



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:31 PM UTC

PDB ID : 6XQ0 / pdb_00006xq0
Title : Human antibody S8V2-18 in complex with the influenza hemagglutinin head domain of A/California/7/2009(NYMC-X181)(H1N1)
Authors : McCarthy, K.R.; Harrison, S.C.
Deposited on : 2020-07-09
Resolution : 2.30 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

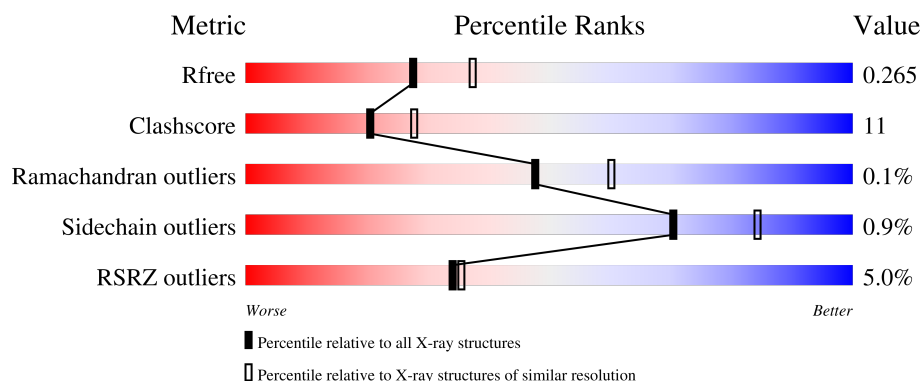
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	225	4% 79% 18% .
1	D	225	4% 80% 16% .
2	C	215	3% 80% 19% ..
2	F	215	8% 77% 22% .
3	B	240	4% 78% 16% ..

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Mol	Chain	Length	Quality of chain
3	E	240	6% 75% 20%
4	G	5	60% 20% 20%
4	H	5	20% 80%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10954 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	216	Total	C	N	O	S	0	0	0
			1711	1090	289	326	6			
1	A	219	Total	C	N	O	S	0	0	0
			1729	1101	292	330	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	54	ALA	-	expression tag	UNP I6T519
D	55	SER	-	expression tag	UNP I6T519
D	268	LEU	-	expression tag	UNP I6T519
D	269	GLU	-	expression tag	UNP I6T519
D	270	VAL	-	expression tag	UNP I6T519
D	271	LEU	-	expression tag	UNP I6T519
D	272	PHE	-	expression tag	UNP I6T519
D	273	GLN	-	expression tag	UNP I6T519
A	54	ALA	-	expression tag	UNP I6T519
A	55	SER	-	expression tag	UNP I6T519
A	268	LEU	-	expression tag	UNP I6T519
A	269	GLU	-	expression tag	UNP I6T519
A	270	VAL	-	expression tag	UNP I6T519
A	271	LEU	-	expression tag	UNP I6T519
A	272	PHE	-	expression tag	UNP I6T519
A	273	GLN	-	expression tag	UNP I6T519

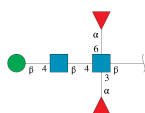
- Molecule 2 is a protein called antibody S8V2-18 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	0	0	0
			1645	1032	281	328	4			
2	F	213	Total	C	N	O	S	0	0	0
			1645	1032	281	328	4			

- Molecule 3 is a protein called antibody S8V2-18 heavy chain.

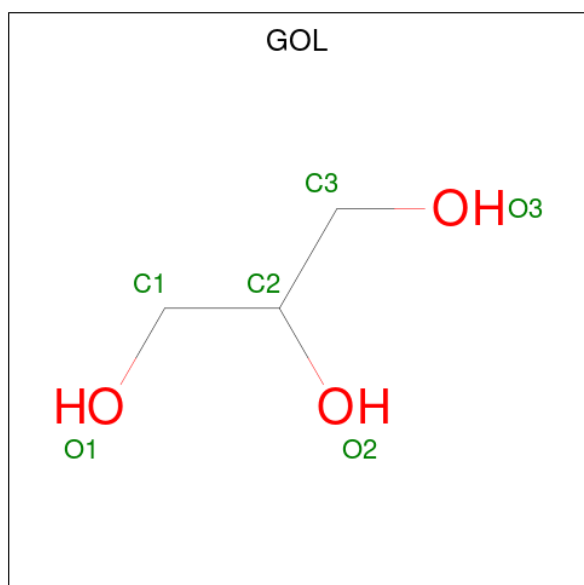
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	230	Total	C	N	O	S	0	0	0
			1729	1090	302	328	9			
3	E	230	Total	C	N	O	S	0	0	0
			1729	1090	302	328	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	0
			59	34	2	23			
4	H	5	Total	C	N	O	0	0	0
			59	34	2	23			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

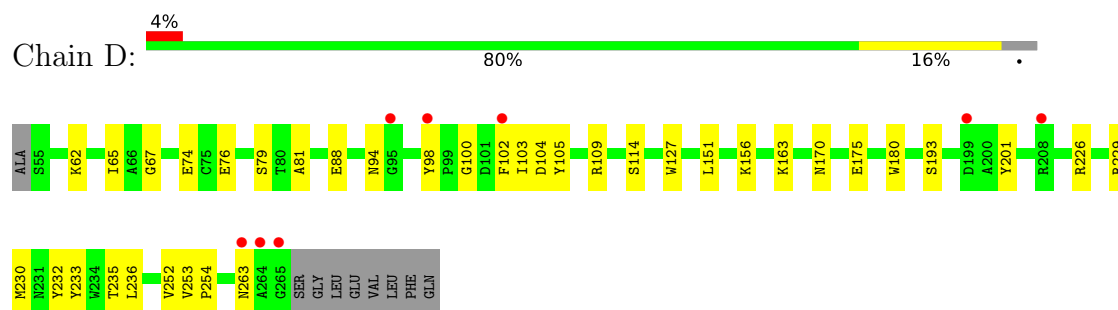
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	132	Total 132	O 132	0	0
6	A	127	Total 127	O 127	0	0
6	C	86	Total 86	O 86	0	0
6	B	114	Total 114	O 114	0	0
6	E	114	Total 114	O 114	0	0
6	F	69	Total 69	O 69	0	0

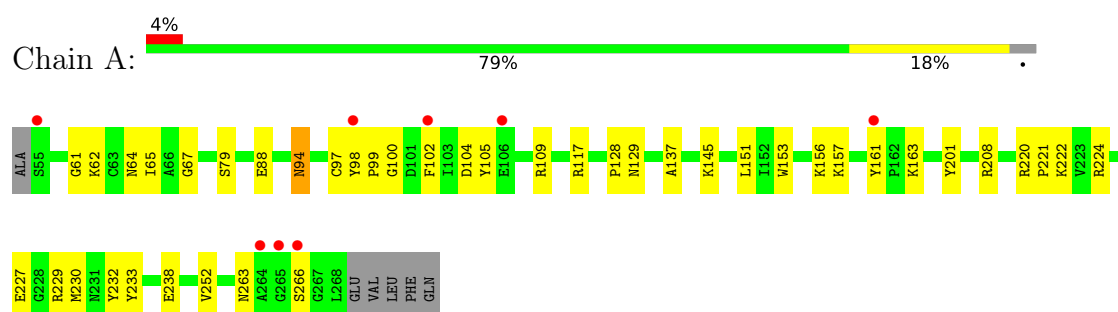
3 Residue-property plots [i](#)

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.

