



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:08 AM UTC

PDB ID : 2NR6 / pdb_00002nr6
Title : Crystal structure of the complex of antibody and the allergen Bla g 2
Authors : Li, M.; Gustchina, A.; Wlodawer, A.; Pomes, A.; Wunschmann, S.
Deposited on : 2006-11-01
Resolution : 2.81 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

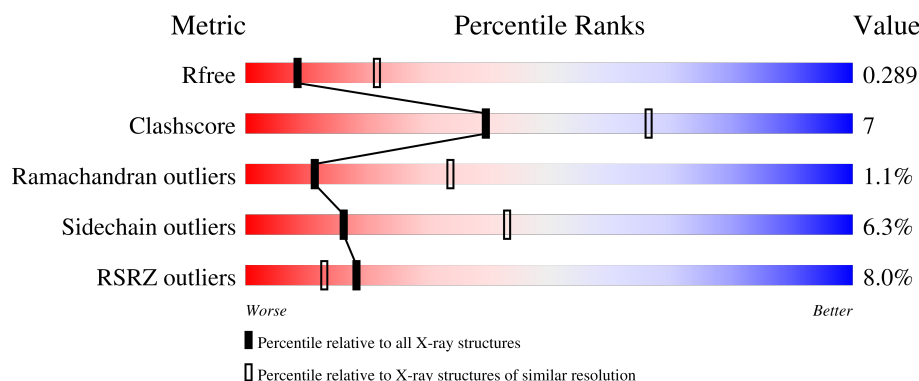
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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.



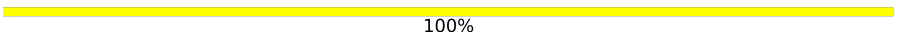
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	A	330	4% 85% 14% .
1	B	330	4% 82% 17% .
2	C	211	10% 83% 13% ..
2	E	211	10% 78% 20% .
3	D	213	18% 79% 17% ..

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Mol	Chain	Length	Quality of chain
3	F	213	 7% 77% 20%
4	G	2	 50% 50%
4	H	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11796 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 Aspartic protease Bla g 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2548	1626	419	491	12			
1	B	330	Total	C	N	O	S	0	0	0
			2548	1626	419	491	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P54958
A	-7	ALA	-	expression tag	UNP P54958
A	-6	SER	-	expression tag	UNP P54958
A	-5	ILE	-	expression tag	UNP P54958
A	98	GLN	ASN	engineered mutation	UNP P54958
B	-8	GLY	-	expression tag	UNP P54958
B	-7	ALA	-	expression tag	UNP P54958
B	-6	SER	-	expression tag	UNP P54958
B	-5	ILE	-	expression tag	UNP P54958
B	98	GLN	ASN	engineered mutation	UNP P54958

- Molecule 2 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1641	1025	276	333	7			
2	E	211	Total	C	N	O	S	0	0	0
			1641	1025	276	333	7			

- Molecule 3 is a protein called Antibody heavy chain.

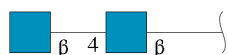
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	213	Total	C	N	O	S	0	0	0
			1611	1017	270	318	6			

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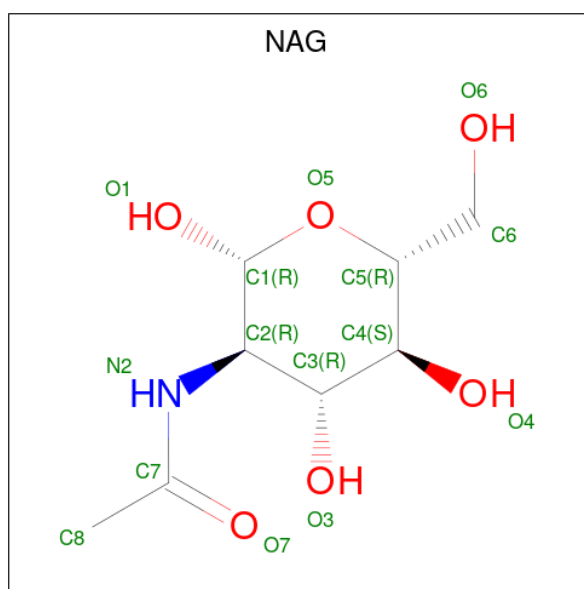
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	213	Total	C	N	O	S	0	0	0
			1611	1017	270	318	6			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Zn 1	0	0
6	B	1	Total 1	Zn 1	0	0

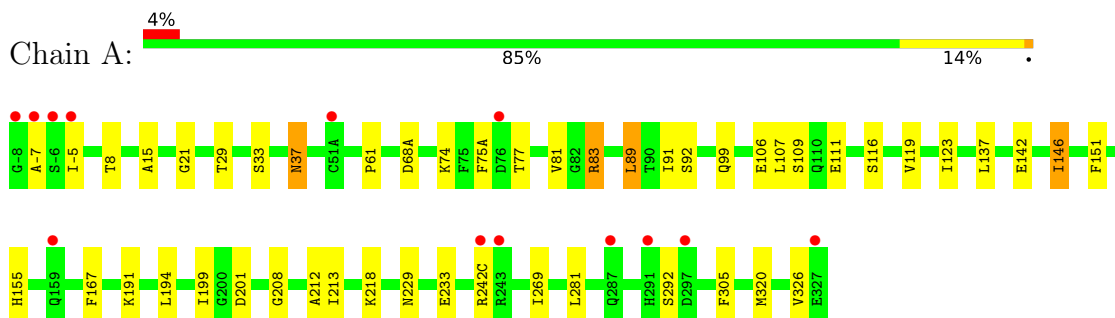
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total 32	O 32	0	0
7	B	26	Total 26	O 26	0	0
7	C	13	Total 13	O 13	0	0
7	D	19	Total 19	O 19	0	0
7	E	11	Total 11	O 11	0	0
7	F	9	Total 9	O 9	0	0

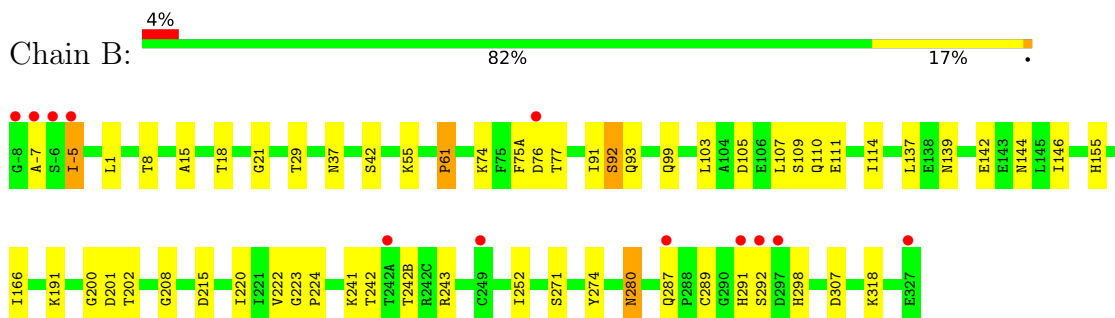
3 Residue-property plots [i](#)

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.

