



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:03 PM EDT

PDB ID : 7KZB  
Title : Potent SARS-CoV-2 binding and neutralization through maturation of iconic SARS-CoV-1 antibodies  
Authors : Langley, D.B.; Christ, D.  
Deposited on : 2020-12-10  
Resolution : 2.83 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

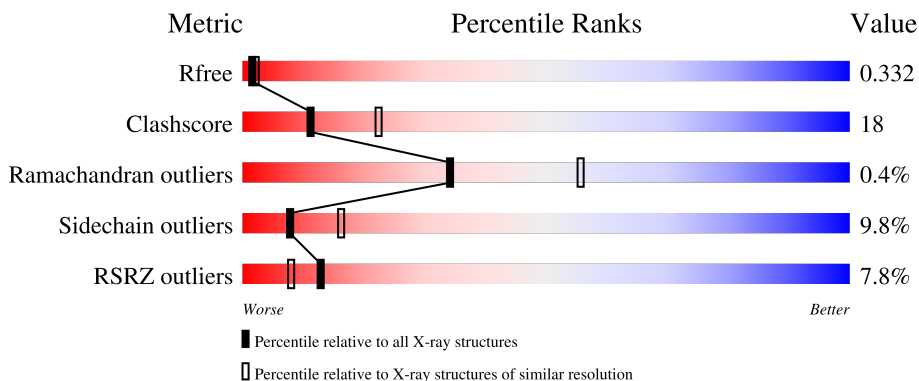
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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))
$R_{free}$	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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  $\geq 3$ , 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	H	231	
2	L	214	
3	C	204	
4	A	230	
5	B	214	

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Mol	Chain	Length	Quality of chain
6	D	3	 100%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7145 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 Fab heavy chain of CR3014-C8 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	214	1567	993	263	305	6	0	0	0

- Molecule 2 is a protein called Fab light chain of CR3014-C8 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1590	994	258	332	6	0	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	192	1463	936	243	276	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	529	GLY	-	expression tag	UNP P0DTC2
C	530	SER	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2

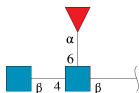
- Molecule 4 is a protein called Fab heavy chain of CR3022-B6 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	170	1095	685	187	216	7	0	0	0

- Molecule 5 is a protein called Fab light chain of CR3022-B6 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	202	1386	862	235	283	6	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	D	3	38	22	2	14	0	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	L	1	1	1	0	0

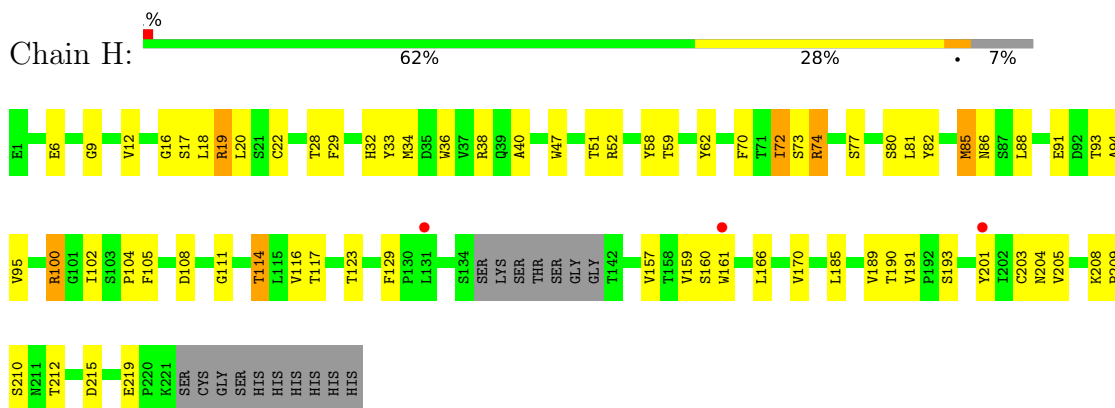
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	L	4	4	4	0	0
8	C	1	1	1	0	0

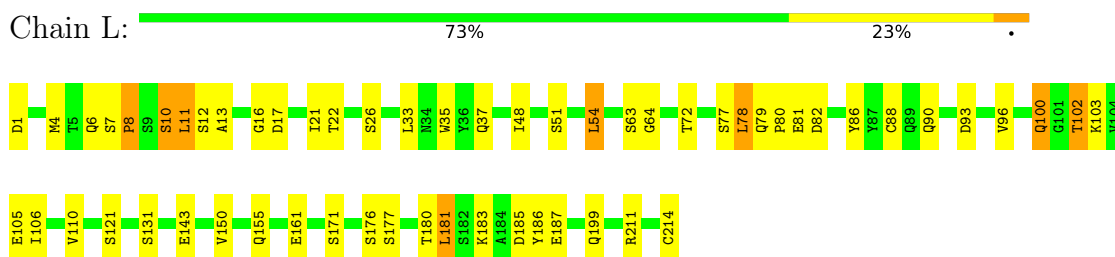
### 3 Residue-property plots [i](#)

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.