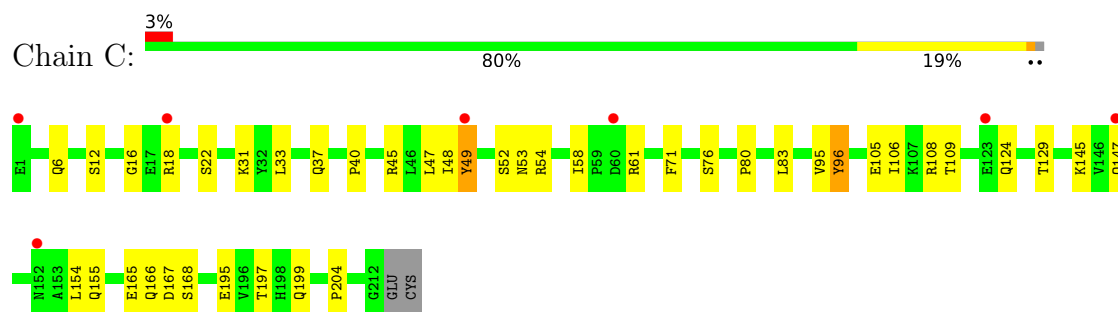
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

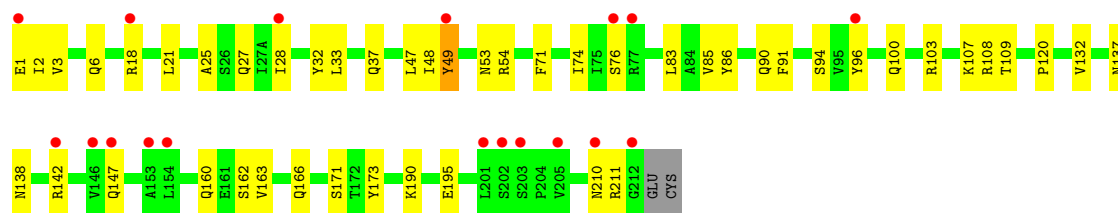


- Molecule 2: antibody S8V2-18 light chain

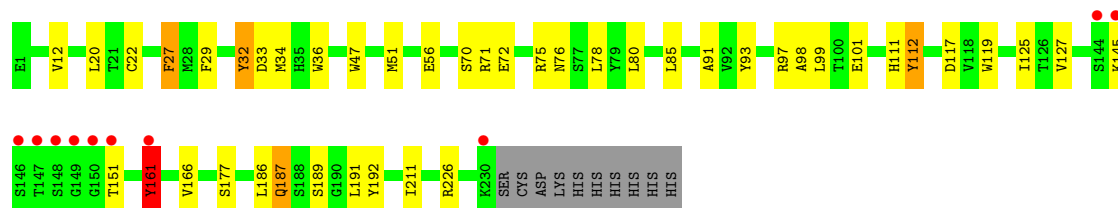
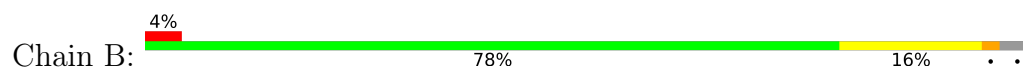


- Molecule 2: antibody S8V2-18 light chain

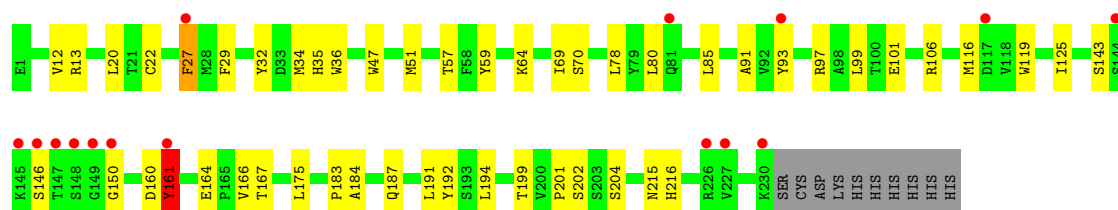
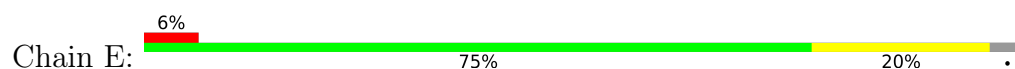




• Molecule 3: antibody S8V2-18 heavy chain



• Molecule 3: antibody S8V2-18 heavy chain



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.20Å 55.26Å 168.00Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	44.88 – 2.30 44.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (44.88-2.30) 95.3 (44.88-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.222 , 0.268 0.225 , 0.265	Depositor DCC
R_{free} test set	3042 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10954	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6264e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, BMA, GOL, FUC

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	0.17	0/1779	0.44	0/2415
1	D	0.22	0/1761	0.46	0/2391
2	C	0.19	0/1679	0.50	0/2278
2	F	0.18	0/1679	0.49	0/2278
3	B	0.20	0/1772	0.54	3/2405 (0.1%)
3	E	0.18	0/1772	0.54	1/2405 (0.0%)
All	All	0.19	0/10442	0.50	4/14172 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	161	TYR	CA-CB-CG	5.21	123.28	113.90
3	B	186	LEU	CA-C-N	-5.14	112.30	122.02
3	B	186	LEU	C-N-CA	-5.14	112.30	122.02
3	B	161	TYR	CA-CB-CG	5.03	122.95	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ASN	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	1729	0	1658	39	1
1	D	1711	0	1639	29	1
2	C	1645	0	1614	40	0
2	F	1645	0	1614	42	0
3	B	1729	0	1690	40	0
3	E	1729	0	1690	50	0
4	G	59	0	52	3	0
4	H	59	0	52	3	0
5	A	6	0	8	3	0
6	A	127	0	0	10	1
6	B	114	0	0	5	1
6	C	86	0	0	7	0
6	D	132	0	0	6	0
6	E	114	0	0	9	1
6	F	69	0	0	3	0
All	All	10954	0	10017	228	4

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 11.

