



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:38 PM UTC

PDB ID : 6YAX / pdb_00006yax
Title : Crystal structure of CD32b (Fc Gamma Receptor IIb) in complex with Human IgG1 Fab fragment (5C05)
Authors : Fisher, H.; Tews, I.; Orr, C.
Deposited on : 2020-03-14
Resolution : 2.80 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

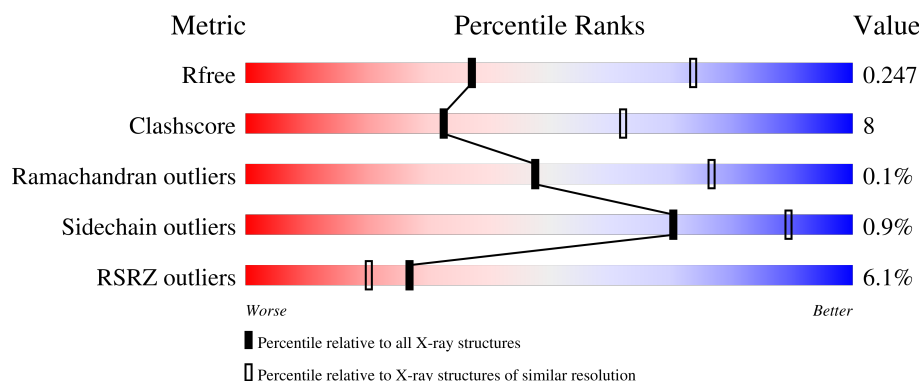
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



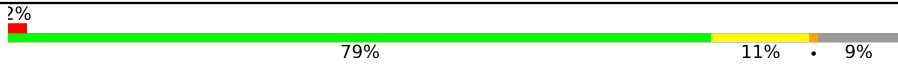
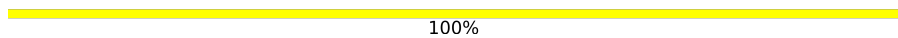
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	HHH	218	5% 78% 14% 6%
1	III	218	11% 62% 14% 23%
2	LLL	218	4% 84% 14% .
2	MMM	218	8% 67% 15% 17%
3	AAA	181	2% 78% 13% 9%

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Mol	Chain	Length	Quality of chain
3	BBB	181	 2% 79% 11% 9%
4	A	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	2	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16762 atoms, of which 8097 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 5C05 F(ab) heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HHH	204	Total	C	H	N	O	S	87	0	0
			3053	981	1509	257	300	6			
1	III	167	Total	C	H	N	O	S	79	0	0
			2441	790	1190	211	246	4			

- Molecule 2 is a protein called 5C05 F(ab) light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	MMM	182	Total	C	H	N	O	S	94	0	0
			2530	811	1225	218	272	4			
2	LLL	214	Total	C	H	N	O	S	100	0	0
			3096	983	1524	264	321	4			

- Molecule 3 is a protein called Low affinity immunoglobulin gamma Fc region receptor II-c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	AAA	165	Total	C	H	N	O	S	98	1	0
			2610	841	1285	232	248	4			
3	BBB	164	Total	C	H	N	O	S	97	2	0
			2595	836	1278	227	250	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	218	HIS	-	expression tag	UNP P31995
AAA	219	HIS	-	expression tag	UNP P31995
AAA	220	HIS	-	expression tag	UNP P31995
AAA	221	HIS	-	expression tag	UNP P31995
AAA	222	HIS	-	expression tag	UNP P31995
AAA	223	HIS	-	expression tag	UNP P31995
BBB	218	HIS	-	expression tag	UNP P31995
BBB	219	HIS	-	expression tag	UNP P31995

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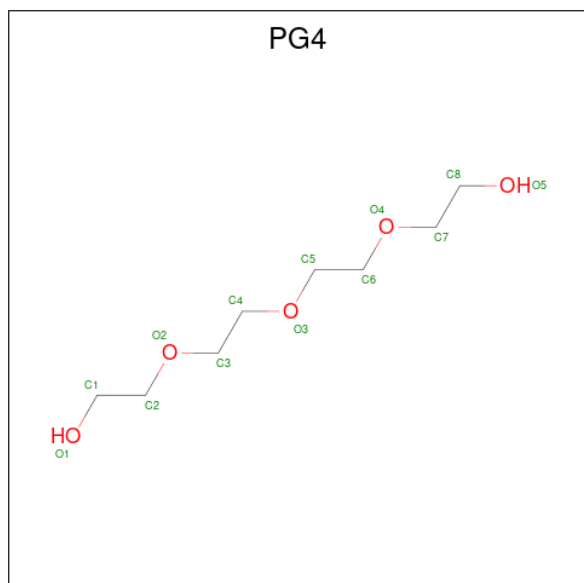
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	220	HIS	-	expression tag	UNP P31995
BBB	221	HIS	-	expression tag	UNP P31995
BBB	222	HIS	-	expression tag	UNP P31995
BBB	223	HIS	-	expression tag	UNP P31995

- 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	A	2	Total	C	H	N	O	5	0	0
			56	16	28	2	10			

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	HHH	1	Total	C	H	O	1	0
			31	8	18	5		
5	III	1	Total	C	H	O	1	0
			31	8	18	5		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	LLL	1	Total	C	H	O	2	0
			14	3	8	3		

