 (94%)	11 (6%)	20	38
1	D	189/194 (97%)	176 (93%)	13 (7%)	15	30
All	All	753/776 (97%)	711 (94%)	42 (6%)	21	40

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	SER
1	A	369	THR
1	A	425	LEU
1	A	436	THR
1	A	477	GLN
1	A	483	VAL
1	A	491	SER
1	A	497	LYS
1	A	501	SER
1	A	505	VAL
1	A	518	GLN
1	B	344	SER
1	B	369	THR
1	B	477	GLN
1	B	483	VAL
1	B	491	SER
1	B	501	SER
1	B	505	VAL
1	C	335	CYS
1	C	344	SER
1	C	369	THR
1	C	436	THR
1	C	477	GLN
1	C	483	VAL

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Mol	Chain	Res	Type
1	C	491	SER
1	C	497	LYS
1	C	501	SER
1	C	505	VAL
1	C	518	GLN
1	D	334	ARG
1	D	344	SER
1	D	369	THR
1	D	425	LEU
1	D	436	THR
1	D	437	SER
1	D	477	GLN
1	D	483	VAL
1	D	491	SER
1	D	497	LYS
1	D	501	SER
1	D	505	VAL
1	D	518	GLN

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

Mol	Chain	Res	Type
1	A	422	HIS
1	A	481	ASN
1	B	481	ASN
1	B	490	HIS
1	C	481	ASN
1	C	518	GLN
1	D	422	HIS
1	D	424	HIS
1	D	481	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)