All (228) 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:D:170:ASN:O	6:D:301:HOH:O	1.80	0.98
2:C:22:SER:O	6:C:301:HOH:O	1.80	0.97
3:E:57:THR:OG1	6:E:301:HOH:O	1.83	0.95
1:A:102:PHE:HD1	1:A:232:TYR:HB2	1.34	0.92
3:E:204:SER:OG	6:E:303:HOH:O	1.88	0.92
1:A:62:LYS:HD2	4:H:5:FUC:H62	1.52	0.89
1:D:88:GLU:OE2	6:D:302:HOH:O	1.91	0.88
3:E:161:TYR:OH	6:E:302:HOH:O	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:GLU:O	6:F:301:HOH:O	1.93	0.86
1:D:127:TRP:CZ2	1:D:253:VAL:HG11	2.11	0.85
1:A:98:TYR:HD1	1:A:99:PRO:HD2	1.43	0.84
3:E:106:ARG:NH1	6:E:307:HOH:O	2.11	0.83
3:E:161:TYR:CE1	3:E:192:TYR:HB2	2.13	0.83
2:C:147:GLN:HE21	2:C:154:LEU:HD11	1.45	0.81
3:B:145:LYS:NZ	3:B:151:THR:O	2.15	0.80
3:E:20:LEU:HD11	3:E:125:ILE:HD11	1.66	0.78
1:A:266:SER:O	6:A:401:HOH:O	2.01	0.78
3:E:119:TRP:O	6:E:304:HOH:O	1.99	0.78
1:A:102:PHE:CD1	1:A:232:TYR:HB2	2.18	0.77
3:B:161:TYR:CE1	3:B:192:TYR:HB2	2.20	0.77
2:C:31:LYS:O	6:C:303:HOH:O	2.03	0.76
3:B:119:TRP:O	6:B:302:HOH:O	2.04	0.75
1:A:229:ARG:NE	3:B:101:GLU:OE2	2.19	0.75
1:D:229:ARG:NE	3:E:101:GLU:OE2	2.15	0.75
1:D:76:GLU:O	6:D:303:HOH:O	2.04	0.74
1:A:98:TYR:HH	5:A:300:GOL:HO2	1.33	0.73
1:A:227:GLU:OE1	6:A:402:HOH:O	2.06	0.73
3:E:22:CYS:HB3	3:E:78:LEU:HB3	1.71	0.72
3:E:143:SER:O	6:E:305:HOH:O	2.07	0.72
3:B:189:SER:O	6:B:303:HOH:O	2.08	0.71
2:C:45:ARG:HD2	6:C:374:HOH:O	1.91	0.71
2:F:83:LEU:HD11	2:F:166:GLN:HB3	1.71	0.70
3:B:20:LEU:HD11	3:B:125:ILE:HD11	1.74	0.70
3:E:175:LEU:O	6:E:306:HOH:O	2.10	0.69
2:F:37:GLN:HG3	2:F:86:TYR:HE1	1.58	0.69
6:A:527:HOH:O	4:H:3:BMA:O3	2.09	0.69
1:A:208:ARG:HH21	1:A:238:GLU:HB3	1.57	0.69
2:F:210:ASN:O	2:F:211:ARG:HG3	1.93	0.69
1:D:62:LYS:HE3	1:D:94:ASN:OD1	1.93	0.68
1:A:220:ARG:HG2	3:B:99:LEU:HD21	1.74	0.68
1:A:208:ARG:NH1	6:A:409:HOH:O	2.27	0.68
2:F:108:ARG:HG2	2:F:109:THR:N	2.12	0.65
2:F:49:TYR:CD1	2:F:53:ASN:HB2	2.33	0.64
3:E:13:ARG:HG2	6:E:377:HOH:O	1.97	0.63
1:D:98:TYR:OH	6:D:304:HOH:O	2.15	0.63
2:C:49:TYR:CE1	2:C:53:ASN:HB2	2.32	0.63
3:B:27:PHE:HD2	3:B:97:ARG:NH1	1.97	0.63
2:C:49:TYR:CD1	2:C:53:ASN:HB2	2.34	0.62
3:E:164:GLU:HG3	6:E:302:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:LEU:HB2	2:C:106:ILE:HD12	1.80	0.62
6:D:428:HOH:O	4:G:4:FUC:O5	2.16	0.62
2:C:145:LYS:HB3	2:C:197:THR:OG1	2.00	0.61
3:E:35:HIS:CE1	2:F:96:TYR:HE2	2.19	0.61
3:B:29:PHE:HB2	3:B:76:ASN:OD1	2.01	0.60
3:B:22:CYS:HB3	3:B:78:LEU:HB3	1.83	0.60
3:E:150:GLY:O	3:E:202:SER:N	2.29	0.60
2:F:190:LYS:NZ	6:F:308:HOH:O	2.29	0.60
2:F:85:VAL:HG22	2:F:103:ARG:HD2	1.83	0.60
2:F:37:GLN:HG3	2:F:86:TYR:CE1	2.36	0.59
1:A:79:SER:HB3	1:A:117:ARG:HH21	1.66	0.59
2:F:91:PHE:HB2	2:F:96:TYR:HE1	1.67	0.59
1:D:103:ILE:HG13	1:D:233:TYR:CE1	2.37	0.59
1:A:98:TYR:OH	5:A:300:GOL:O2	2.11	0.59
3:B:161:TYR:CD1	3:B:192:TYR:HB2	2.38	0.59
1:D:62:LYS:NZ	1:D:74:GLU:OE1	2.26	0.58
1:A:153:TRP:HH2	5:A:300:GOL:H31	1.69	0.57
3:B:51:MET:HE3	3:B:71:ARG:HD2	1.86	0.57
3:B:177:SER:O	6:B:304:HOH:O	2.17	0.57
3:E:27:PHE:HD2	3:E:97:ARG:NH1	2.02	0.57
3:E:51:MET:HG3	3:E:57:THR:HG22	1.85	0.57
1:D:62:LYS:HD2	4:G:5:FUC:H62	1.88	0.56
2:C:95:VAL:HG23	3:B:47:TRP:CZ3	2.40	0.56
1:A:97:CYS:HA	1:A:224:ARG:NH1	2.20	0.56
2:C:37:GLN:OE1	2:C:45:ARG:HD3	2.05	0.56
3:B:34:MET:HB3	3:B:78:LEU:HD22	1.87	0.56
3:E:187:GLN:HG2	3:E:191:LEU:O	2.06	0.56
2:F:33:LEU:HD22	2:F:71:PHE:CG	2.41	0.56
3:B:97:ARG:HE	3:B:117:ASP:HB3	1.71	0.56
1:A:128:PRO:O	1:A:157:LYS:NZ	2.25	0.56
2:F:18:ARG:HG3	2:F:76:SER:HA	1.88	0.55
1:A:109:ARG:NH1	6:A:418:HOH:O	2.38	0.55
1:D:163:LYS:NZ	1:D:201:TYR:OH	2.39	0.55
2:C:199:GLN:HG2	6:C:317:HOH:O	2.06	0.55
2:F:49:TYR:CE1	2:F:53:ASN:HB2	2.42	0.55
1:D:81:ALA:HB3	6:D:319:HOH:O	2.06	0.55
3:B:56:GLU:HG2	6:B:373:HOH:O	2.07	0.54
1:D:102:PHE:HD2	1:D:105:TYR:HB2	1.73	0.54
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.90	0.54
1:D:62:LYS:HD2	4:G:5:FUC:C6	2.38	0.54
2:C:33:LEU:HD22	2:C:71:PHE:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:ILE:HG21	2:F:28:ILE:HD11	1.89	0.54
2:C:105:GLU:HG2	6:C:356:HOH:O	2.06	0.54
2:C:197:THR:HG22	2:C:204:PRO:HB3	1.90	0.53
1:A:222:LYS:NZ	6:A:420:HOH:O	2.41	0.53
3:B:51:MET:HE1	3:B:70:SER:C	2.34	0.53
3:E:27:PHE:HE1	3:E:29:PHE:HD1	1.56	0.53
3:E:199:THR:HG21	2:F:137:ASN:ND2	2.23	0.53
2:C:49:TYR:HD1	2:C:49:TYR:O	1.91	0.53
3:B:187:GLN:HG3	3:B:191:LEU:O	2.08	0.53
1:A:102:PHE:CE2	1:A:105:TYR:HD1	2.26	0.52
3:E:161:TYR:CD1	3:E:192:TYR:HB2	2.43	0.52
1:A:163:LYS:NZ	1:A:201:TYR:OH	2.42	0.52
2:F:138:ASN:ND2	6:F:312:HOH:O	2.42	0.52
2:C:16:GLY:O	2:F:1:GLU:HB2	2.10	0.52
2:F:49:TYR:C	2:F:49:TYR:HD1	2.18	0.52
1:A:98:TYR:CD1	1:A:99:PRO:HD2	2.35	0.52
3:B:91:ALA:HB3	3:B:93:TYR:HE1	1.75	0.52
3:B:211:ILE:CD1	3:B:226:ARG:HG2	2.39	0.52
2:F:49:TYR:CD1	2:F:49:TYR:C	2.88	0.51
2:F:147:GLN:HB3	2:F:195:GLU:HB3	1.92	0.51
1:D:98:TYR:HE1	1:D:226:ARG:HD3	1.74	0.51
1:A:97:CYS:O	1:A:224:ARG:HD2	2.11	0.51
3:E:161:TYR:HD1	3:E:161:TYR:O	1.93	0.51
2:F:49:TYR:HD1	2:F:49:TYR:O	1.93	0.51