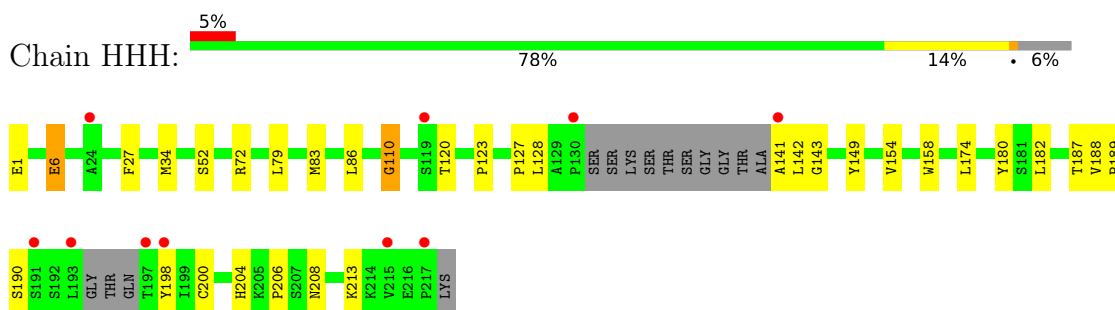
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	HHH	53	Total 53	O 53	0	0
8	MMM	34	Total 34	O 34	0	0
8	AAA	34	Total 34	O 34	0	0
8	LLL	40	Total 40	O 40	0	0
8	III	42	Total 42	O 42	0	0
8	BBB	74	Total 74	O 74	0	0

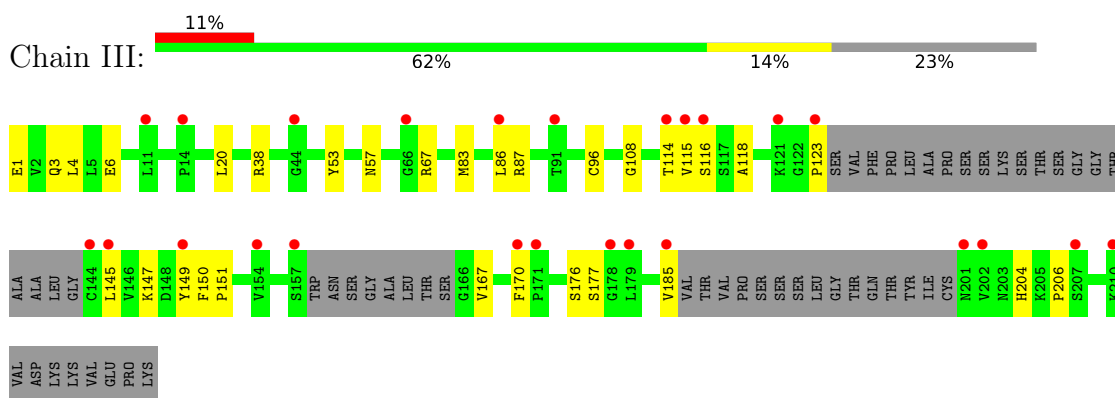
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