19 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
2	NAG	E	1	1,2	14,14,15	0.52	0	17,19,21	1.52	2 (11%)
2	NAG	E	2	2	14,14,15	0.45	0	17,19,21	1.13	1 (5%)
2	BMA	E	3	2	11,11,12	1.33	1 (9%)	15,15,17	1.40	1 (6%)
2	MAN	E	4	2	11,11,12	0.54	0	15,15,17	1.15	2 (13%)
2	MAN	E	5	2	11,11,12	0.52	0	15,15,17	1.57	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.53	0	17,19,21	1.14	2 (11%)
2	NAG	F	2	2	14,14,15	0.48	0	17,19,21	1.39	2 (11%)
2	BMA	F	3	2	11,11,12	1.06	0	15,15,17	1.53	3 (20%)
2	MAN	F	4	2	11,11,12	0.59	0	15,15,17	1.03	1 (6%)
2	MAN	F	5	2	11,11,12	0.67	0	15,15,17	1.32	3 (20%)
2	NAG	G	1	1,2	14,14,15	0.49	0	17,19,21	0.85	0
2	NAG	G	2	2	14,14,15	0.50	0	17,19,21	1.04	1 (5%)
2	BMA	G	3	2	11,11,12	1.28	1 (9%)	15,15,17	1.41	2 (13%)
2	MAN	G	4	2	11,11,12	0.59	0	15,15,17	1.26	2 (13%)
2	MAN	G	5	2	11,11,12	0.66	0	15,15,17	0.94	0
3	NAG	H	1	1,3	14,14,15	0.62	0	17,19,21	0.91	1 (5%)
3	NAG	H	2	3	14,14,15	0.59	0	17,19,21	0.91	0
3	BMA	H	3	3	11,11,12	0.93	0	15,15,17	0.78	0