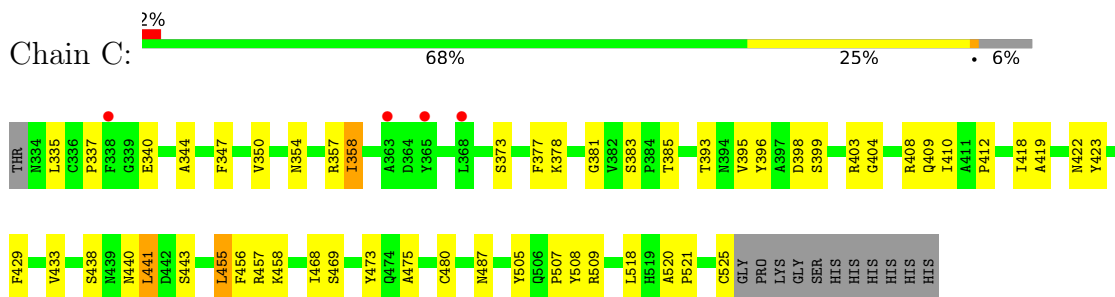
- Molecule 1: Fab heavy chain of CR3014-C8 antibody



- Molecule 2: Fab light chain of CR3014-C8 antibody

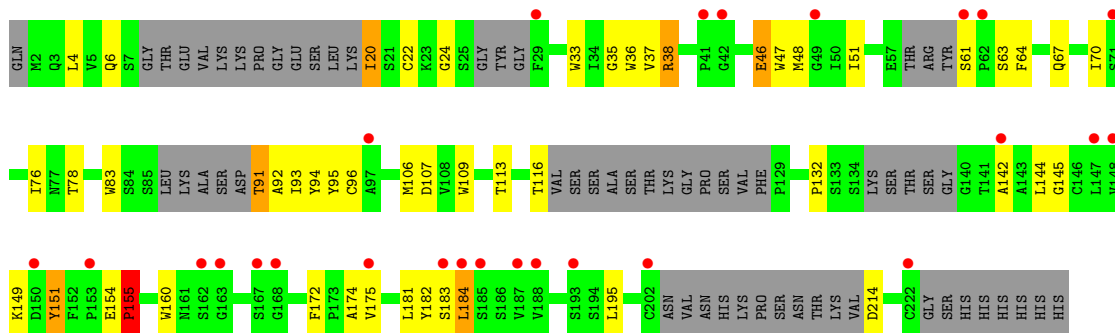


- Molecule 3: Spike glycoprotein

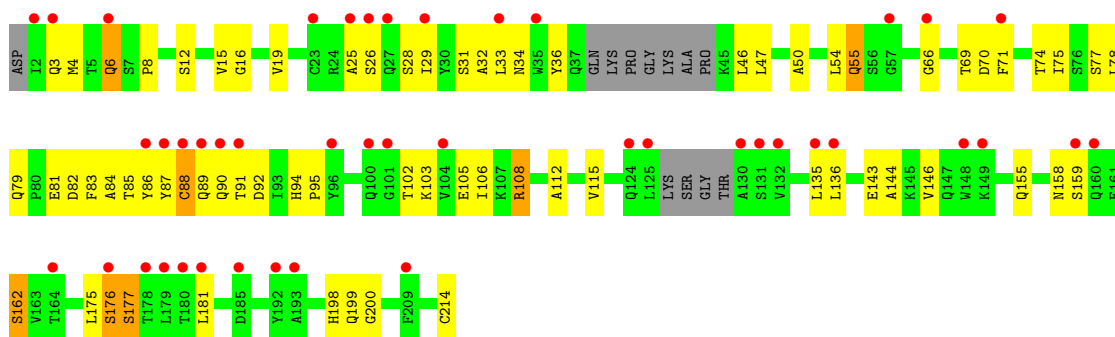


- Molecule 4: Fab heavy chain of CR3022-B6 antibody





- Molecule 5: Fab light chain of CR3022-B6 antibody



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.18Å 147.67Å 157.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.83 49.38 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.38-2.83) 99.7 (49.38-2.83)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.251 , 0.336 0.251 , 0.332	Depositor DCC
$R_{free}$ test set	1462 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.2	Xtrriage
Anisotropy	0.567	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, FUC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	H	0.73	0/1606	0.97	1/2195 (0.0%)
2	L	0.76	0/1627	1.02	0/2227
3	C	0.73	0/1504	0.95	0/2052
4	A	0.76	0/1117	0.85	1/1535 (0.1%)
5	B	0.74	0/1412	0.85	0/1938
All	All	0.74	0/7266	0.94	2/9947 (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
2	L	0	1
3	C	0	2
4	A	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	155	PRO	N-CA-CB	-7.14	94.73	103.30
1	H	74	ARG	NE-CZ-NH2	-6.27	117.17	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	154	GLU	Peptide
3	C	335	LEU	Peptide
3	C	381	GLY	Peptide
2	L	51	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1567	0	1469	47	1
2	L	1590	0	1444	46	1
3	C	1463	0	1323	31	0
4	A	1095	0	858	50	0
5	B	1386	0	1180	75	0
6	D	38	0	34	7	0
7	L	1	0	0	0	0
8	C	1	0	0	0	0
8	L	4	0	0	0	0
All	All	7145	0	6308	241	1

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 18.