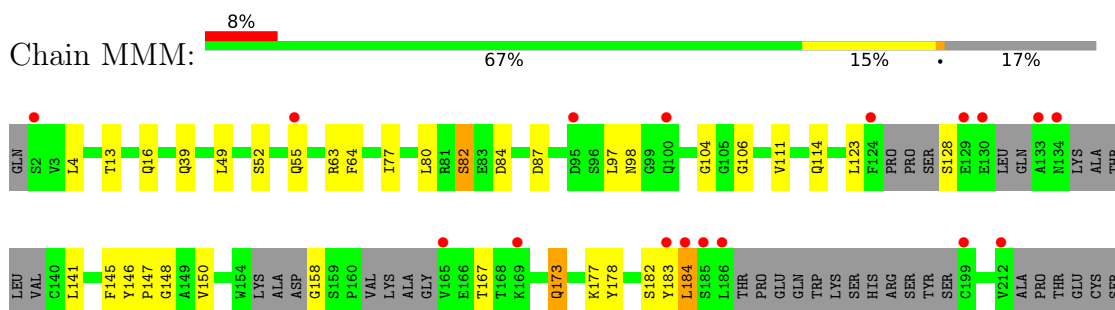
- Molecule 1: 5C05 F(ab) heavy chain



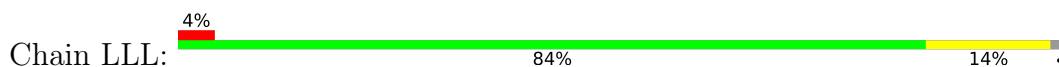
- Molecule 1: 5C05 F(ab) heavy chain

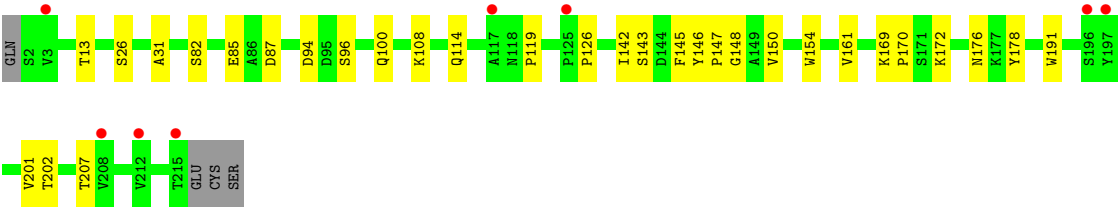


- Molecule 2: 5C05 F(ab) light chain

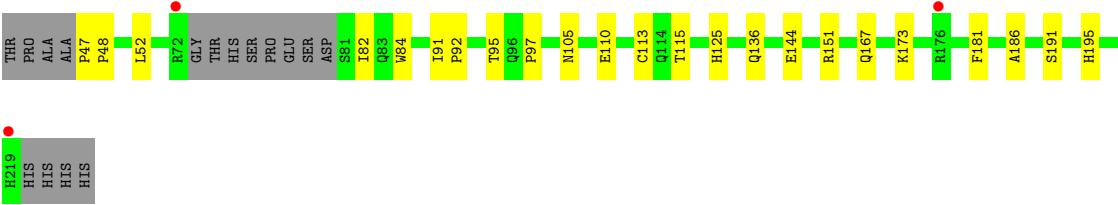
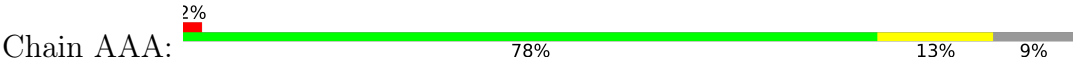


- Molecule 2: 5C05 F(ab) light chain

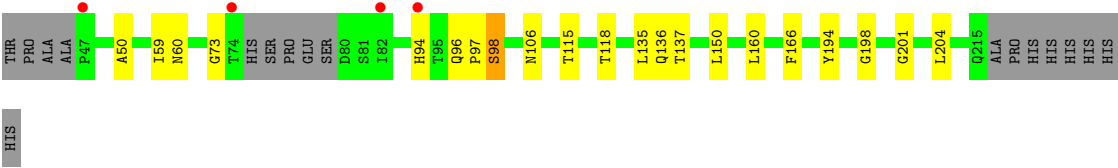
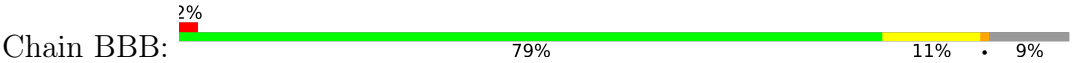




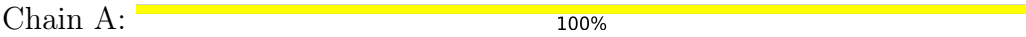
● Molecule 3: Low affinity immunoglobulin gamma Fc region receptor II-c



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● Molecule 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 43	Depositor
Cell constants a, b, c, α , β , γ	95.73Å 95.73Å 186.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.86 – 2.80 47.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.86-2.80) 99.6 (47.86-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.230 , 0.264 (Not available) , 0.247	Depositor DCC
R_{free} test set	1972 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 84.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16762	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: NAG, PG4, GOL

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	HHH	0.99	0/1581	1.28	1/2152 (0.0%)
1	III	1.11	4/1279 (0.3%)	1.30	0/1738
2	LLL	1.02	0/1611	1.32	1/2202 (0.0%)
2	MMM	1.04	0/1330	1.36	3/1814 (0.2%)
3	AAA	0.98	0/1368	1.24	2/1865 (0.1%)
3	BBB	0.96	0/1361	1.23	0/1855
All	All	1.01	4/8530 (0.0%)	1.29	7/11626 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	III	67	ARG	CZ-NH2	10.61	1.47	1.33
1	III	38	ARG	CZ-NH2	-7.86	1.23	1.33
1	III	67	ARG	CZ-NH1	7.02	1.42	1.32
1	III	67	ARG	CD-NE	6.84	1.55	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MMM	183	TYR	CA-C-N	6.05	131.24	122.16
2	MMM	183	TYR	C-N-CA	6.05	131.24	122.16
2	LLL	13	THR	CB-CA-C	5.52	117.06	108.61
2	MMM	106	GLY	CA-C-O	-5.45	118.47	122.23
3	AAA	105	ASN	CA-C-N	5.25	127.83	120.28
3	AAA	105	ASN	C-N-CA	5.25	127.83	120.28
1	HHH	110	GLY	CA-C-O	-5.00	118.24	122.29