1:A:102:PHE:HE2	1:A:105:TYR:HD1	1.57	0.51
2:C:49:TYR:CD1	2:C:49:TYR:C	2.88	0.51
3:E:51:MET:HE2	3:E:69:ILE:HG12	1.93	0.51
1:A:137:ALA:HA	1:A:145:LYS:HG2	1.92	0.51
3:B:33:ASP:OD1	6:B:305:HOH:O	2.19	0.51
3:B:97:ARG:NH2	3:B:117:ASP:OD2	2.37	0.51
2:C:61:ARG:HD2	2:C:76:SER:O	2.11	0.51
2:F:107:LYS:NZ	4:H:2:NAG:H83	2.26	0.51
3:E:201:PRO:HG2	3:E:204:SER:OG	2.11	0.51
2:C:106:ILE:O	2:C:166:GLN:NE2	2.41	0.50
2:C:52:SER:OG	6:C:302:HOH:O	2.03	0.50
1:A:98:TYR:HD1	1:A:99:PRO:CD	2.20	0.50
2:C:49:TYR:HD1	2:C:49:TYR:C	2.20	0.50
3:B:12:VAL:HG11	3:B:85:LEU:HD13	1.94	0.50
3:B:211:ILE:HD12	3:B:226:ARG:HG2	1.92	0.50
3:E:161:TYR:CD1	3:E:161:TYR:C	2.90	0.50
3:E:51:MET:CE	3:E:69:ILE:HG12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:183:PRO:HG2	2:F:162:SER:HB2	1.94	0.50
3:E:150:GLY:O	3:E:201:PRO:HA	2.12	0.49
2:C:18:ARG:NE	2:F:3:VAL:HG22	2.27	0.49
1:D:98:TYR:CD2	1:D:230:MET:HB2	2.48	0.49
2:C:76:SER:HB3	2:F:3:VAL:HG21	1.95	0.49
1:D:114:SER:OG	1:D:263:ASN:HB3	2.12	0.49
3:B:161:TYR:CD1	3:B:161:TYR:C	2.91	0.49
3:B:161:TYR:HE2	3:B:166:VAL:HG22	1.78	0.49
3:E:51:MET:HE1	3:E:70:SER:C	2.38	0.48
1:D:253:VAL:HG12	1:D:254:PRO:O	2.12	0.48
1:A:64:ASN:HA	1:A:88:GLU:HG3	1.94	0.48
3:E:161:TYR:HE2	3:E:166:VAL:HG22	1.79	0.48
2:F:166:GLN:HE21	2:F:171:SER:HB3	1.77	0.48
3:E:27:PHE:CD2	3:E:97:ARG:NH1	2.81	0.48
2:F:6:GLN:O	2:F:100:GLN:NE2	2.46	0.48
1:A:102:PHE:HD2	1:A:105:TYR:HB2	1.78	0.48
3:E:12:VAL:HG11	3:E:85:LEU:HD13	1.96	0.48
2:C:80:PRO:HA	2:C:106:ILE:HD13	1.95	0.47
3:E:47:TRP:CG	2:F:96:TYR:HB2	2.49	0.47
3:E:36:TRP:NE1	3:E:80:LEU:HB2	2.30	0.47
3:B:161:TYR:HD1	3:B:161:TYR:O	1.97	0.47
2:C:108:ARG:HG2	2:C:109:THR:O	2.15	0.47
1:A:129:ASN:ND2	6:A:417:HOH:O	2.35	0.47
3:B:72:GLU:OE1	3:B:75:ARG:HD2	2.15	0.47
3:E:32:TYR:CE1	3:E:99:LEU:HG	2.50	0.46
1:A:62:LYS:NZ	1:A:94:ASN:OD1	2.49	0.46
2:C:96:TYR:HD1	2:C:96:TYR:N	2.13	0.46
3:E:187:GLN:HA	2:F:160:GLN:HE22	1.81	0.46
2:C:95:VAL:HG23	3:B:47:TRP:HZ3	1.81	0.46
3:E:59:TYR:HB2	3:E:64:LYS:HG2	1.98	0.46
2:C:96:TYR:N	2:C:96:TYR:CD1	2.84	0.46
2:C:48:ILE:HD13	2:C:54:ARG:HA	1.98	0.46
1:A:151:LEU:HB3	1:A:252:VAL:HG12	1.97	0.45
3:B:32:TYR:HB3	3:B:98:ALA:O	2.15	0.45
1:A:263:ASN:ND2	6:A:430:HOH:O	2.49	0.45
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.99	0.45
2:F:142:ARG:HH21	2:F:163:VAL:HB	1.82	0.45
3:E:35:HIS:CG	3:E:116:MET:HE2	2.51	0.45
1:D:65:ILE:HD12	1:D:109:ARG:HG2	1.98	0.45
2:C:154:LEU:HD12	2:C:155:GLN:H	1.81	0.45
3:E:161:TYR:HD1	3:E:161:TYR:C	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:27:PHE:C	3:E:27:PHE:CD1	2.94	0.45
2:F:142:ARG:HB2	2:F:173:TYR:CE2	2.52	0.45
1:D:98:TYR:HD2	1:D:230:MET:CB	2.29	0.45
1:A:102:PHE:CE2	1:A:105:TYR:CD1	3.04	0.45
3:B:111:HIS:C	3:B:112:TYR:HD1	2.25	0.45
3:B:91:ALA:HB3	3:B:93:TYR:CE1	2.51	0.44
3:E:91:ALA:HB3	3:E:93:TYR:HE1	1.83	0.44
2:C:12:SER:HA	2:C:105:GLU:O	2.17	0.44
1:D:156:LYS:HE2	1:D:193:SER:O	2.18	0.44
1:A:221:PRO:HB3	2:C:49:TYR:OH	2.18	0.44
3:B:161:TYR:CE2	3:B:166:VAL:HG13	2.52	0.44
1:D:102:PHE:CD1	1:D:232:TYR:HB2	2.53	0.44
3:B:32:TYR:CD2	3:B:97:ARG:HD3	2.53	0.44
1:D:98:TYR:CE1	1:D:226:ARG:HD3	2.53	0.43
2:C:83:LEU:HD11	2:C:166:GLN:HB3	2.00	0.43
3:B:161:TYR:C	3:B:161:TYR:HD1	2.26	0.43
3:E:167:THR:OG1	3:E:215:ASN:HB2	2.18	0.43
1:D:67:GLY:HA3	1:D:94:ASN:O	2.18	0.43
1:A:65:ILE:HD12	1:A:109:ARG:HG2	1.99	0.43
1:A:100:GLY:HA3	1:A:230:MET:O	2.18	0.43
2:C:147:GLN:HB3	2:C:195:GLU:HB3	2.00	0.43
3:E:34:MET:HB3	3:E:78:LEU:HD22	2.01	0.43
3:E:51:MET:HE2	3:E:69:ILE:HG23	1.99	0.43
3:B:36:TRP:NE1	3:B:80:LEU:HB2	2.34	0.43
2:F:18:ARG:HE	2:F:74:ILE:CG2	2.32	0.43
3:B:12:VAL:O	3:B:127:VAL:HA	2.19	0.43
1:D:180:TRP:HZ3	1:D:235:THR:HG22	1.84	0.43
2:C:6:GLN:HG2	6:C:301:HOH:O	2.19	0.42
3:B:27:PHE:CD1	3:B:27:PHE:C	2.97	0.42
1:D:102:PHE:CE2	1:D:105:TYR:HD1	2.37	0.42
2:C:40:PRO:HB3	2:C:165:GLU:OE1	2.19	0.42
3:E:27:PHE:HE1	3:E:29:PHE:CD1	2.38	0.42
2:F:48:ILE:HD13	2:F:54:ARG:HA	2.02	0.42
2:F:91:PHE:CD1	2:F:96:TYR:CE1	3.08	0.42
1:D:100:GLY:HA3	1:D:230:MET:O	2.20	0.42
1:A:233:TYR:OH	6:A:404:HOH:O	2.21	0.42
3:B:27:PHE:CD2	3:B:97:ARG:NH1	2.84	0.41
1:A:156:LYS:HA	1:A:161:TYR:HD1	1.85	0.41
3:E:160:ASP:OD1	3:E:187:GLN:NE2	2.53	0.41
2:F:25:ALA:C	2:F:27:GLN:H	2.28	0.41
3:E:161:TYR:CE2	3:E:166:VAL:HG13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:GLN:HB2	2:F:47:LEU:HD11	2.02	0.41
2:F:91:PHE:CE1	2:F:94:SER:HA	2.56	0.41
1:A:61:GLY:O	6:A:405:HOH:O	2.22	0.41
2:C:124:GLN:HG2	2:C:129:THR:O	2.20	0.41
3:E:91:ALA:HB3	3:E:93:TYR:CE1	2.56	0.41
2:F:21:LEU:HD21	2:F:86:TYR:HD2	1.85	0.41
1:D:151:LEU:HB3	1:D:252:VAL:HG12	2.03	0.41
2:C:167:ASP:OD1	2:C:168:SER:N	2.54	0.41
3:E:166:VAL:HG12	3:E:216:HIS:HB2	2.03	0.41
2:F:32:TYR:O	2:F:90:GLN:HA	2.21	0.41
1:A:67:GLY:HA3	1:A:94:ASN:O	2.21	0.41
2:F:91:PHE:HE1	2:F:94:SER:HA	1.86	0.41
1:D:175:GLU:OE1	1:D:236:LEU:HB3	2.20	0.40
2:C:45:ARG:HH11	2:C:58:ILE:HD13	1.86	0.40
3:E:184:ALA:HA	3:E:194:LEU:HB3	2.04	0.40