3	MAN	H	4	3	11,11,12	0.62	0	15,15,17	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	2/2/19/22	0/1/1/1
2	MAN	F	5	2	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	BMA	O3-C3	3.23	1.50	1.43
2	G	3	BMA	O3-C3	2.79	1.49	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	O3-C3-C2	4.51	118.63	109.99
2	E	5	MAN	C1-O5-C5	4.31	118.03	112.19
2	F	3	BMA	C1-C2-C3	4.19	114.81	109.67
2	G	3	BMA	O3-C3-C2	4.06	117.77	109.99
2	F	2	NAG	C1-O5-C5	3.93	117.51	112.19
2	E	2	NAG	O5-C5-C6	3.79	113.14	107.20
2	E	1	NAG	C2-N2-C7	-3.77	117.53	122.90
2	E	5	MAN	C1-C2-C3	3.45	113.91	109.67
2	E	1	NAG	C1-O5-C5	3.35	116.73	112.19
2	E	4	MAN	O5-C1-C2	-3.04	106.07	110.77
2	F	1	NAG	O5-C1-C2	-3.02	106.52	111.29
2	G	4	MAN	O5-C5-C6	2.77	111.55	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	NAG	C2-N2-C7	-2.52	119.31	122.90
2	G	4	MAN	O5-C1-C2	-2.52	106.89	110.77
2	F	5	MAN	O5-C5-C6	2.46	111.07	107.20
2	F	5	MAN	C2-C3-C4	-2.45	106.66	110.89
2	F	1	NAG	C2-N2-C7	-2.43	119.44	122.90
2	F	4	MAN	C1-O5-C5	2.37	115.40	112.19