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	HHH	1544	1509	1504	25	1
1	III	1251	1190	1170	19	0
2	LLL	1572	1524	1514	27	0
2	MMM	1305	1225	1196	30	0
3	AAA	1325	1285	1273	14	1
3	BBB	1317	1278	1268	16	0
4	A	28	28	25	0	0
5	HHH	13	18	18	0	0
5	III	13	18	18	1	0
6	AAA	14	14	13	0	0
7	LLL	6	8	8	0	0
8	AAA	34	0	0	1	1
8	BBB	74	0	0	1	1
8	HHH	53	0	0	0	0
8	III	42	0	0	1	0
8	LLL	40	0	0	2	0
8	MMM	34	0	0	2	0
All	All	8665	8097	8007	129	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (129) 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:HHH:188:VAL:HB	1:HHH:189:PRO:HD2	1.34	1.06
2:MMM:82:SER:HA	2:MMM:111:VAL:HG21	1.61	0.80
1:HHH:188:VAL:HB	1:HHH:189:PRO:CD	2.12	0.80
2:LLL:172:LYS:HD3	2:LLL:178:TYR:CZ	2.17	0.79
2:LLL:87:ASP:OD1	2:LLL:108:LYS:HG2	1.88	0.74
1:III:83:MET:HB3	1:III:86:LEU:HD21	1.69	0.73
2:LLL:114:GLN:HE22	2:LLL:176:ASN:ND2	1.85	0.72
2:MMM:184:LEU:H	2:MMM:184:LEU:HD12	1.55	0.72
3:BBB:96:GLN:HB3	3:BBB:97:PRO:HD2	1.72	0.72
3:BBB:73:GLY:HA3	3:BBB:115:THR:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MMM:173:GLN:HB2	2:MMM:177:LYS:O	1.91	0.70
2:LLL:94:ASP:OD2	2:LLL:96:SER:HB3	1.92	0.69
2:MMM:80:LEU:HD21	2:MMM:111:VAL:HG12	1.75	0.67
3:AAA:52:LEU:HD13	3:AAA:113:CYS:SG	2.34	0.67
3:AAA:136:GLN:OE1	3:AAA:151:ARG:NH1	2.27	0.67
3:AAA:47:PRO:HB2	3:AAA:48:PRO:HD2	1.76	0.67
3:BBB:115:THR:HG22	3:BBB:118:THR:HG22	1.77	0.66
2:LLL:114:GLN:HE22	2:LLL:176:ASN:HD21	1.42	0.65
2:MMM:123:LEU:HD11	2:MMM:184:LEU:HD23	1.80	0.64
1:HHH:182:LEU:C	1:HHH:182:LEU:HD12	2.22	0.64
1:III:57:ASN:ND2	8:III:402:HOH:O	2.31	0.63
1:HHH:142:LEU:HD21	1:HHH:198:TYR:CD2	2.33	0.63
2:LLL:100:GLN:HG3	8:LLL:438:HOH:O	2.00	0.62
2:MMM:39:GLN:HB2	2:MMM:49:LEU:HD11	1.82	0.61
1:HHH:6:GLU:OE1	1:HHH:110:GLY:N	2.26	0.61
2:MMM:167:THR:HG22	2:MMM:182:SER:CB	2.31	0.60
1:III:204:HIS:CD2	1:III:206:PRO:HD2	2.36	0.60
2:MMM:173:GLN:CB	2:MMM:177:LYS:O	2.49	0.60
2:LLL:142:ILE:HG22	2:LLL:145:PHE:CE1	2.37	0.59
5:III:301:PG4:H22	3:BBB:201:GLY:HA2	1.83	0.59
1:III:87:ARG:O	1:III:115:VAL:HG11	2.01	0.59
1:HHH:127:PRO:HD3	1:HHH:213:LYS:HE2	1.85	0.58
2:MMM:148:GLY:HA3	2:MMM:178:TYR:CD2	2.38	0.58
2:MMM:158:GLY:HA2	8:MMM:323:HOH:O	2.03	0.58
3:BBB:115:THR:HG22	3:BBB:118:THR:CG2	2.34	0.57
1:HHH:188:VAL:HG21	1:HHH:198:TYR:CE2	2.39	0.57
2:MMM:63:ARG:NH2	2:MMM:84:ASP:OD2	2.34	0.57
2:MMM:141:LEU:HD22	1:III:170:PHE:CE1	2.39	0.57
3:BBB:115:THR:CG2	3:BBB:118:THR:HG22	2.35	0.56
3:AAA:82:ILE:HD12	3:AAA:115:THR:HG22	1.87	0.56
2:LLL:85:GLU:OE1	2:LLL:172:LYS:NZ	2.30	0.56
3:AAA:82:ILE:CD1	3:AAA:115:THR:HG22	2.37	0.55
2:MMM:145:PHE:CE1	2:MMM:150:VAL:HG23	2.43	0.54
2:LLL:148:GLY:HA3	2:LLL:178:TYR:CG	2.43	0.53
2:MMM:167:THR:HG22	2:MMM:182:SER:HB2	1.91	0.53
3:BBB:106:ASN:ND2	8:BBB:401:HOH:O	2.42	0.53
2:LLL:150:VAL:CG1	2:LLL:201:VAL:HG13	2.38	0.52
2:MMM:145:PHE:CE1	2:MMM:150:VAL:CG2	2.91	0.52
3:BBB:50:ALA:HB2	3:BBB:118:THR:HG21	1.92	0.52
1:III:167:VAL:CB	1:III:185:VAL:O	2.58	0.52
2:LLL:154:TRP:HB2	2:LLL:161:VAL:CG2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:III:1:GLU:OE1	1:III:3:GLN:NE2	2.43	0.51
1:HHH:188:VAL:HG21	1:HHH:198:TYR:CZ	2.45	0.51
3:BBB:94[B]:HIS:NE2	3:BBB:98:SER:O	2.44	0.50
1:HHH:188:VAL:CB	1:HHH:189:PRO:HD2	2.25	0.49
2:MMM:114:GLN:HB2	2:MMM:146:TYR:CE2	2.47	0.49
1:III:167:VAL:CB	1:III:185:VAL:C	2.86	0.48
2:MMM:13:THR:HB	2:MMM:16:GLN:HG2	1.96	0.48
1:III:6:GLU:OE2	1:III:108:GLY:HA3	2.14	0.48