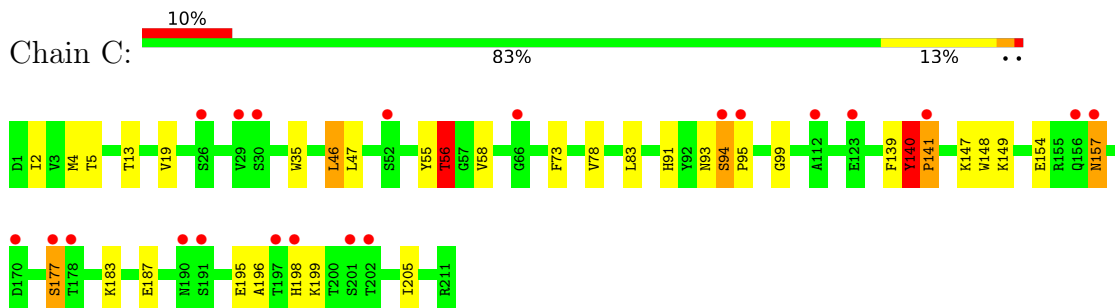
- Molecule 1: Aspartic protease Bla g 2



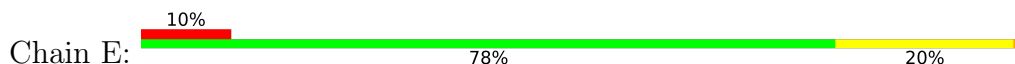
- Molecule 1: Aspartic protease Bla g 2

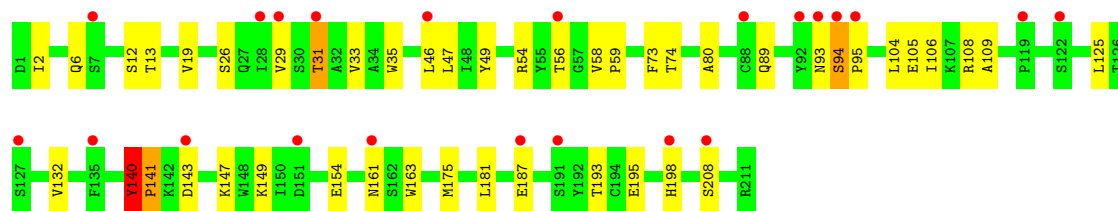


- Molecule 2: Antibody light chain

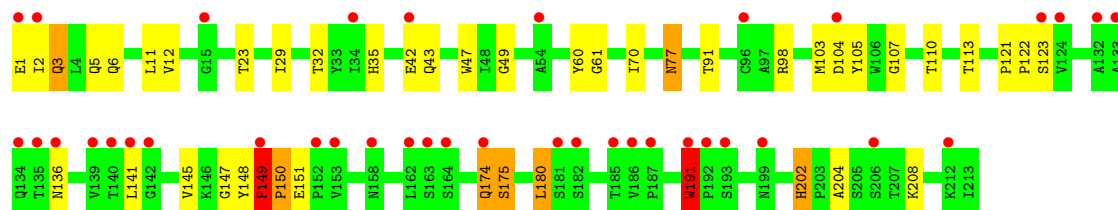
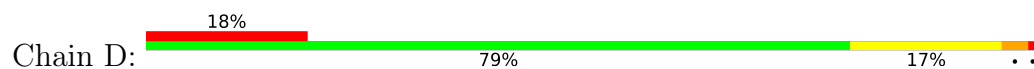


- Molecule 2: Antibody light chain

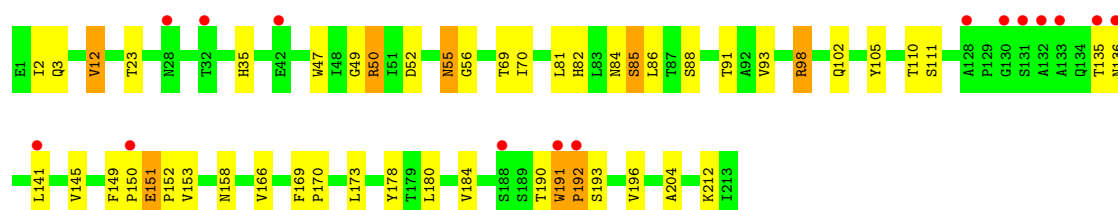
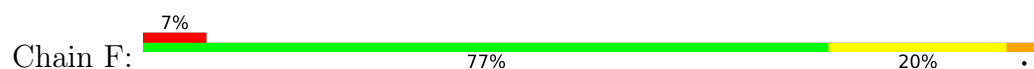




• Molecule 3: Antibody heavy chain



• Molecule 3: Antibody heavy chain



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



• 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.00Å 103.19Å 146.33Å 90.00° 94.83° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-2.81) 92.8 (50.00-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.232 , 0.281 0.246 , 0.289	Depositor DCC
R_{free} test set	2610 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.801	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11796	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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, ZN, CSX

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	0.77	7/2598 (0.3%)	0.76	4/3527 (0.1%)
1	B	0.80	9/2598 (0.3%)	0.79	3/3527 (0.1%)
2	C	0.43	0/1679	0.76	1/2278 (0.0%)
2	E	0.43	0/1679	0.80	3/2278 (0.1%)
3	D	0.49	0/1653	0.88	9/2262 (0.4%)
3	F	0.45	0/1653	0.77	2/2262 (0.1%)
All	All	0.62	16/11860 (0.1%)	0.79	22/16134 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	E	0	1
3	D	0	1
3	F	0	1
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	SER	C-N	16.01	1.55	1.33
1	A	146	ILE	C-N	15.30	1.56	1.33
1	B	208	GLY	C-N	14.18	1.53	1.33
1	A	292	SER	C-N	13.61	1.51	1.33
1	A	107	LEU	C-N	13.24	1.50	1.33
1	B	21	GLY	C-N	13.17	1.54	1.33
1	B	107	LEU	C-N	12.58	1.50	1.33
1	A	8	THR	C-N	12.52	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLY	C-N	12.05	1.50	1.33
1	B	8	THR	C-N	11.94	1.49	1.33
1	B	61	PRO	C-N	11.32	1.49	1.33
1	A	21	GLY	C-N	9.55	1.49	1.33
1	B	146	ILE	C-N	7.18	1.53	1.33
1	A	61	PRO	C-N	6.94	1.45	1.33
1	B	110	GLN	CD-OE1	5.48	1.33	1.23
1	B	252	ILE	CA-CB	5.31	1.56	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	149	PHE	N-CA-C	8.85	123.43	108.82
2	C	140	TYR	N-CA-C	8.09	122.51	108.75
2	E	140	TYR	N-CA-C	7.84	122.74	108.94
3	D	191	TRP	CA-C-N	-6.92	111.19	119.84
3	D	191	TRP	C-N-CA	-6.92	111.19	119.84
3	D	149	PHE	CA-C-N	6.85	128.41	119.84
3	D	149	PHE	C-N-CA	6.85	128.41	119.84
1	B	292	SER	CA-C-N	-6.82	111.74	122.65
1	B	292	SER	C-N-CA	-6.82	111.74	122.65
3	D	202	HIS	CA-C-N	6.56	126.06	119.24
3	D	202	HIS	C-N-CA	6.56	126.06	119.24
2	E	140	TYR	CA-C-N	6.11	127.47	119.84
2	E	140	TYR	C-N-CA	6.11	127.47	119.84
1	A	242(C)	ARG	N-CA-C	5.67	116.03	108.38
3	F	149	PHE	CA-C-N	-5.58	113.97	119.99
3	F	149	PHE	C-N-CA	-5.58	113.97	119.99
1	A	292	SER	CA-C-N	-5.53	113.81	122.65
1	A	292	SER	C-N-CA	-5.53	113.81	122.65
1	A	37	ASN	N-CA-C	5.52	116.65	108.86
1	B	292	SER	O-C-N	5.18	129.28	123.27
3	D	121	PRO	CA-C-N	5.01	124.18	118.97
3	D	121	PRO	C-N-CA	5.01	124.18	118.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	140	TYR	Peptide
3	D	149	PHE	Peptide
2	E	140	TYR	Peptide