2	F	2	NAG	C2-N2-C7	-2.34	119.58	122.90
2	E	4	MAN	O5-C5-C6	2.18	110.62	107.20
2	F	3	BMA	C2-C3-C4	2.05	114.44	110.89
2	F	5	MAN	C1-O5-C5	-2.04	109.43	112.19
3	H	1	NAG	O5-C1-C2	-2.03	108.09	111.29
2	G	3	BMA	O2-C2-C3	-2.03	106.08	110.14
2	F	3	BMA	O2-C2-C3	-2.01	106.12	110.14

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	5	MAN	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	F	4	MAN	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	F	5	MAN	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	5	MAN	C4-C5-C6-O6
2	G	4	MAN	C4-C5-C6-O6
2	F	4	MAN	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	BMA	1	0
2	E	3	BMA	1	0
2	F	3	BMA	1	0
2	E	5	MAN	1	0
2	F	4	MAN	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.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
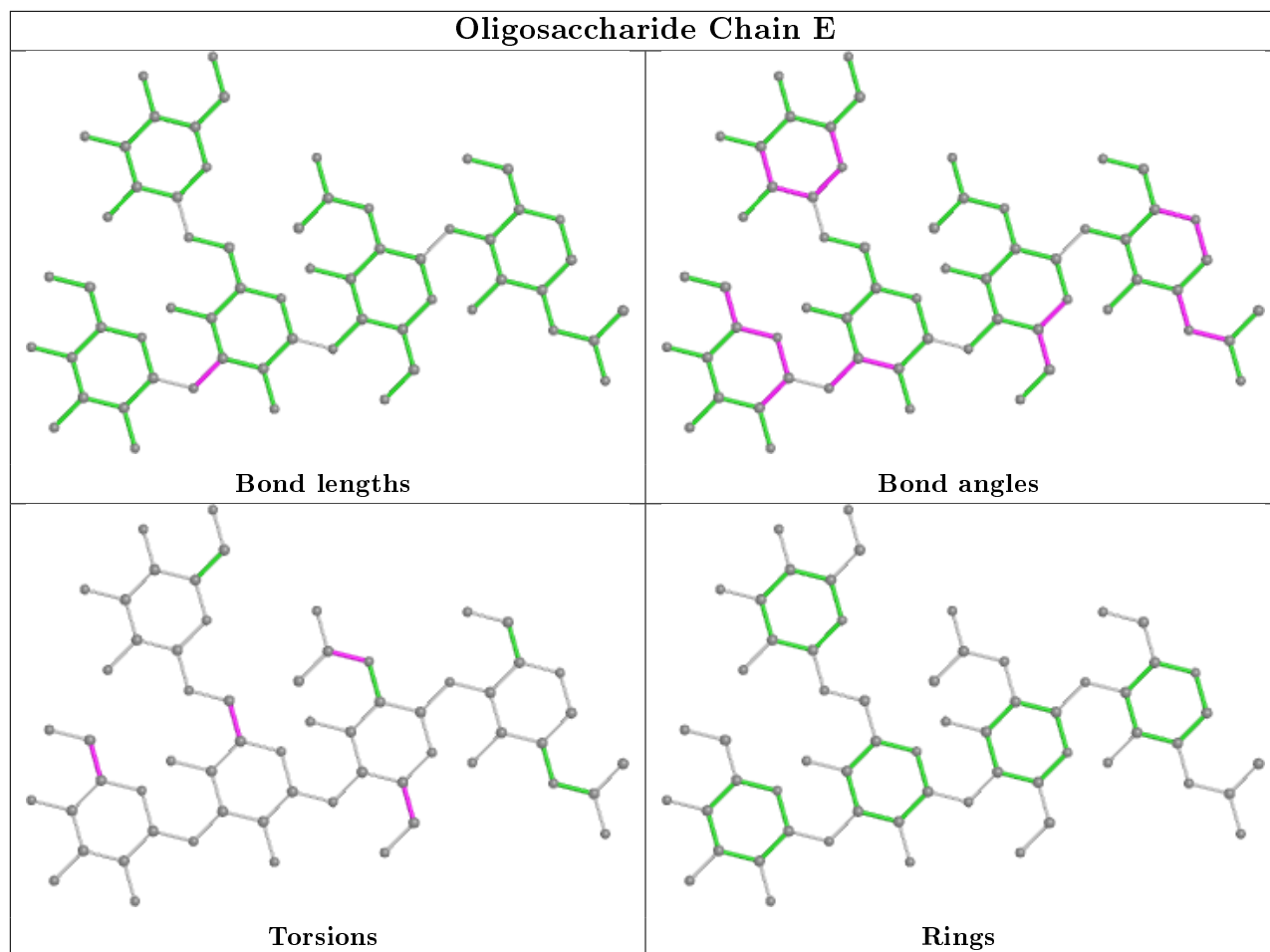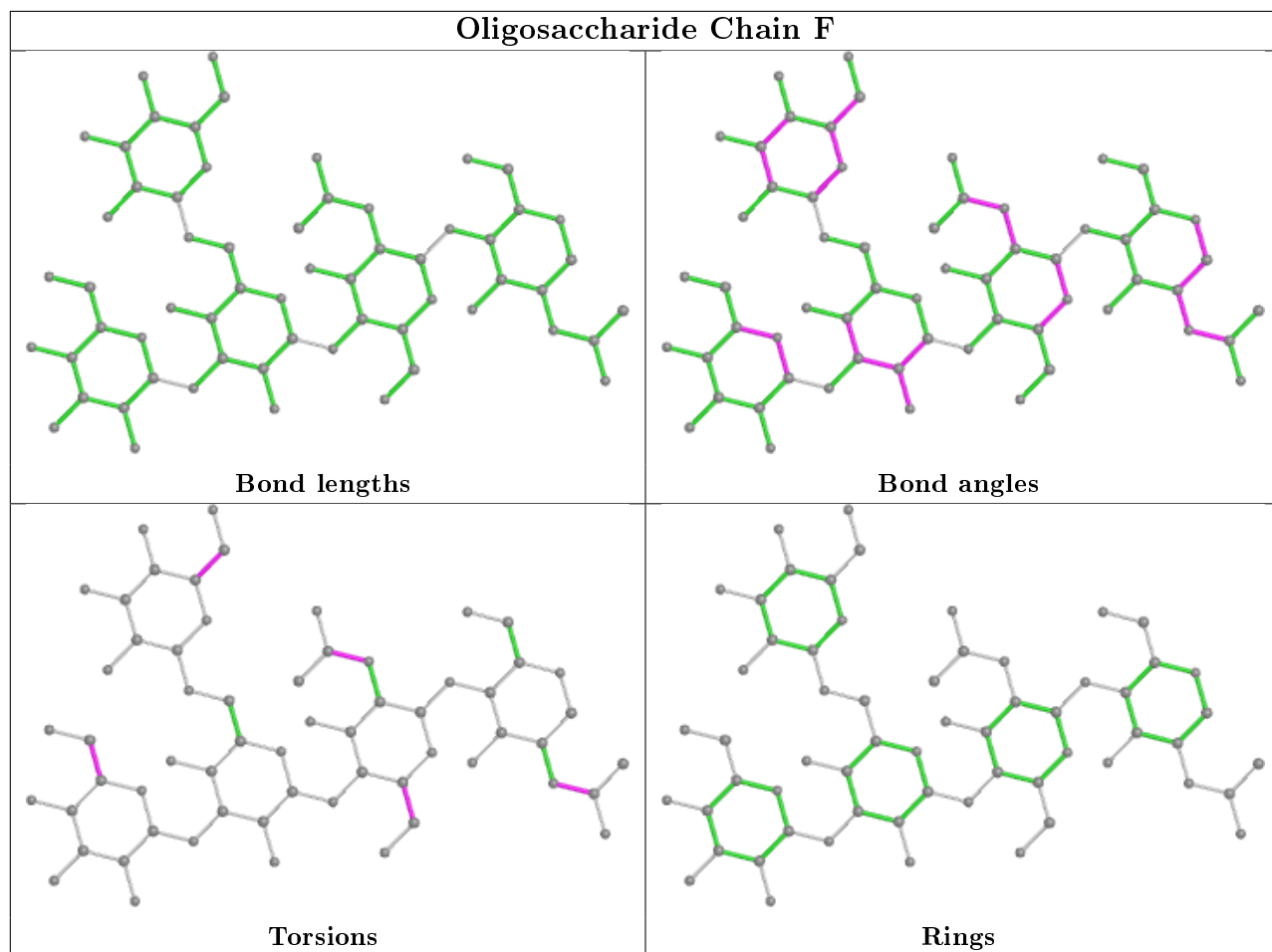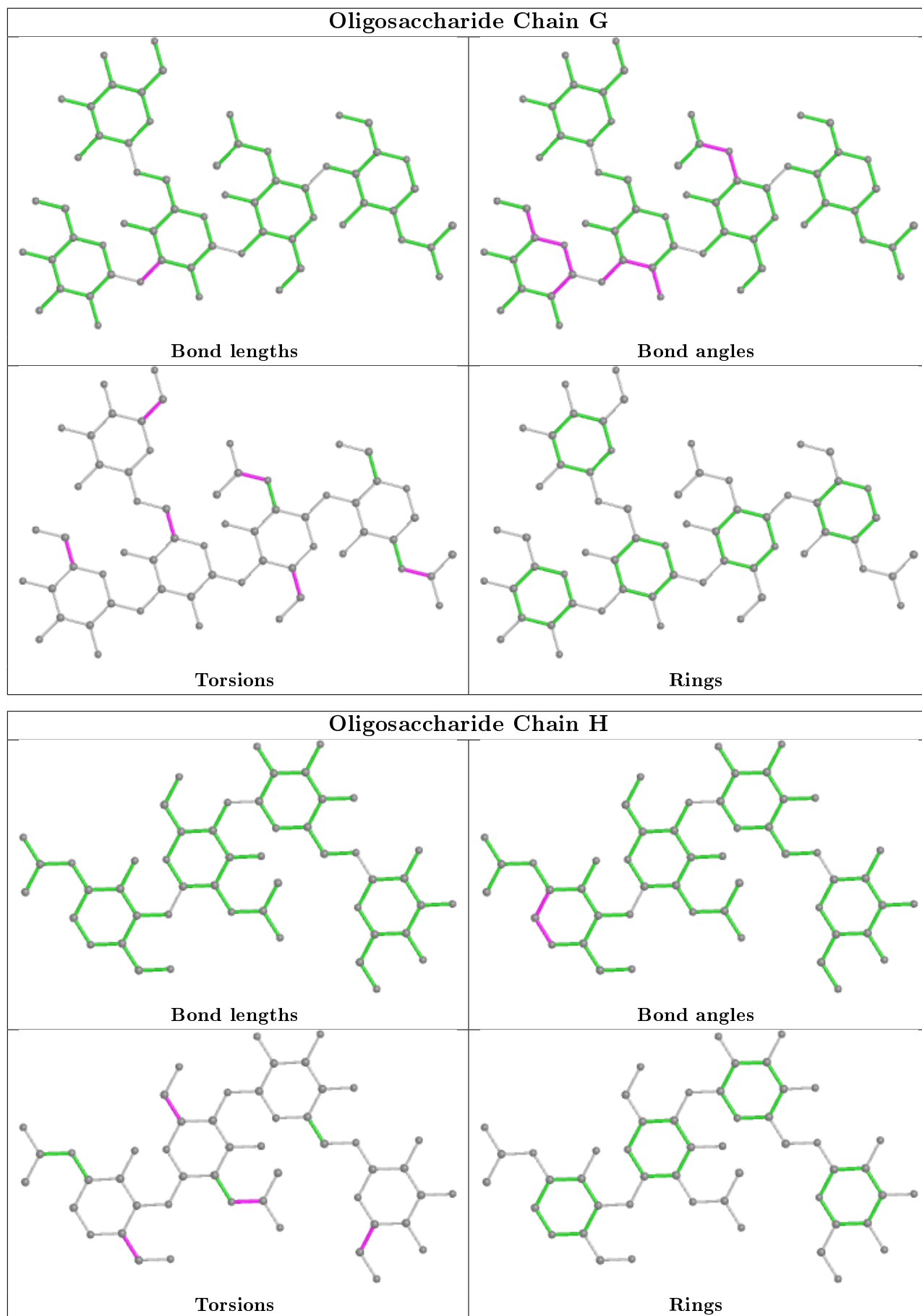
5.6 Ligand geometry (i)

There are no ligands in this entry.