3:AAA:82:ILE:N	3:AAA:95:THR:O	2.44	0.48
2:MMM:184:LEU:H	2:MMM:184:LEU:CD1	2.20	0.48
2:LLL:126:PRO:HD2	2:LLL:191:TRP:CZ2	2.49	0.47
2:MMM:64:PHE:CE2	2:MMM:77:ILE:HG12	2.48	0.47
1:HHH:52:SER:O	1:HHH:72:ARG:NH2	2.47	0.47
2:LLL:146:TYR:HA	2:LLL:147:PRO:C	2.38	0.47
2:MMM:82:SER:HA	2:MMM:111:VAL:CG2	2.38	0.47
2:MMM:52:SER:HB2	2:MMM:55:GLN:HG3	1.95	0.47
1:III:4:LEU:HB3	1:III:96:CYS:SG	2.55	0.47
1:HHH:34:MET:HB3	1:HHH:79:LEU:HD22	1.96	0.46
3:AAA:82:ILE:HG13	3:AAA:97:PRO:HA	1.97	0.46
3:BBB:166:PHE:O	3:BBB:194:TYR:HA	2.15	0.46
1:III:114:THR:HG21	1:III:151:PRO:HB3	1.96	0.46
2:LLL:94:ASP:HB3	2:LLL:100:GLN:HE21	1.80	0.46
2:LLL:126:PRO:HG2	2:LLL:191:TRP:CD2	2.51	0.46
1:HHH:142:LEU:C	1:HHH:142:LEU:HD12	2.41	0.46
3:BBB:60:ASN:OD1	3:BBB:136:GLN:HA	2.16	0.46
2:LLL:148:GLY:HA3	2:LLL:178:TYR:CD1	2.50	0.46
1:III:145:LEU:CD2	1:III:147:LYS:HB2	2.46	0.46
2:LLL:150:VAL:HG11	2:LLL:201:VAL:HG13	1.97	0.46
1:III:176:SER:O	1:III:177:SER:OG	2.28	0.46
2:MMM:13:THR:HB	2:MMM:16:GLN:CG	2.46	0.45
3:AAA:110:GLU:HG3	3:AAA:125:HIS:NE2	2.32	0.45
1:HHH:174:LEU:HD13	1:HHH:180:TYR:CZ	2.52	0.45
1:HHH:83:MET:HE3	1:HHH:86:LEU:HD11	1.98	0.45
3:AAA:52:LEU:HD11	3:AAA:84:TRP:CZ3	2.52	0.45
2:LLL:119:PRO:HB3	2:LLL:142:ILE:HG23	1.98	0.45
2:LLL:148:GLY:HA3	2:LLL:178:TYR:CD2	2.51	0.45
3:BBB:135:LEU:HD21	3:BBB:150:LEU:HD13	1.98	0.45
3:AAA:110:GLU:CG	3:AAA:125:HIS:NE2	2.80	0.44
1:III:116:SER:C	1:III:118:ALA:H	2.25	0.44
2:LLL:143:SER:HB2	8:LLL:413:HOH:O	2.18	0.44
2:LLL:82:SER:OG	2:LLL:114:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:141:ALA:N	1:HHH:187:THR:HA	2.33	0.44
1:III:53:TYR:CE2	3:BBB:204:LEU:HD13	2.52	0.43
3:BBB:96:GLN:HB3	3:BBB:97:PRO:CD	2.45	0.43
1:HHH:174:LEU:HD13	1:HHH:180:TYR:CE1	2.54	0.43
2:MMM:97:LEU:HB3	2:MMM:98:ASN:H	1.66	0.43
1:HHH:128:LEU:N	1:HHH:143:GLY:O	2.42	0.43
2:LLL:148:GLY:CA	2:LLL:178:TYR:CG	3.02	0.43
1:HHH:27:PHE:CD1	1:HHH:27:PHE:N	2.87	0.43
1:HHH:6:GLU:H	1:HHH:6:GLU:HG2	1.65	0.43
2:MMM:146:TYR:CD1	2:MMM:147:PRO:HA	2.53	0.43
1:III:20:LEU:HG	1:III:83:MET:HE2	2.00	0.42
1:III:123:PRO:HG3	1:III:149:TYR:HB3	1.99	0.42
3:AAA:167:GLN:NE2	3:AAA:191:SER:O	2.51	0.42
2:MMM:80:LEU:HD11	2:MMM:111:VAL:HG12	2.01	0.42
3:AAA:173:LYS:HE2	8:AAA:407:HOH:O	2.19	0.42
2:LLL:26:SER:O	2:LLL:31:ALA:HB2	2.19	0.42
2:MMM:4:LEU:O	2:MMM:104:GLY:HA2	2.19	0.42
2:MMM:146:TYR:CG	2:MMM:147:PRO:HA	2.55	0.42
2:MMM:87:ASP:OD2	8:MMM:301:HOH:O	2.22	0.42
1:III:86:LEU:HD23	1:III:86:LEU:HA	1.91	0.42
2:LLL:169:LYS:HA	2:LLL:170:PRO:HD3	1.94	0.41
1:HHH:120:THR:HG21	1:HHH:206:PRO:O	2.20	0.41
1:HHH:154:VAL:HG23	1:HHH:204:HIS:HB2	2.01	0.41
1:III:150:PHE:HA	1:III:151:PRO:HA	1.83	0.41
3:AAA:144:GLU:HA	3:AAA:186:ALA:O	2.21	0.41
3:BBB:59:ILE:HG12	3:BBB:137:THR:O	2.20	0.41
1:HHH:123:PRO:HB3	1:HHH:149:TYR:HB3	2.03	0.41
1:HHH:127:PRO:HG3	1:HHH:213:LYS:HG3	2.02	0.41
1:HHH:120:THR:HG21	1:HHH:206:PRO:C	2.46	0.41
2:MMM:80:LEU:HD11	2:MMM:111:VAL:CG1	2.51	0.41
1:HHH:158:TRP:CZ3	1:HHH:200:CYS:HB3	2.57	0.40
2:LLL:154:TRP:HB2	2:LLL:161:VAL:HG22	2.04	0.40
2:LLL:202:THR:HA	2:LLL:207:THR:HA	2.02	0.40
3:BBB:160:LEU:HD11	3:BBB:198:GLY:HA3	2.04	0.40
2:MMM:145:PHE:CE1	2:MMM:150:VAL:HG21	2.56	0.40
2:LLL:145:PHE:CE2	2:LLL:150:VAL:HG23	2.56	0.40
3:AAA:91:ILE:HA	3:AAA:92:PRO:HD3	1.92	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:208:ASN:HD22	3:AAA:195:HIS:HD2[4_555]	1.19	0.41
8:AAA:433:HOH:O	8:BBB:466:HOH:O[1_655]	2.19	0.01