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Mol	Chain	Res	Type	Group
3	F	191	TRP	Peptide

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	2548	0	2469	18	0
1	B	2548	0	2469	23	0
2	C	1641	0	1573	26	0
2	E	1641	0	1573	31	0
3	D	1611	0	1578	27	0
3	F	1611	0	1578	32	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	32	0	0	2	0
7	B	26	0	0	2	0
7	C	13	0	0	0	0
7	D	19	0	0	5	0
7	E	11	0	0	1	0
7	F	9	0	0	0	0
All	All	11796	0	11316	154	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 7.

All (154) 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)
3:F:191:TRP:CD1	3:F:192:PRO:HD3	1.70	1.26
2:E:94:SER:HB2	2:E:95:PRO:HD3	1.46	0.97
3:F:191:TRP:HD1	3:F:192:PRO:HD3	1.12	0.94
3:F:191:TRP:CD1	3:F:192:PRO:CD	2.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:PRO:HD2	2:C:198:HIS:CE1	2.09	0.88
2:E:141:PRO:HD2	2:E:198:HIS:CE1	2.09	0.86
2:E:147:LYS:HB2	2:E:195:GLU:HB3	1.55	0.86
3:F:191:TRP:HD1	3:F:192:PRO:CD	1.88	0.85
3:D:49:GLY:HA2	7:D:229:HOH:O	1.75	0.85
2:E:94:SER:HB2	2:E:95:PRO:CD	2.09	0.81
2:E:94:SER:CB	2:E:95:PRO:HD3	2.09	0.81
3:F:141:LEU:HD22	3:F:191:TRP:HZ3	1.47	0.80
3:D:35:HIS:HD2	3:D:47:TRP:HE1	1.32	0.76
2:C:141:PRO:CD	2:C:198:HIS:CE1	2.69	0.75
2:E:141:PRO:HD2	2:E:198:HIS:HE1	1.50	0.75
3:F:150:PRO:HG3	3:F:204:ALA:HB3	1.69	0.74
2:C:141:PRO:HD2	2:C:198:HIS:HE1	1.52	0.74
1:A:83:ARG:HD2	7:A:630:HOH:O	1.87	0.73
2:C:94:SER:OG	2:C:95:PRO:HD3	1.87	0.73
2:E:141:PRO:CD	2:E:198:HIS:CE1	2.71	0.73
1:A:320:MET:HE2	7:A:603:HOH:O	1.90	0.71
3:F:35:HIS:HD2	3:F:47:TRP:HE1	1.39	0.70
3:D:104:ASP:HB3	3:D:105:TYR:CD2	2.26	0.70
3:D:29:ILE:H	3:D:77:ASN:HD21	1.39	0.68
3:D:6:GLN:HE21	3:D:107:GLY:HA3	1.60	0.67
3:F:145:VAL:HB	3:F:180:LEU:HD23	1.79	0.64
2:E:94:SER:CB	2:E:95:PRO:CD	2.73	0.63
1:A:89:LEU:HD23	1:A:99:GLN:HG2	1.81	0.63
3:F:141:LEU:HD22	3:F:191:TRP:CZ3	2.31	0.62
3:D:35:HIS:CD2	3:D:47:TRP:HE1	2.17	0.60
3:D:61:GLY:N	7:D:229:HOH:O	2.34	0.60
2:C:140:TYR:CD1	2:C:140:TYR:O	2.55	0.59
2:E:141:PRO:HD3	2:E:198:HIS:HE2	1.68	0.59
2:E:108:ARG:HG2	2:E:109:ALA:N	2.18	0.58
3:D:42:GLU:O	3:D:43:GLN:HG2	2.02	0.58
2:E:141:PRO:HD3	2:E:198:HIS:NE2	2.21	0.56
3:F:93:VAL:HG22	3:F:111:SER:HB3	1.87	0.56
1:B:105:ASP:HA	7:B:620:HOH:O	2.05	0.56
3:F:173:LEU:HD12	3:F:178:TYR:CZ	2.41	0.56
3:D:47:TRP:CZ3	7:D:229:HOH:O	2.53	0.56
2:E:149:LYS:HA	2:E:154:GLU:HA	1.87	0.55
3:D:60:TYR:HA	7:D:229:HOH:O	2.07	0.55
3:D:150:PRO:HG2	3:D:204:ALA:CB	2.36	0.55
3:D:1:GLU:HG3	3:D:3:GLN:HE22	1.70	0.54
3:F:52:ASP:HB3	3:F:55:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:88:SER:O	3:F:91:THR:HG22	2.08	0.54
2:E:80:ALA:HA	2:E:106:ILE:HD11	1.89	0.54
1:B:280:ASN:C	1:B:280:ASN:HD22	2.15	0.54
1:B:242:THR:C	1:B:242(B):THR:H	2.13	0.54
1:B:1:LEU:HD23	1:B:166:ILE:HG21	1.89	0.54
3:F:141:LEU:HD13	3:F:191:TRP:CH2	2.43	0.53
2:C:141:PRO:HG3	2:C:199:LYS:HG2	1.89	0.53
3:D:191:TRP:CG	3:D:191:TRP:O	2.61	0.53
2:E:80:ALA:HA	2:E:106:ILE:CD1	2.39	0.53
3:F:141:LEU:HB2	3:F:184:VAL:HG13	1.91	0.53
1:A:33:SER:HA	1:A:123:ILE:HG13	1.91	0.52
2:C:94:SER:CB	2:C:95:PRO:HD3	2.38	0.52
3:D:174:GLN:O	3:D:175:SER:C	2.52	0.52
3:D:149:PHE:O	3:D:149:PHE:CD2	2.63	0.52
3:F:35:HIS:CD2	3:F:50:ARG:HB3	2.45	0.52
1:B:15:ALA:HA	1:B:29:THR:O	2.10	0.51
3:D:35:HIS:HD2	3:D:47:TRP:NE1	2.05	0.51
1:A:29:THR:HG23	1:A:119:VAL:HG12	1.93	0.51
3:D:32:THR:HG21	3:D:98:ARG:HG2	1.91	0.51
3:D:91:THR:HG23	3:D:113:THR:HA	1.93	0.51
2:C:139:PHE:HB2	2:C:198:HIS:CE1	2.46	0.50
2:E:49:TYR:CG	3:F:102:GLN:HG2	2.47	0.50
3:D:122:PRO:HA	3:D:148:TYR:HB3	1.93	0.50
2:E:141:PRO:CD	2:E:198:HIS:NE2	2.75	0.50
1:A:146:ILE:HD13	1:A:167:PHE:HB3	1.94	0.50
2:E:108:ARG:HG2	2:E:109:ALA:H	1.77	0.49
2:C:157:ASN:H	2:C:157:ASN:ND2	2.10	0.49
1:B:222:VAL:HG22	1:B:287:GLN:HB3	1.95	0.49
2:E:140:TYR:O	2:E:140:TYR:CD1	2.65	0.49
1:A:75(A):PHE:C	1:A:77:THR:H	2.21	0.49
2:C:147:LYS:HB2	2:C:195:GLU:HB3	1.95	0.49
3:D:150:PRO:CG	3:D:204:ALA:CB	2.91	0.49