All (4) 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)
6:A:503:HOH:O	6:A:515:HOH:O[4_557]	2.06	0.14
1:D:79:SER:OG	1:D:104:ASP:OD1[4_546]	2.14	0.06
6:B:406:HOH:O	6:E:405:HOH:O[3_455]	2.16	0.04
1:A:79:SER:OG	1:A:104:ASP:OD1[4_547]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	217/225 (96%)	211 (97%)	6 (3%)	0	100	100
1	D	214/225 (95%)	206 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
2	F	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
3	B	228/240 (95%)	224 (98%)	4 (2%)	0	100	100
3	E	228/240 (95%)	224 (98%)	3 (1%)	1 (0%)	30	38
All	All	1309/1360 (96%)	1273 (97%)	35 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	146	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	188/193 (97%)	188 (100%)	0	100	100
1	D	186/193 (96%)	186 (100%)	0	100	100
2	C	184/186 (99%)	182 (99%)	2 (1%)	65	81
2	F	184/186 (99%)	183 (100%)	1 (0%)	81	90
3	B	185/195 (95%)	180 (97%)	5 (3%)	39	58
3	E	185/195 (95%)	183 (99%)	2 (1%)	65	81
All	All	1112/1148 (97%)	1102 (99%)	10 (1%)	70	84