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	HHH	198/218 (91%)	188 (95%)	9 (4%)	1 (0%)	24	55
1	III	159/218 (73%)	147 (92%)	12 (8%)	0	100	100
2	LLL	212/218 (97%)	202 (95%)	10 (5%)	0	100	100
2	MMM	168/218 (77%)	155 (92%)	13 (8%)	0	100	100
3	AAA	162/181 (90%)	157 (97%)	5 (3%)	0	100	100
3	BBB	162/181 (90%)	155 (96%)	7 (4%)	0	100	100
All	All	1061/1234 (86%)	1004 (95%)	56 (5%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	HHH	190	SER

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	HHH	172/182 (94%)	170 (99%)	2 (1%)	63	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	III	132/182 (72%)	132 (100%)	0	100	100
2	LLL	174/181 (96%)	174 (100%)	0	100	100
2	MMM	139/181 (77%)	135 (97%)	4 (3%)	37	73
3	AAA	153/166 (92%)	152 (99%)	1 (1%)	76	91
3	BBB	153/166 (92%)	152 (99%)	1 (1%)	76	91
All	All	923/1058 (87%)	915 (99%)	8 (1%)	70	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	1	GLU
1	HHH	6	GLU
2	MMM	82	SER
2	MMM	128	SER
2	MMM	173	GLN
2	MMM	184	LEU
3	AAA	181	PHE
3	BBB	98	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

2 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	A	1	3,4	14,14,15	0.50	0	17,19,21	1.07	2 (11%)
4	NAG	A	2	4	14,14,15	0.63	0	17,19,21	2.37	3 (17%)

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	A	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	1/1/7/7	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	NAG	C1-O5-C5	6.67	121.13	112.19
4	A	2	NAG	C1-C2-N2	4.71	117.86	110.43
4	A	2	NAG	C2-N2-C7	3.97	128.22	122.90
4	A	1	NAG	C1-O5-C5	2.98	116.17	112.19
4	A	1	NAG	O4-C4-C5	2.01	114.27	109.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2	NAG	C1

All (3) torsion outliers are listed below:

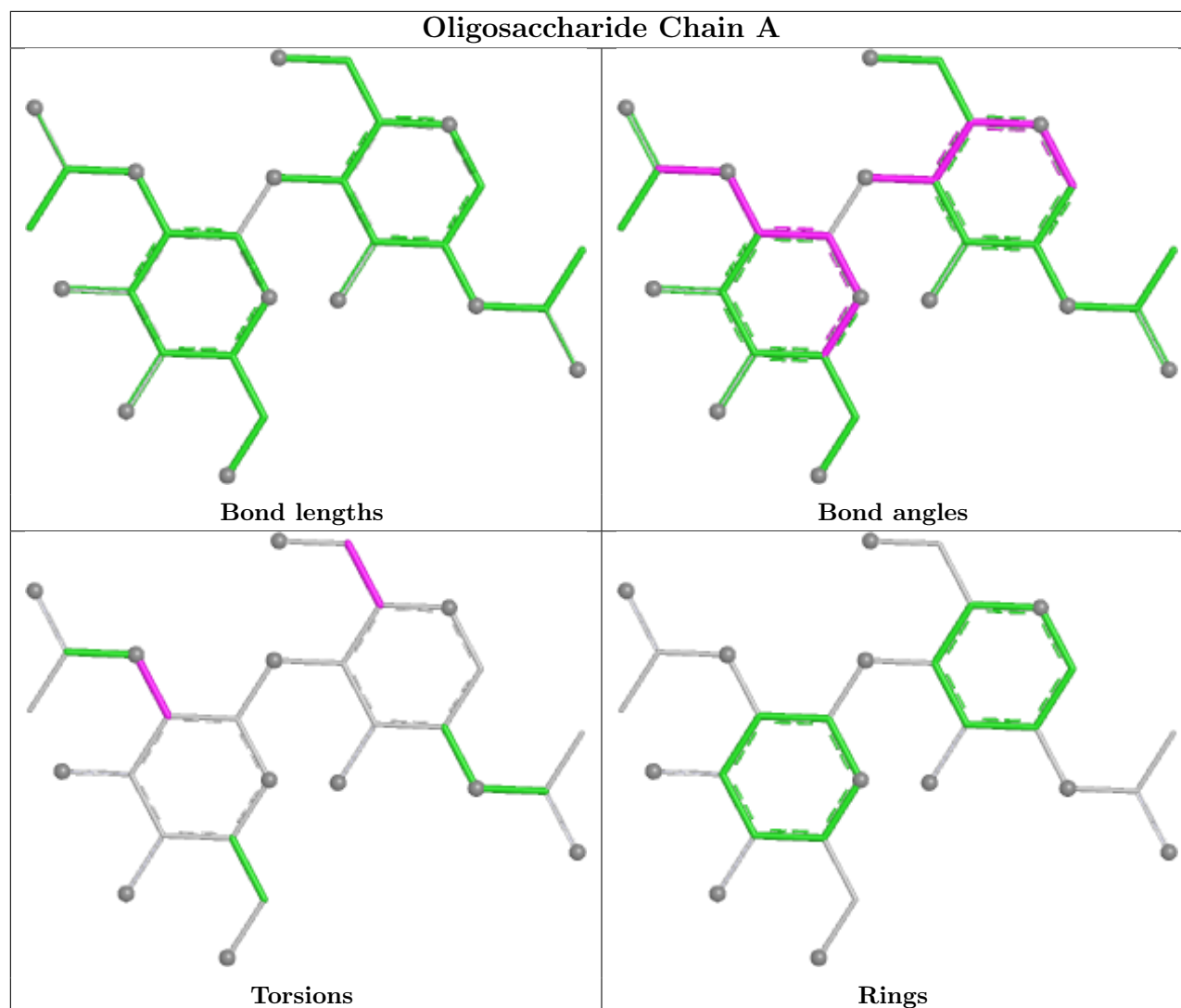
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C1-C2-N2-C7
4	A	1	NAG	C4-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6