3:D:150:PRO:HD2	3:D:202:HIS:NE2	2.27	0.49
3:F:69:THR:HB	3:F:82:HIS:HB3	1.95	0.49
1:B:75(A):PHE:HD2	1:B:111:GLU:HB3	1.78	0.48
2:E:163:TRP:CD1	2:E:175:MET:HB3	2.49	0.48
2:C:47:LEU:HA	2:C:58:VAL:HG21	1.95	0.48
2:C:141:PRO:HD3	2:C:198:HIS:NE2	2.28	0.48
3:F:12:VAL:HG11	3:F:86:LEU:HD12	1.96	0.48
1:A:15:ALA:HA	1:A:29:THR:O	2.14	0.47
1:A:109:SER:HB3	1:A:111:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:VAL:HA	2:E:89:GLN:O	2.15	0.47
2:E:13:THR:HG22	2:E:104:LEU:HD11	1.98	0.46
2:C:55:TYR:O	2:C:56:THR:C	2.58	0.46
1:B:75(A):PHE:C	1:B:77:THR:H	2.23	0.46
2:C:149:LYS:HA	2:C:154:GLU:HA	1.98	0.46
2:E:193:THR:HG23	2:E:208:SER:HB3	1.98	0.46
1:A:123:ILE:HD12	1:A:151:PHE:CE2	2.51	0.45
2:C:196:ALA:HB3	2:C:205:ILE:HB	1.98	0.45
2:C:141:PRO:HD3	2:C:198:HIS:CE1	2.52	0.45
3:F:191:TRP:O	3:F:193:SER:N	2.50	0.45
3:F:150:PRO:HG3	3:F:204:ALA:CB	2.43	0.45
3:F:151:GLU:N	3:F:152:PRO:CD	2.79	0.45
1:B:155:HIS:O	1:B:307:ASP:HA	2.17	0.45
2:E:35:TRP:CE2	2:E:73:PHE:HB2	2.52	0.45
3:F:141:LEU:CD2	3:F:191:TRP:CZ3	2.99	0.45
3:F:55:ASN:HD22	3:F:56:GLY:N	2.15	0.45
1:B:-5:ILE:HB	1:B:144:ASN:HD21	1.81	0.44
2:C:46:LEU:HD13	2:C:55:TYR:HB2	1.99	0.44
2:C:157:ASN:H	2:C:157:ASN:HD22	1.65	0.44
3:D:150:PRO:HG2	3:D:204:ALA:HB3	1.99	0.44
2:C:148:TRP:HE1	2:C:177:SER:HB3	1.82	0.44
2:E:35:TRP:CD2	2:E:73:PHE:HB2	2.53	0.44
2:E:47:LEU:HA	2:E:58:VAL:HG21	1.99	0.44
3:F:98:ARG:HD2	3:F:105:TYR:HB2	1.99	0.44
3:F:84:ASN:O	3:F:85:SER:C	2.61	0.43
1:B:291:HIS:CE1	7:B:623:HOH:O	2.72	0.43
1:B:42:SER:HB3	1:B:103:LEU:HG	2.00	0.43
1:B:109:SER:HB3	1:B:111:GLU:OE1	2.18	0.43
1:B:271:SER:HA	1:B:274:TYR:CE2	2.53	0.43
1:A:269:ILE:HD11	1:A:305:PHE:HD1	1.84	0.43
1:B:224:PRO:HA	1:B:289:CSX:O	2.19	0.43
2:E:58:VAL:HA	2:E:59:PRO:HD3	1.89	0.43
3:F:158:ASN:HD21	3:F:196:VAL:HA	1.84	0.42
1:B:99:GLN:OE1	1:B:139:ASN:ND2	2.49	0.42
3:F:35:HIS:CD2	3:F:47:TRP:HE1	2.26	0.42
1:A:229:ASN:O	1:A:233:GLU:HG2	2.19	0.42
1:B:191:LYS:HE2	1:B:298:HIS:CE1	2.54	0.42
1:B:223:GLY:O	1:B:289:CSX:N	2.53	0.42
2:E:54:ARG:NH1	7:E:221:HOH:O	2.50	0.42
1:B:18:THR:HG22	1:B:91:ILE:HG12	2.02	0.42
2:E:2:ILE:HD11	2:E:93:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:MET:O	2:C:99:GLY:HA2	2.19	0.42
1:B:242:THR:C	1:B:242(B):THR:N	2.78	0.41
2:E:12:SER:HA	2:E:105:GLU:O	2.20	0.41
3:D:49:GLY:CA	7:D:229:HOH:O	2.49	0.41
3:D:145:VAL:HB	3:D:180:LEU:HD23	2.02	0.41
1:A:81:VAL:HB	1:A:106:GLU:HB2	2.02	0.41
1:A:91:ILE:O	1:A:92:SER:C	2.64	0.41
2:C:35:TRP:CD2	2:C:73:PHE:HB2	2.55	0.41
1:B:61:PRO:O	2:E:31:THR:HG21	2.20	0.41
2:C:94:SER:OG	2:C:95:PRO:CD	2.64	0.41
3:D:60:TYR:HE1	3:D:70:ILE:HG13	1.85	0.41
2:C:13:THR:HG21	2:C:78:VAL:HG21	2.02	0.41
1:A:68(A):ASP:HA	2:C:91:HIS:HB2	2.02	0.41
3:D:122:PRO:O	3:D:123:SER:HB2	2.20	0.41
1:A:191:LYS:HG2	1:A:213:ILE:HB	2.03	0.41
1:B:76:ASP:OD2	1:B:215:ASP:OD2	2.39	0.41
3:F:166:VAL:HG22	3:F:184:VAL:HG23	2.02	0.41
1:B:91:ILE:O	1:B:92:SER:C	2.64	0.41
3:D:150:PRO:CG	3:D:204:ALA:HB3	2.51	0.41
2:E:140:TYR:O	2:E:140:TYR:CG	2.74	0.41
3:F:47:TRP:CZ2	3:F:49:GLY:HA2	2.56	0.41
2:C:2:ILE:HD13	2:C:93:ASN:HB2	2.02	0.41
2:C:140:TYR:O	2:C:140:TYR:CG	2.73	0.41
1:A:194:LEU:HD11	1:A:212:ALA:HB2	2.02	0.40
1:A:305:PHE:CD2	1:A:305:PHE:C	2.99	0.40
3:F:141:LEU:HD13	3:F:191:TRP:HH2	1.86	0.40
3:F:169:PHE:HA	3:F:170:PRO:HD3	1.98	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	327/330 (99%)	316 (97%)	9 (3%)	2 (1%)	21	48
1	B	327/330 (99%)	308 (94%)	16 (5%)	3 (1%)	14	38
2	C	209/211 (99%)	197 (94%)	9 (4%)	3 (1%)	9	27
2	E	209/211 (99%)	196 (94%)	11 (5%)	2 (1%)	12	36
3	D	211/213 (99%)	196 (93%)	11 (5%)	4 (2%)	6	20
3	F	211/213 (99%)	198 (94%)	11 (5%)	2 (1%)	14	38
All	All	1494/1508 (99%)	1411 (94%)	67 (4%)	16 (1%)	11	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	94	SER
2	E	94	SER
1	A	-7	ALA
1	B	92	SER
3	D	150	PRO
3	F	192	PRO
2	C	56	THR
3	D	147	GLY
2	E	141	PRO
3	F	85	SER
2	C	141	PRO
3	D	191	TRP
1	B	-7	ALA
1	A	326	VAL
1	B	200	GLY
3	D	175	SER