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

Mol	Chain	Res	Type
2	C	49	TYR
2	C	96	TYR
3	B	27	PHE
3	B	32	TYR
3	B	112	TYR
3	B	161	TYR

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Mol	Chain	Res	Type
3	B	187	GLN
3	E	27	PHE
3	E	161	TYR
2	F	49	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	147	GLN
3	B	187	GLN
2	F	30	ASN
2	F	53	ASN
2	F	90	GLN
2	F	160	GLN
2	F	189	HIS

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](#)

10 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	1,4	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	G	2	4	14,14,15	0.44	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	G	3	4	11,11,12	0.61	0	15,15,17	0.68	0
4	FUC	G	4	4	10,10,11	0.68	0	14,14,16	0.78	0
4	FUC	G	5	4	10,10,11	0.64	0	14,14,16	1.44	2 (14%)
4	NAG	H	1	1,4	14,14,15	0.36	0	17,19,21	0.70	1 (5%)
4	NAG	H	2	4	14,14,15	0.30	0	17,19,21	0.43	0
4	BMA	H	3	4	11,11,12	0.54	0	15,15,17	0.67	0
4	FUC	H	4	4	10,10,11	0.63	0	14,14,16	0.79	0
4	FUC	H	5	4	10,10,11	0.82	0	14,14,16	0.90	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
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
4	FUC	G	5	4	-	-	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	FUC	H	4	4	-	-	0/1/1/1
4	FUC	H	5	4	-	-	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	5	FUC	C1-O5-C5	3.02	120.08	112.97
4	G	5	FUC	O5-C5-C6	-2.22	102.59	107.40
4	H	1	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6

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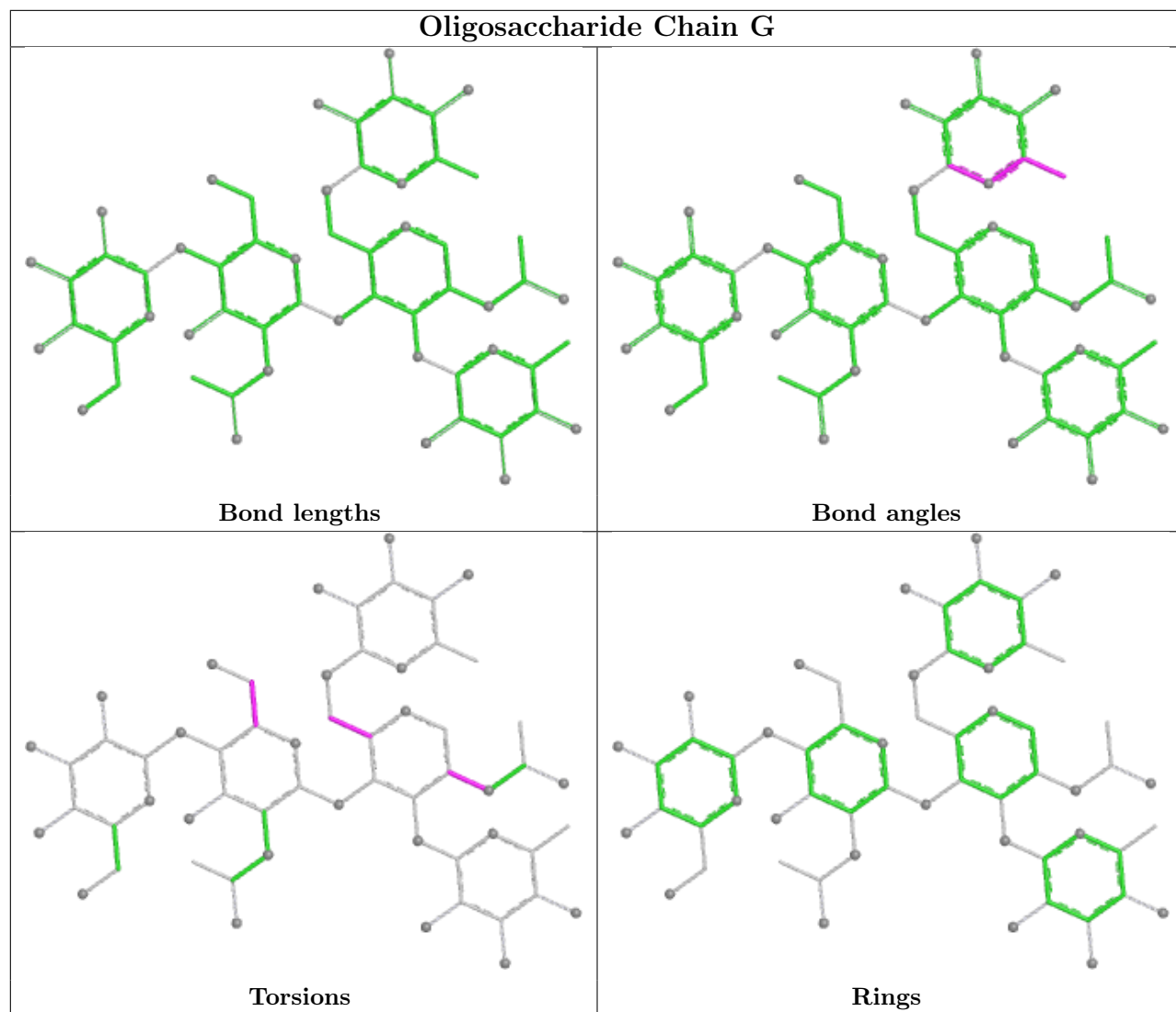
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C1-C2-N2-C7