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](#)

4 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	$\# Z > 2$
5	PG4	HHH	301	-	12,12,12	0.15	0	11,11,11	0.17	0
5	PG4	III	301	-	12,12,12	0.14	0	11,11,11	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	AAA	301	3	14,14,15	0.56	0	17,19,21	1.31	2 (11%)
7	GOL	LLL	301	-	5,5,5	0.11	0	5,5,5	0.33	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
5	PG4	HHH	301	-	-	6/10/10/10	-
5	PG4	III	301	-	-	5/10/10/10	-
6	NAG	AAA	301	3	-	0/6/23/26	0/1/1/1
7	GOL	LLL	301	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AAA	301	NAG	C1-C2-N2	-2.68	106.21	110.43
6	AAA	301	NAG	C1-O5-C5	2.17	115.09	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	HHH	301	PG4	O3-C5-C6-O4
5	III	301	PG4	O3-C5-C6-O4
5	HHH	301	PG4	O1-C1-C2-O2
5	III	301	PG4	O2-C3-C4-O3
5	HHH	301	PG4	O4-C7-C8-O5
5	III	301	PG4	C3-C4-O3-C5
5	HHH	301	PG4	C3-C4-O3-C5
5	III	301	PG4	O1-C1-C2-O2
5	HHH	301	PG4	C6-C5-O3-C4
5	III	301	PG4	C4-C3-O2-C2
5	HHH	301	PG4	O2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	III	301	PG4	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

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	HHH	204/218 (93%)	0.50	10 (4%) 35 27	50, 70, 107, 133	0
1	III	167/218 (76%)	0.88	25 (14%) 5 4	45, 75, 116, 124	0
2	LLL	214/218 (98%)	0.46	8 (3%) 45 36	47, 77, 103, 121	0
2	MMM	182/218 (83%)	0.92	17 (9%) 14 10	52, 85, 112, 139	0
3	AAA	165/181 (91%)	0.27	3 (1%) 67 58	41, 71, 104, 131	1 (0%)
3	BBB	164/181 (90%)	0.08	4 (2%) 59 49	30, 59, 90, 109	2 (1%)
All	All	1096/1234 (88%)	0.52	67 (6%) 27 20	30, 73, 107, 139	3 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	MMM	165	VAL	6.0
2	MMM	186	LEU	5.0
1	III	144	CYS	4.9
2	MMM	185	SER	4.4
1	III	201	ASN	4.3
1	III	157	SER	4.2
2	MMM	184	LEU	4.0
1	HHH	193	LEU	3.8
3	BBB	94[A]	HIS	3.8
1	III	210	LYS	3.7
3	AAA	176[A]	ARG	3.5
2	MMM	130	GLU	3.4
2	MMM	212	VAL	3.3
1	III	14	PRO	3.3
2	MMM	133	ALA	3.2
2	LLL	125	PRO	3.2
2	LLL	208	VAL	3.1
2	MMM	199	CYS	3.1
1	HHH	215	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	HHH	141	ALA	3.0
2	LLL	215	THR	3.0
2	LLL	3	VAL	3.0
2	MMM	55	GLN	2.9
1	III	202	VAL	2.9
2	MMM	124	PHE	2.9
3	AAA	72	ARG	2.8
3	BBB	74	THR	2.8
1	III	121	LYS	2.8
1	III	154	VAL	2.7
1	III	114	THR	2.7
1	III	115	VAL	2.7
2	LLL	196	SER	2.6
1	III	66	GLY	2.6
1	HHH	197	THR	2.6
1	III	179	LEU	2.6
1	HHH	217	PRO	2.5
1	HHH	24	ALA	2.4
2	MMM	183	TYR	2.4
2	LLL	197	TYR	2.4
1	III	11	LEU	2.4
1	III	123	PRO	2.4
1	III	116	SER	2.4
1	III	207	SER	2.4
3	BBB	47	PRO	2.4
1	III	44	GLY	2.3
1	HHH	119	SER	2.3
2	MMM	2	SER	2.3
1	HHH	130	PRO	2.3
2	MMM	134	ASN	2.3
1	III	178	GLY	2.3
1	III	86	LEU	2.3
1	III	185	VAL	2.3
2	LLL	117	ALA	2.2
1	HHH	198	TYR	2.2
2	MMM	95	ASP	2.2
1	III	171	PRO	2.2
1	III	91	THR	2.2
2	MMM	169	LYS	2.2
1	III	170	PHE	2.1
3	BBB	82	ILE	2.1
1	III	145	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	MMM	100	GLN	2.1
3	AAA	219	HIS	2.1
2	MMM	129	GLU	2.0
1	III	149	TYR	2.0
1	HHH	191	SER	2.0
2	LLL	212	VAL	2.0