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	212/221 (95%)	0.09	8 (3%)	40	34	25, 50, 110, 158	0
1	B	213/221 (96%)	0.14	8 (3%)	40	34	27, 51, 112, 157	0
1	C	214/221 (96%)	0.26	16 (7%)	14	10	26, 56, 127, 164	0
1	D	213/221 (96%)	0.05	5 (2%)	60	55	22, 50, 112, 157	0
All	All	852/884 (96%)	0.13	37 (4%)	35	29	22, 52, 115, 164	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	366	SER	8.8
1	B	334	ARG	6.6
1	B	366	SER	6.3
1	B	333	PRO	5.3
1	C	367	LYS	5.1
1	C	456	SER	4.4
1	C	422	HIS	3.7
1	A	457	ARG	3.3
1	A	393	ARG	3.1
1	A	427	ARG	3.1
1	B	336	VAL	2.9
1	C	332	ASN	2.9
1	C	365	PRO	2.8
1	C	412	GLU	2.7
1	A	426	PRO	2.7
1	A	424	HIS	2.7
1	D	333	PRO	2.6
1	A	455	GLY	2.6
1	C	396	THR	2.6
1	C	427	ARG	2.6
1	D	393	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	544	ASN	2.5
1	D	456	SER	2.4
1	B	368	GLY	2.4
1	C	333	PRO	2.4
1	A	396	THR	2.3
1	C	368	GLY	2.3
1	B	424	HIS	2.2
1	C	335	CYS	2.2
1	C	455	GLY	2.2
1	C	457	ARG	2.2
1	D	457	ARG	2.1
1	B	335	CYS	2.1
1	C	393	ARG	2.1
1	A	367	LYS	2.0
1	C	334	ARG	2.0
1	D	455	GLY	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
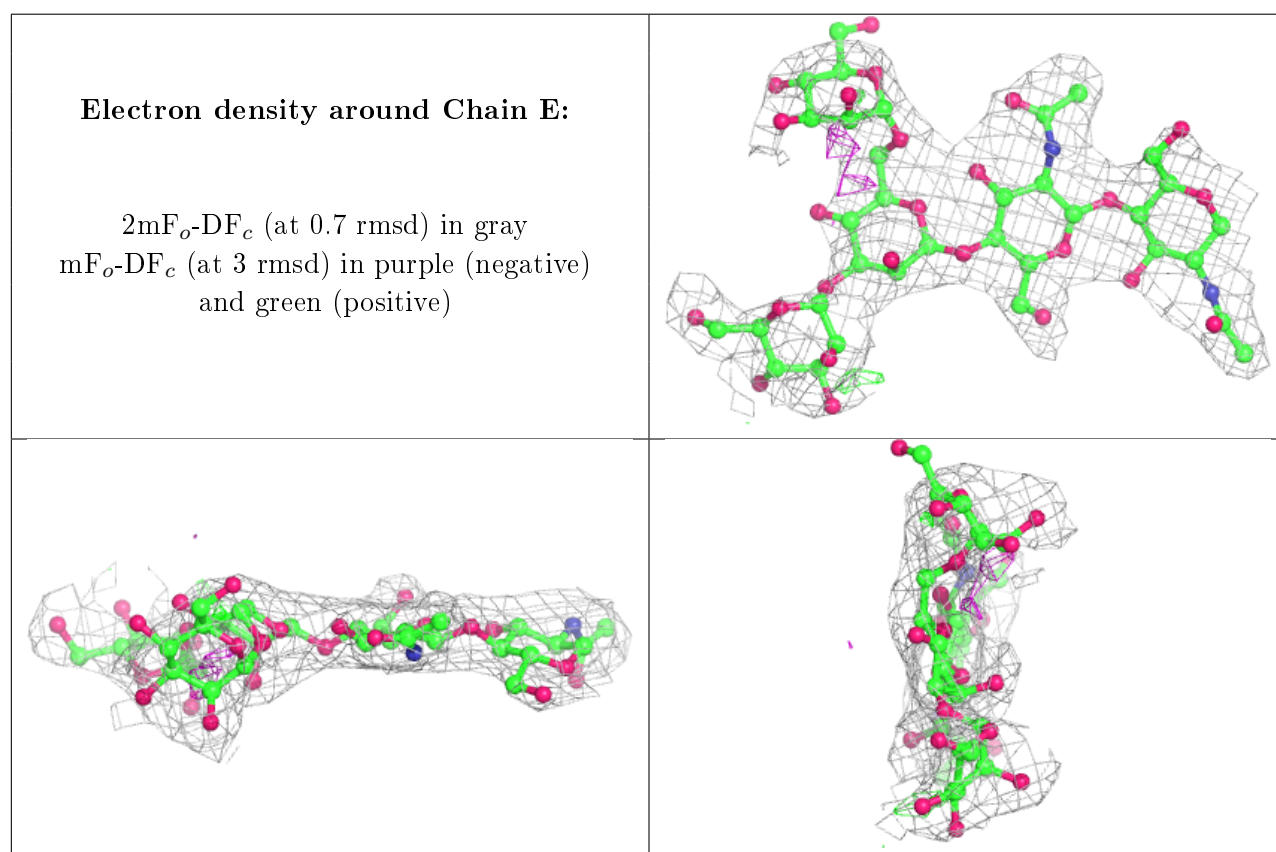
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	MAN	G	4	11/12	0.68	0.20	54,114,137,145	0
3	MAN	H	4	11/12	0.71	0.30	78,107,143,143	0
2	MAN	F	4	11/12	0.74	0.33	56,115,136,148	0