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	281/281 (100%)	268 (95%)	13 (5%)	24	56
1	B	281/281 (100%)	266 (95%)	15 (5%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	187/187 (100%)	178 (95%)	9 (5%)	23	54
2	E	187/187 (100%)	173 (92%)	14 (8%)	12	35
3	D	182/182 (100%)	167 (92%)	15 (8%)	10	31
3	F	182/182 (100%)	166 (91%)	16 (9%)	9	28
All	All	1300/1300 (100%)	1218 (94%)	82 (6%)	16	43

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	ILE
1	A	37	ASN
1	A	74	LYS
1	A	83	ARG
1	A	89	LEU
1	A	116	SER
1	A	137	LEU
1	A	142	GLU
1	A	155	HIS
1	A	199	ILE
1	A	201	ASP
1	A	218	LYS
1	A	281	LEU
1	B	-5	ILE
1	B	37	ASN
1	B	55	LYS
1	B	74	LYS
1	B	93	GLN
1	B	114	ILE
1	B	137	LEU
1	B	142	GLU
1	B	201	ASP
1	B	202	THR
1	B	220	ILE
1	B	241	LYS
1	B	243	ARG
1	B	280	ASN
1	B	318	LYS
2	C	5	THR
2	C	19	VAL
2	C	46	LEU
2	C	56	THR

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Mol	Chain	Res	Type
2	C	83	LEU
2	C	157	ASN
2	C	177	SER
2	C	183	LYS
2	C	187	GLU
3	D	2	ILE
3	D	3	GLN
3	D	5	GLN
3	D	11	LEU
3	D	12	VAL
3	D	23	THR
3	D	77	ASN
3	D	103	MET
3	D	110	THR
3	D	136	ASN
3	D	141	LEU
3	D	151	GLU
3	D	174	GLN
3	D	180	LEU
3	D	208	LYS
2	E	6	GLN
2	E	19	VAL
2	E	26	SER
2	E	29	VAL
2	E	31	THR
2	E	46	LEU
2	E	56	THR
2	E	74	THR
2	E	125	LEU
2	E	132	VAL
2	E	143	ASP
2	E	161	ASN
2	E	181	LEU
2	E	187	GLU
3	F	2	ILE
3	F	3	GLN
3	F	12	VAL
3	F	23	THR
3	F	50	ARG
3	F	55	ASN
3	F	70	ILE
3	F	81	LEU

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Mol	Chain	Res	Type
3	F	98	ARG
3	F	110	THR
3	F	135	THR
3	F	136	ASN
3	F	151	GLU
3	F	153	VAL
3	F	190	THR
3	F	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	13	GLN
1	A	26	ASN
1	A	52	ASN
1	A	98	GLN
1	A	211	GLN
1	A	229	ASN
1	A	232	ASN
1	A	278	ASN
1	A	298	HIS
1	B	72	GLN
1	B	144	ASN
1	B	159	GLN
1	B	211	GLN
1	B	229	ASN
1	B	232	ASN
1	B	266	ASN
1	B	280	ASN
1	B	291	HIS
2	C	27	GLN
2	C	79	GLN
2	C	198	HIS
3	D	3	GLN
3	D	6	GLN
3	D	28	ASN
3	D	35	HIS
3	D	77	ASN
3	D	84	ASN
3	D	136	ASN
2	E	89	GLN

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Mol	Chain	Res	Type
2	E	93	ASN
2	E	96	GLN
2	E	124	GLN
2	E	138	ASN
2	E	145	ASN
2	E	198	HIS
3	F	3	GLN
3	F	35	HIS
3	F	55	ASN
3	F	57	ASN
3	F	174	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSX	A	289	1	3,6,7	0.75	0	1,6,8	0.67	0
1	CSX	B	289	1	3,6,7	0.77	0	1,6,8	1.20	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
1	CSX	A	289	1	-	0/2/5/7	-
1	CSX	B	289	1	-	0/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	289	CSX	2	0

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	1	4,1	14,14,15	0.54	0	17,19,21	0.96	0
4	NAG	G	2	4	14,14,15	0.51	0	17,19,21	1.04	1 (5%)
4	NAG	H	1	4,1	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
4	NAG	H	2	4	14,14,15	0.59	0	17,19,21	0.77	1 (5%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C4-C3-C2	2.34	114.45	111.02
4	H	1	NAG	C1-O5-C5	2.08	114.97	112.19
4	H	2	NAG	O5-C5-C6	2.07	111.69	107.66

There are no chirality outliers.