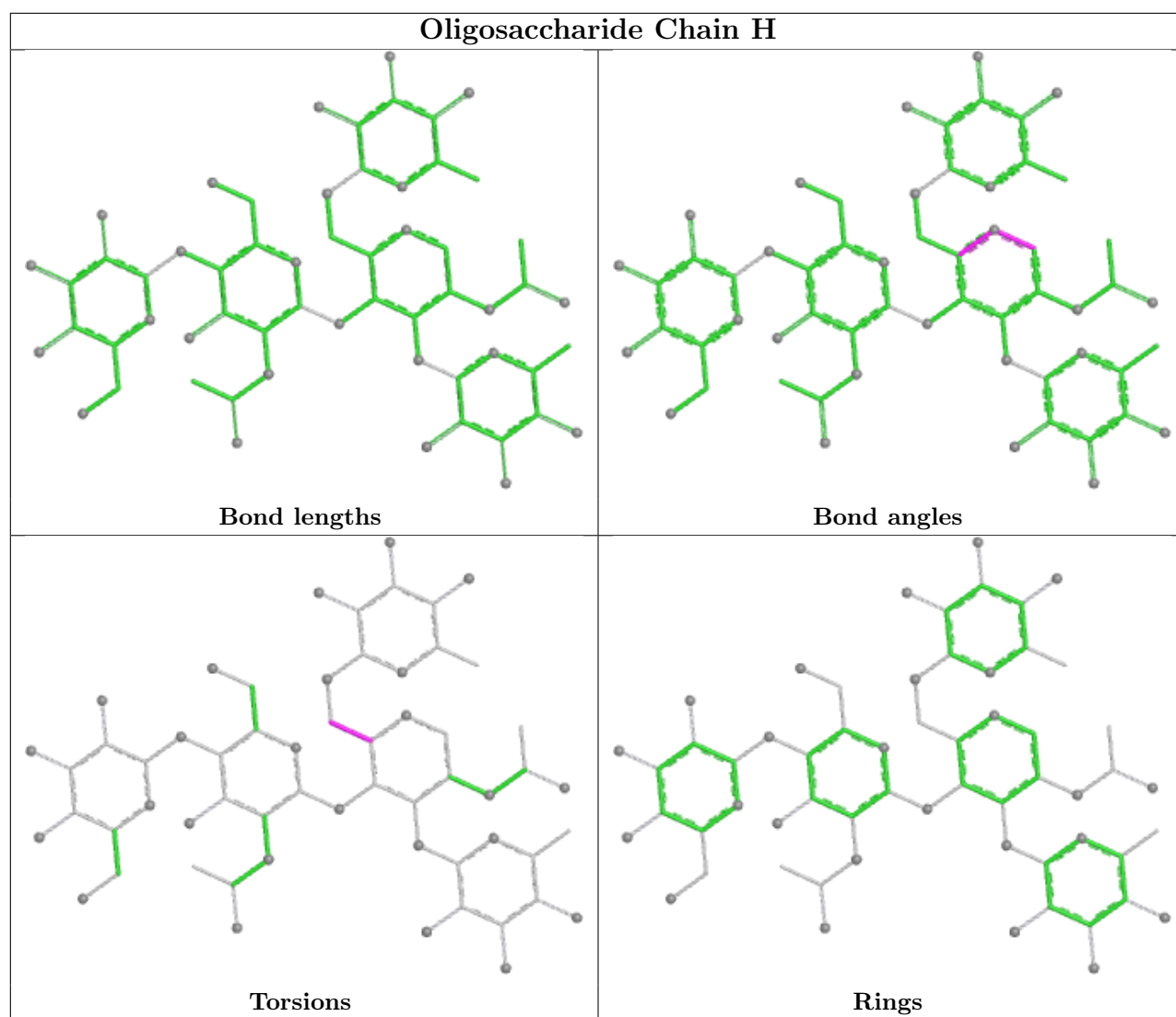
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
4	H	5	FUC	1	0
4	G	4	FUC	1	0
4	H	3	BMA	1	0
4	G	5	FUC	2	0

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





5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	A	300	-	5,5,5	0.93	0	5,5,5	1.33	1 (20%)

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	GOL	A	300	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	300	GOL	C3-C2-C1	-2.28	103.44	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	300	GOL	O1-C1-C2-C3
5	A	300	GOL	C1-C2-C3-O3
5	A	300	GOL	O2-C2-C3-O3
5	A	300	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	300	GOL	3	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	A	219/225 (97%)	0.22	8 (3%) 45 48	24, 34, 55, 76	0
1	D	216/225 (96%)	0.16	8 (3%) 45 48	19, 32, 48, 71	0
2	C	213/215 (99%)	0.47	7 (3%) 49 51	29, 41, 66, 88	0
2	F	213/215 (99%)	0.84	18 (8%) 16 18	31, 56, 89, 108	0
3	B	230/240 (95%)	0.40	10 (4%) 40 41	24, 38, 70, 186	0
3	E	230/240 (95%)	0.48	15 (6%) 25 27	26, 42, 70, 195	0
All	All	1321/1360 (97%)	0.43	66 (4%) 34 35	19, 39, 74, 195	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	95	GLY	4.6
3	B	161	TYR	4.2
3	B	147	THR	4.1
3	E	149	GLY	4.0
3	E	145	LYS	3.8
3	B	150	GLY	3.8
2	F	49	TYR	3.7
3	B	145	LYS	3.6
3	E	147	THR	3.6
3	E	148	SER	3.4
1	A	266	SER	3.3
1	A	102	PHE	3.3
3	B	151	THR	3.1
1	D	263	ASN	3.1
3	E	146	SER	3.0
3	B	146	SER	3.0
2	F	76	SER	2.9
1	A	98	TYR	2.9
1	A	106	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	96	TYR	2.9
2	C	18	ARG	2.9
1	D	102	PHE	2.8
3	B	148	SER	2.8
2	F	203	SER	2.8
2	F	210	ASN	2.7
2	C	49	TYR	2.7
3	E	117	ASP	2.7
2	F	28	ILE	2.7
2	F	1	GLU	2.7
3	E	230	LYS	2.6
2	F	142	ARG	2.6
1	A	55	SER	2.6
3	B	230	LYS	2.5
3	E	144	SER	2.5
2	F	147	GLN	2.5
3	E	161	TYR	2.5
1	D	199	ASP	2.5
3	E	27	PHE	2.4
3	E	227	VAL	2.4
1	A	264	ALA	2.3
1	A	161	TYR	2.3
2	C	1	GLU	2.3
2	F	154	LEU	2.3
2	F	201	LEU	2.3
2	C	60	ASP	2.3
2	F	202	SER	2.3
1	D	265	GLY	2.2
3	B	149	GLY	2.2
1	D	264	ALA	2.2
2	F	153	ALA	2.2
2	F	77	ARG	2.2
1	D	208	ARG	2.1
2	C	147	GLN	2.1
2	F	212	GLY	2.1
3	E	150	GLY	2.1
2	F	18	ARG	2.1
2	C	152	ASN	2.1
3	E	81	GLN	2.1
2	F	205	VAL	2.1
2	C	123	GLU	2.1
1	D	98	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	93	TYR	2.1
2	F	146	VAL	2.1
1	A	265	GLY	2.1
3	B	144	SER	2.0
3	E	226	ARG	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](#)