2	MAN	E	5	11/12	0.75	0.29	72,124,156,166	0
2	MAN	E	4	11/12	0.78	0.19	52,108,130,133	0
2	MAN	G	5	11/12	0.82	0.19	60,85,105,115	0
2	MAN	F	5	11/12	0.83	0.23	47,89,131,146	0
2	BMA	G	3	11/12	0.84	0.19	63,83,97,134	0
3	BMA	H	3	11/12	0.87	0.18	63,82,122,135	0
2	BMA	F	3	11/12	0.88	0.15	54,75,96,105	0
2	BMA	E	3	11/12	0.90	0.15	65,78,122,135	0
2	NAG	F	1	14/15	0.91	0.24	51,93,120,136	0

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| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	NAG	G	1	14/15	0.91	0.28	67,83,100,115	0
2	NAG	F	2	14/15	0.91	0.16	32,58,81,91	0
2	NAG	E	2	14/15	0.92	0.19	41,61,80,80	0
2	NAG	G	2	14/15	0.92	0.25	74,94,101,102	0
3	NAG	H	2	14/15	0.93	0.19	44,53,85,87	0
2	NAG	E	1	14/15	0.94	0.20	28,73,91,119	0
3	NAG	H	1	14/15	0.94	0.17	35,70,87,106	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 F:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
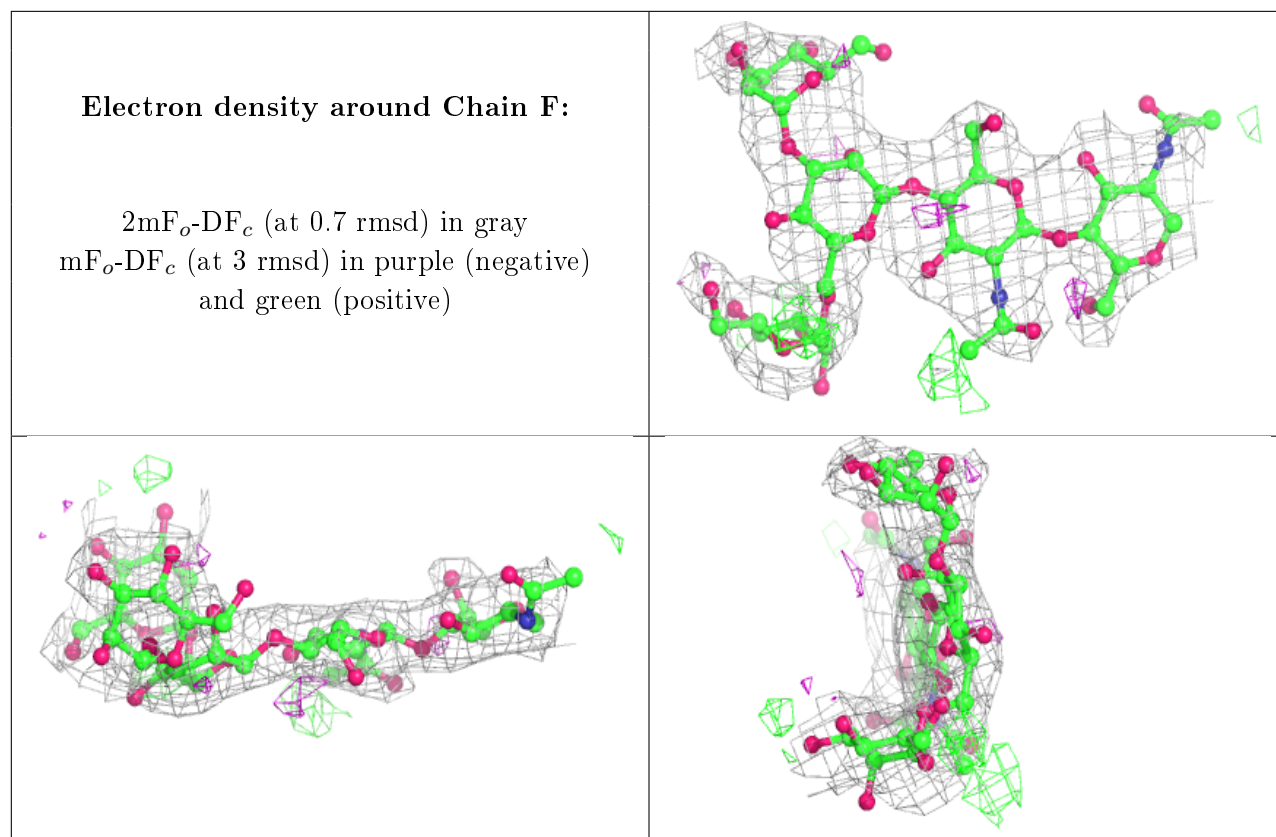
Electron density around Chain G:

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

Electron density around Chain H:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
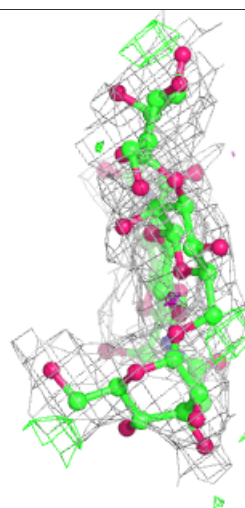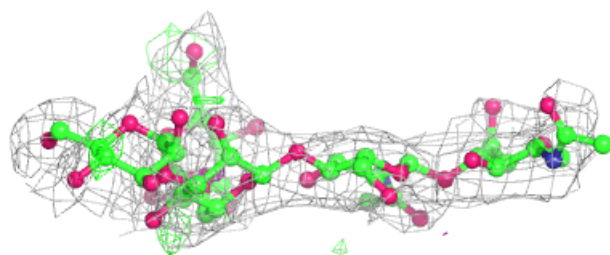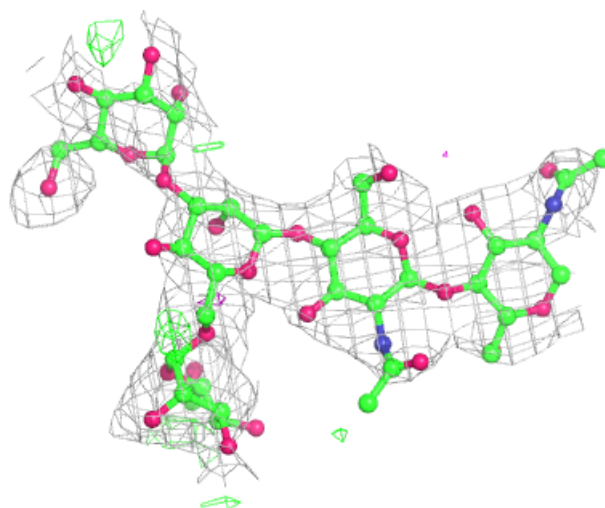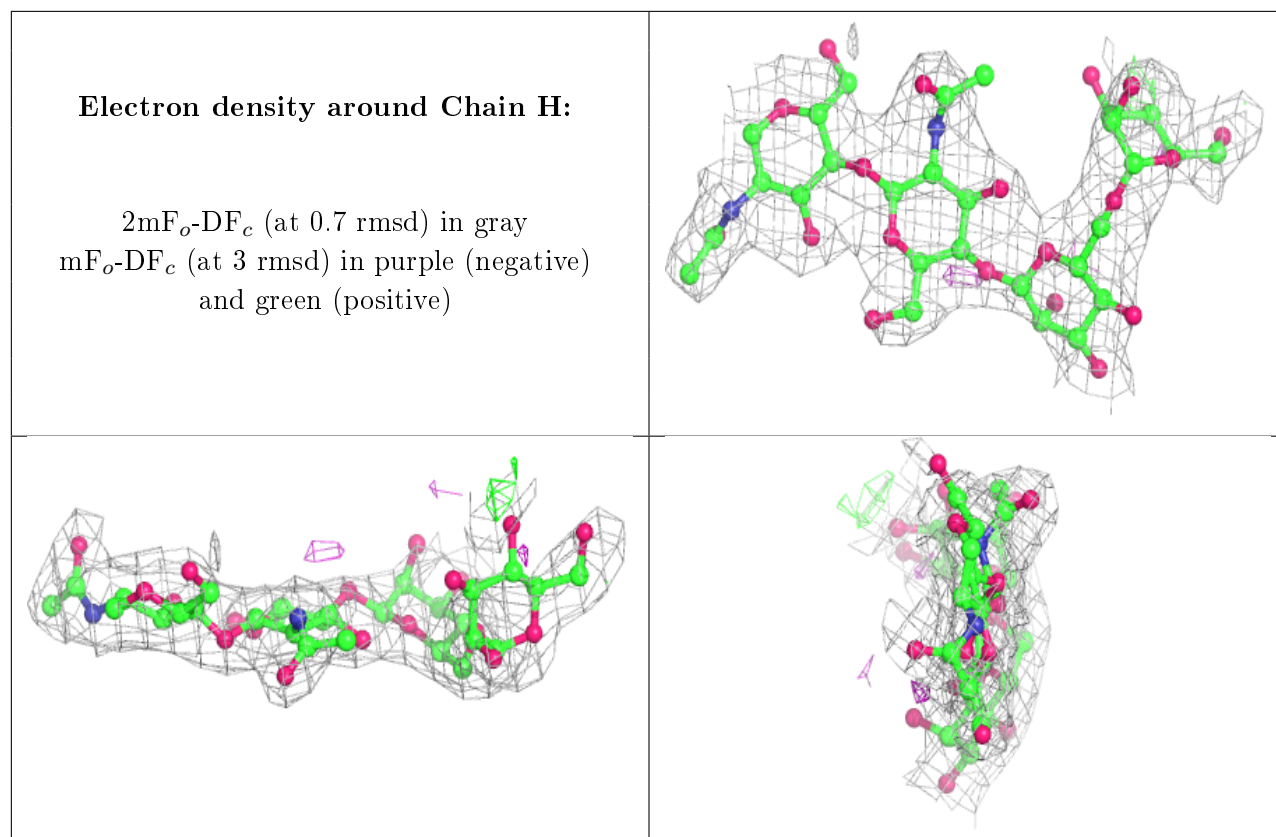
6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.