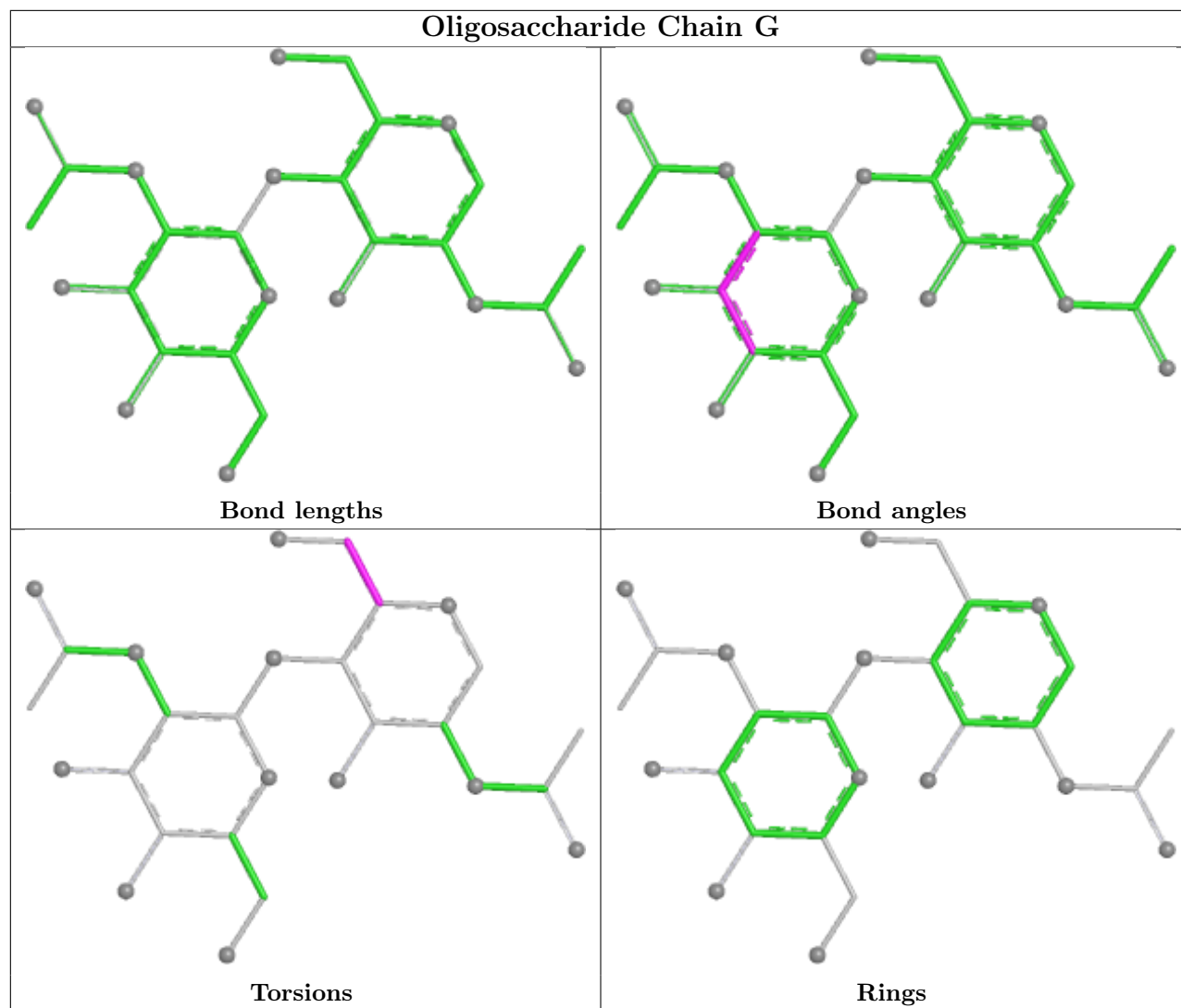
All (3) torsion outliers are listed below:

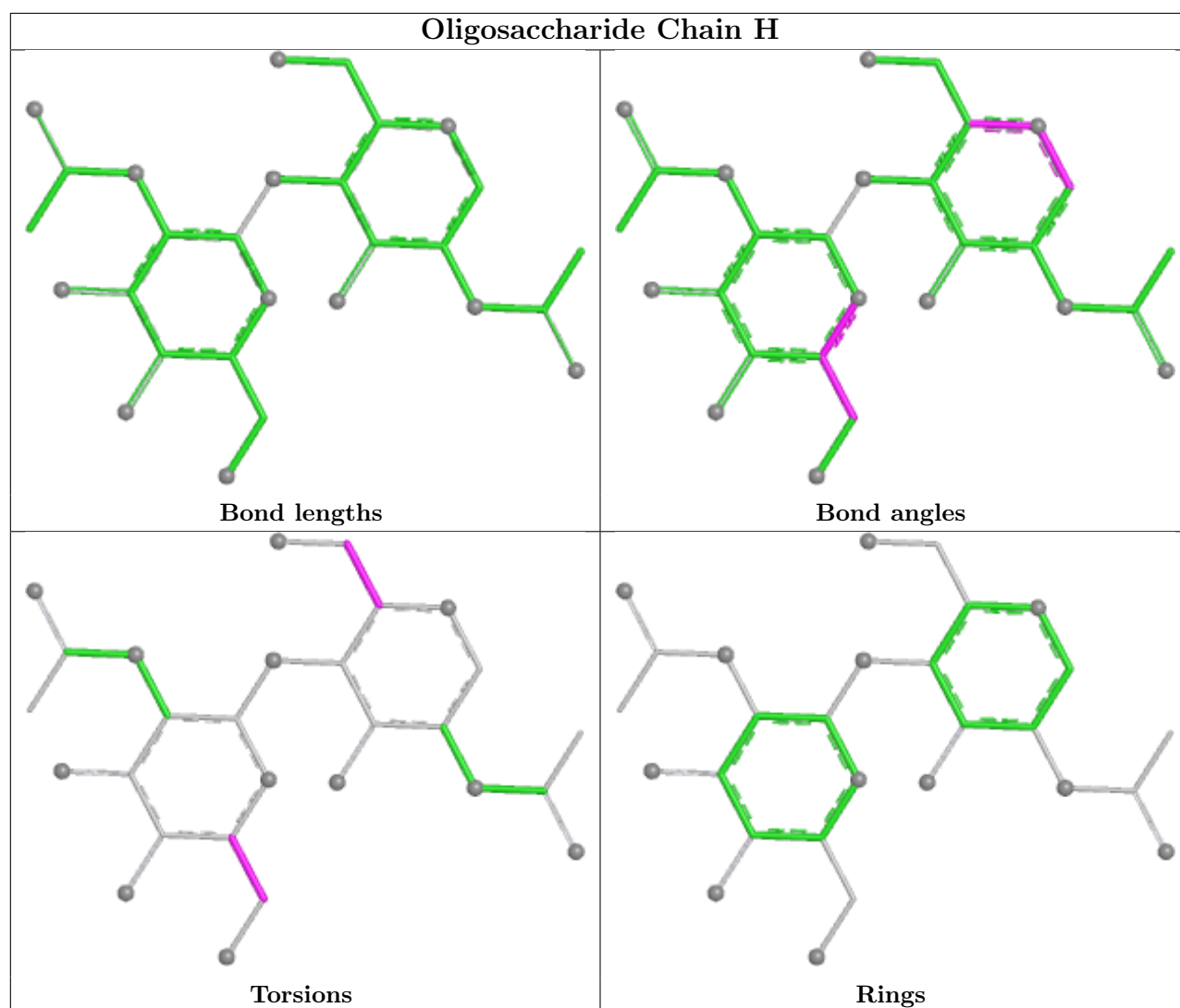
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	601	1	14,14,15	0.51	0	17,19,21	0.68	0
5	NAG	B	601	1	14,14,15	0.52	0	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	NAG	O4-C4-C5	3.42	117.74	109.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	NAG	C8-C7-N2-C2
5	B	601	NAG	O7-C7-N2-C2
5	A	601	NAG	C8-C7-N2-C2
5	A	601	NAG	O7-C7-N2-C2