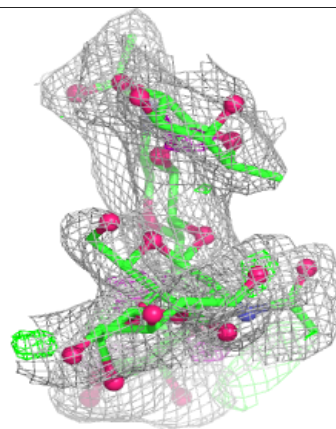
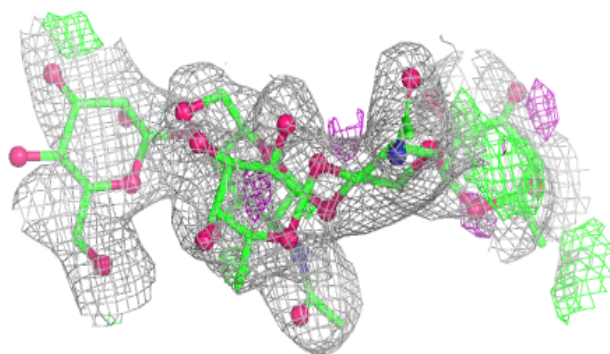
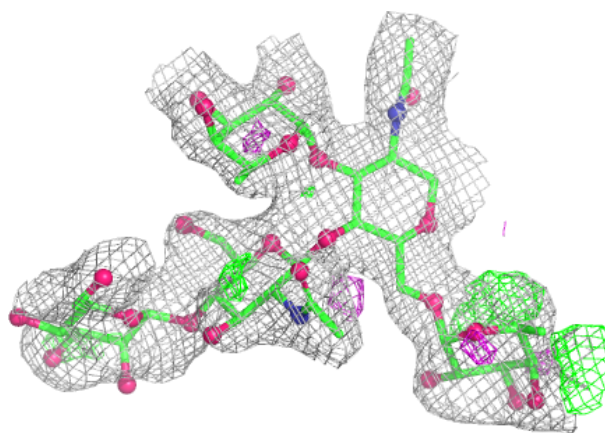
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

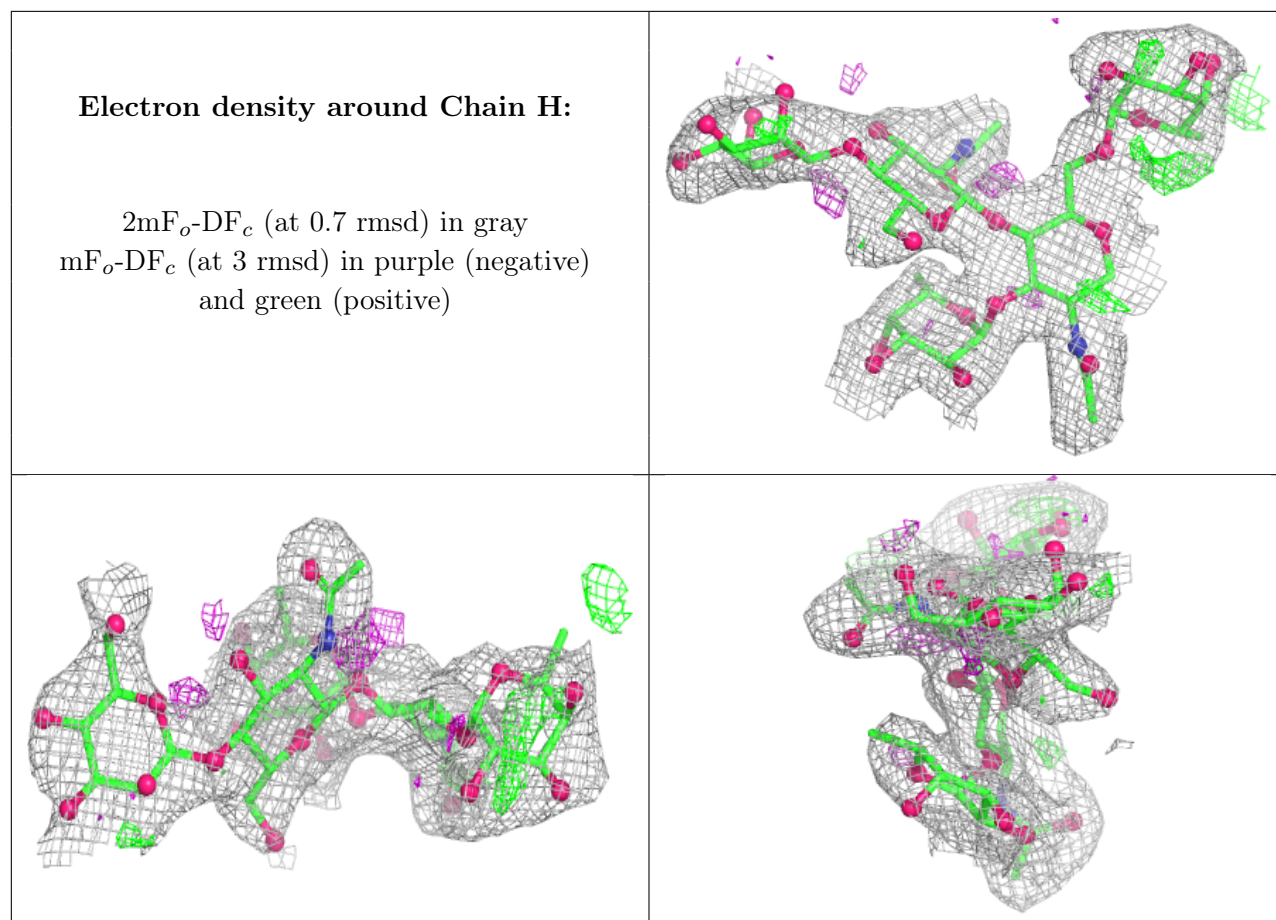
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	H	3	11/12	0.57	0.16	61,66,68,69	0
4	BMA	G	3	11/12	0.69	0.13	66,69,73,76	0
4	FUC	G	5	10/11	0.73	0.18	43,48,55,62	0
4	FUC	H	5	10/11	0.73	0.17	53,57,61,64	0
4	NAG	G	2	14/15	0.82	0.12	40,49,58,62	0
4	FUC	G	4	10/11	0.88	0.12	40,48,50,52	0
4	FUC	H	4	10/11	0.88	0.13	44,49,52,52	0
4	NAG	H	2	14/15	0.88	0.10	43,50,55,56	0
4	NAG	H	1	14/15	0.90	0.09	24,33,44,53	0
4	NAG	G	1	14/15	0.91	0.09	27,36,45,45	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 G:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	300	6/6	0.82	0.22	40,53,54,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.