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

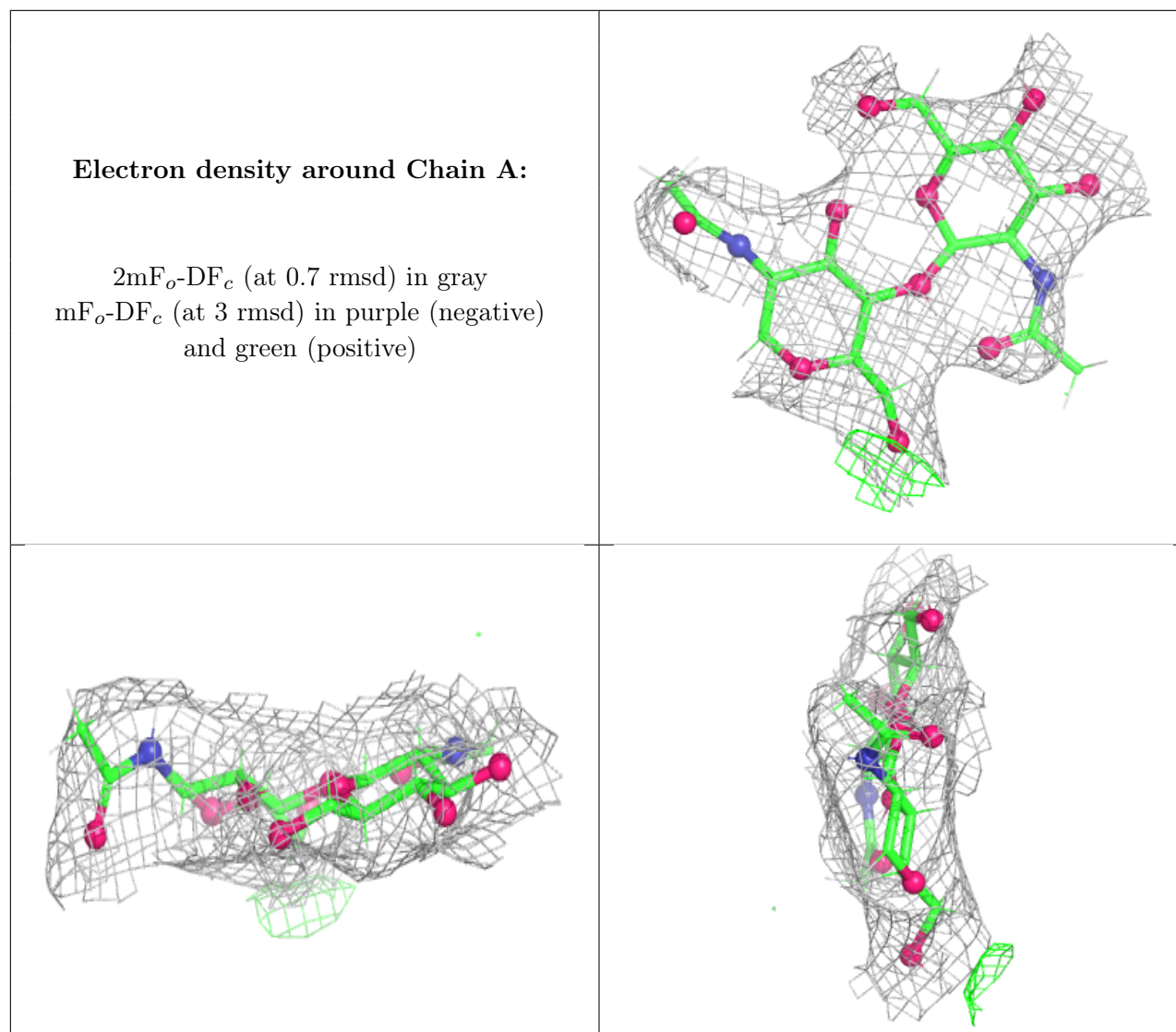
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	A	1	14/15	-	-	86,100,112,112	2
4	NAG	A	2	14/15	-	-	104,106,116,119	3

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(Å ²)	Q<0.9
6	NAG	AAA	301	14/15	0.66	0.15	105,108,112,113	3
7	GOL	LLL	301	6/6	0.90	0.12	69,75,81,81	2
5	PG4	III	301	13/13	0.91	0.17	63,71,79,79	1
5	PG4	HHH	301	13/13	0.93	0.14	69,73,83,83	1

6.5 Other polymers [i](#)

There are no such residues in this entry.