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	329/330 (99%)	0.13	13 (3%) 42 33	15, 15, 15, 15	0
1	B	329/330 (99%)	0.11	12 (3%) 46 37	15, 15, 15, 15	0
2	C	211/211 (100%)	0.88	21 (9%) 12 9	15, 15, 15, 15	0
2	E	211/211 (100%)	1.03	22 (10%) 11 8	15, 15, 15, 15	0
3	D	213/213 (100%)	1.17	38 (17%) 4 2	15, 15, 15, 15	0
3	F	213/213 (100%)	0.86	15 (7%) 22 16	15, 15, 15, 15	0
All	All	1506/1508 (99%)	0.61	121 (8%) 18 13	15, 15, 15, 15	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	135	THR	6.5
3	F	191	TRP	6.4
1	B	-7	ALA	6.2
1	A	327	GLU	5.7
1	A	297	ASP	5.6
1	B	291	HIS	5.0
3	D	133	ALA	4.8
3	F	133	ALA	4.6
2	C	197	THR	4.3
3	F	150	PRO	4.2
1	B	327	GLU	4.2
1	A	76	ASP	4.0
1	A	-7	ALA	3.9
1	A	-8	GLY	3.8
2	E	93	ASN	3.8
1	A	-6	SER	3.8
2	E	191	SER	3.6
3	F	130	GLY	3.6
3	F	135	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	-5	ILE	3.5
3	D	132	ALA	3.5
3	D	134	GLN	3.5
1	A	291	HIS	3.5
3	D	163	SER	3.4
2	C	156	GLN	3.4
3	D	42	GLU	3.4
2	C	157	ASN	3.4
1	A	243	ARG	3.4
3	D	141	LEU	3.3
2	C	201	SER	3.3
2	E	187	GLU	3.2
2	C	190	ASN	3.2
2	C	177	SER	3.1
1	A	-5	ILE	3.0
2	E	127	SER	3.0
1	B	287	GLN	3.0
2	C	94	SER	3.0
2	E	31	THR	3.0
3	D	158	ASN	2.9
2	C	29	VAL	2.9
1	A	287	GLN	2.9
3	D	124	VAL	2.9
2	C	141	PRO	2.8
2	C	198	HIS	2.8
3	F	136	ASN	2.8
2	E	143	ASP	2.8
1	B	-6	SER	2.8
2	E	135	PHE	2.8
3	D	162	LEU	2.8
2	E	94	SER	2.8
3	F	131	SER	2.7
3	D	192	PRO	2.7
3	F	132	ALA	2.7
2	C	30	SER	2.7
2	E	198	HIS	2.7
3	F	192	PRO	2.7
2	C	178	THR	2.6
3	D	186	VAL	2.6
3	F	141	LEU	2.6
1	B	-8	GLY	2.6
2	C	112	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	136	ASN	2.6
1	B	76	ASP	2.6
3	D	1	GLU	2.5
3	F	128	ALA	2.5
1	B	297	ASP	2.5
2	E	119	PRO	2.5
2	C	170	ASP	2.5
3	D	191	TRP	2.5
3	D	174	GLN	2.5
2	C	66	GLY	2.5
2	E	151	ASP	2.4
3	D	104	ASP	2.4
3	D	193	SER	2.4
3	D	139	VAL	2.4
2	E	29	VAL	2.4
3	D	142	GLY	2.4
3	D	187	PRO	2.4
1	B	292	SER	2.3
2	E	7	SER	2.3
2	E	28	ILE	2.3
2	C	95	PRO	2.3
1	A	242(C)	ARG	2.3
2	E	56	THR	2.3
2	E	46	LEU	2.3
3	D	185	THR	2.3
3	D	15	GLY	2.3
1	A	51(A)	CYS	2.3
3	F	32	THR	2.3
3	D	54	ALA	2.2
2	C	191	SER	2.2
3	D	149	PHE	2.2
3	D	199	ASN	2.2
3	D	152	PRO	2.2
3	F	188	SER	2.2
3	F	42	GLU	2.2
2	C	202	THR	2.2
3	D	123	SER	2.2
3	D	181	SER	2.2
3	D	2	ILE	2.2
1	B	249	CYS	2.2
2	E	95	PRO	2.1
1	B	242(A)	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	88	CYS	2.1
3	D	212	LYS	2.1
3	D	140	THR	2.1
3	D	182	SER	2.1
2	E	122	SER	2.1
2	E	92	TYR	2.1
2	C	26	SER	2.0
3	D	153	VAL	2.0
2	E	161	ASN	2.0
1	A	159	GLN	2.0
2	C	52	SER	2.0
2	E	208	SER	2.0
3	D	164	SER	2.0
3	D	206	SER	2.0
3	D	96	CYS	2.0
3	F	28	ASN	2.0
3	D	34	ILE	2.0
2	C	123	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSX	B	289	7/8	0.87	0.23	15,15,15,15	0
1	CSX	A	289	7/8	0.90	0.20	15,15,15,15	0

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.

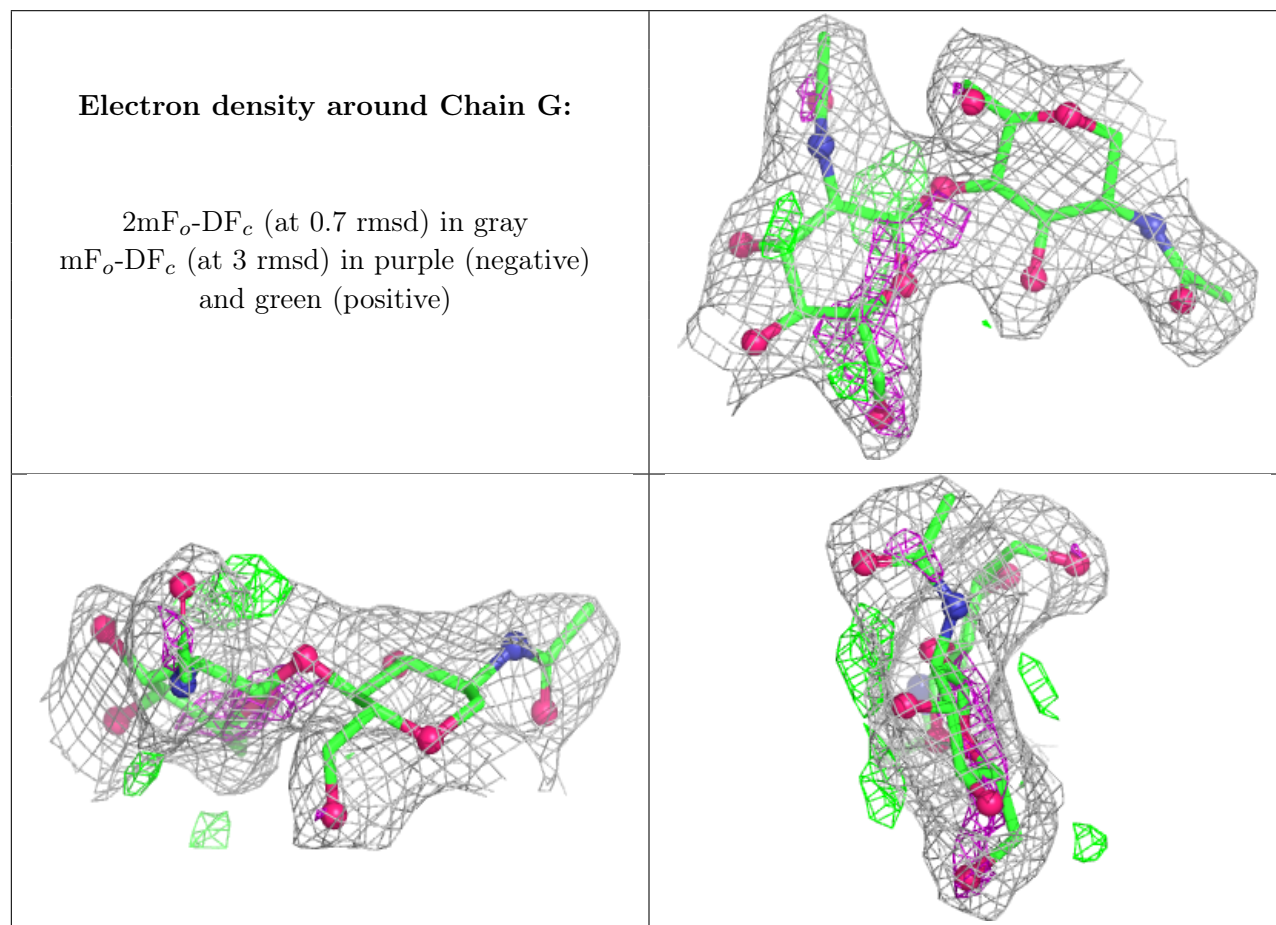
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	H	2	14/15	0.78	0.15	15,15,15,15	0
4	NAG	G	2	14/15	0.87	0.12	15,15,15,15	0
4	NAG	H	1	14/15	0.89	0.10	15,15,15,15	0

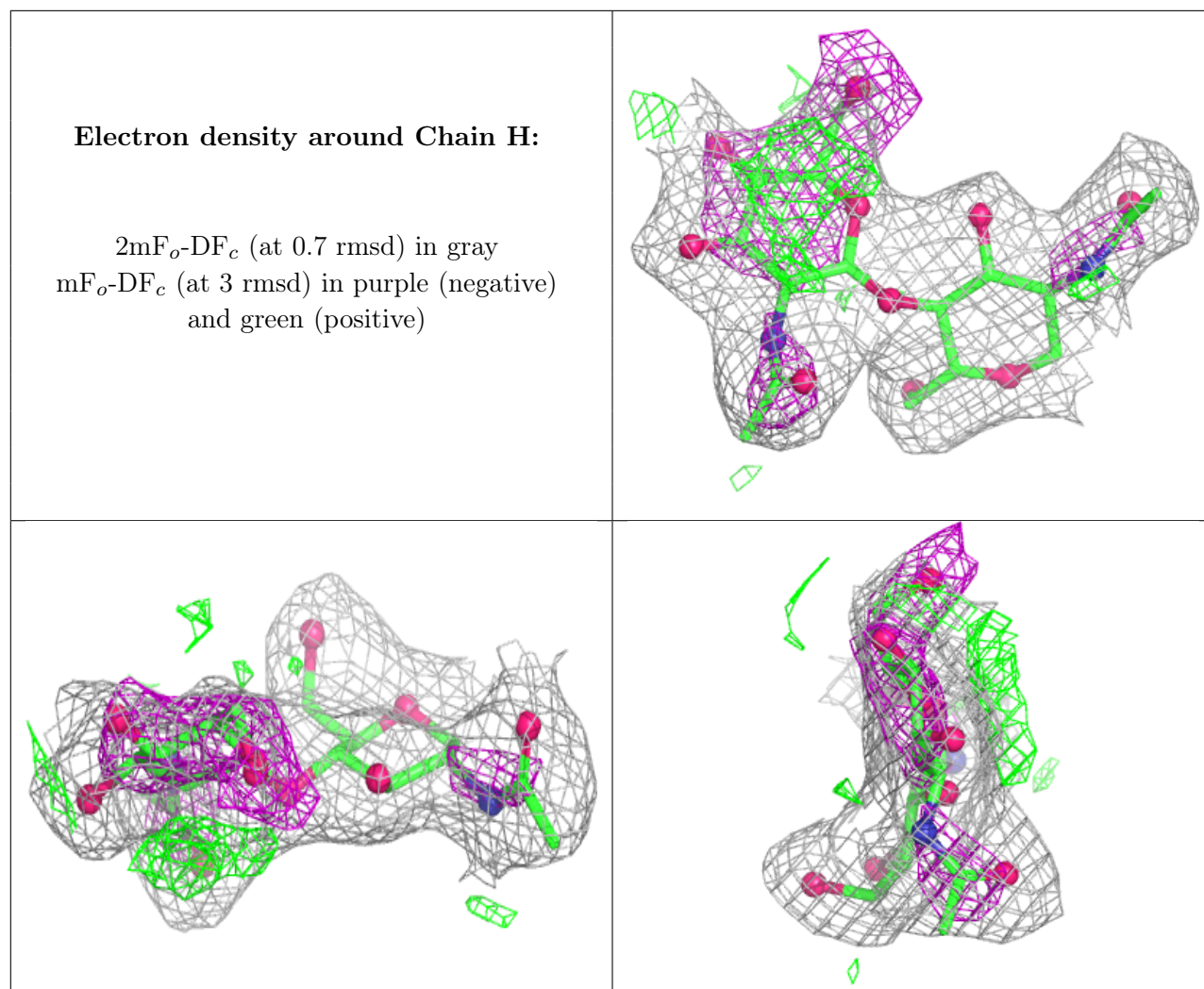
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	G	1	14/15	0.91	0.10	15,15,15,15	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	601	14/15	0.85	0.26	15,15,15,15	13
5	NAG	B	601	14/15	0.91	0.16	15,15,15,15	0
6	ZN	B	602	1/1	0.99	0.06	15,15,15,15	0
6	ZN	A	602	1/1	1.00	0.06	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.