All (241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:175:VAL:O	4:A:182:TYR:CB	1.84	1.25
5:B:6:GLN:NE2	5:B:86:TYR:O	1.77	1.16
4:A:151:TYR:OH	4:A:174:ALA:CB	1.99	1.10
2:L:6:GLN:NE2	2:L:102:THR:HG23	1.68	1.06
4:A:6:GLN:NE2	4:A:94:TYR:O	1.88	1.05
4:A:151:TYR:OH	4:A:174:ALA:HB1	1.54	1.04
5:B:33:LEU:HD12	5:B:89:GLN:O	1.61	0.98
2:L:79:GLN:HB3	2:L:80:PRO:HD2	1.45	0.98
5:B:29:ILE:HD13	5:B:90:GLN:HB2	1.49	0.95
4:A:20:ILE:HG21	4:A:83:TRP:HZ3	1.34	0.93
2:L:6:GLN:HE21	2:L:102:THR:HG23	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:29:ILE:HG23	5:B:92:ASP:HB2	1.54	0.88
2:L:8:PRO:O	2:L:102:THR:HB	1.74	0.87
1:H:34:MET:SD	1:H:100:ARG:HB3	2.16	0.86
1:H:52:ARG:HE	1:H:59:THR:HG23	1.43	0.83
4:A:20:ILE:HD12	4:A:113:THR:HG21	1.61	0.82
5:B:4:MET:CE	5:B:90:GLN:HB3	2.10	0.82
2:L:4:MET:HE1	2:L:90:GLN:H	1.46	0.78
4:A:93:ILE:HA	4:A:113:THR:O	1.83	0.78
5:B:29:ILE:CG2	5:B:92:ASP:HB2	2.14	0.77
5:B:29:ILE:HG23	5:B:92:ASP:CB	2.14	0.76
3:C:398:ASP:OD2	3:C:423:TYR:OH	2.03	0.75
5:B:16:GLY:HA2	5:B:77:SER:OG	1.87	0.74
4:A:151:TYR:OH	4:A:174:ALA:HB2	1.86	0.73
5:B:33:LEU:CD1	5:B:89:GLN:O	2.36	0.73
1:H:9:GLY:H	1:H:114:THR:HG21	1.53	0.73
2:L:6:GLN:HE21	2:L:102:THR:CG2	2.01	0.72
4:A:61:SER:HA	5:B:95:PRO:HG3	1.70	0.72
4:A:20:ILE:CG2	4:A:83:TRP:HZ3	2.01	0.72
6:D:2:NAG:H3	6:D:2:NAG:H83	1.72	0.72
5:B:81:GLU:OE2	5:B:81:GLU:N	2.21	0.72
4:A:20:ILE:HG21	4:A:83:TRP:CZ3	2.21	0.72
2:L:12:SER:HA	2:L:105:GLU:O	1.91	0.71
5:B:85:THR:HA	5:B:102:THR:O	1.91	0.71
1:H:20:LEU:HD11	1:H:85:MET:HE1	1.73	0.71
1:H:93:THR:HG23	1:H:117:THR:HA	1.74	0.69
6:D:2:NAG:H3	6:D:2:NAG:C8	2.23	0.68
5:B:33:LEU:HD11	5:B:88:CYS:HB2	1.75	0.68
5:B:176:SER:OG	5:B:176:SER:O	2.10	0.68
1:H:32:HIS:NE2	1:H:102:ILE:HD12	2.10	0.67
2:L:54:LEU:HD23	2:L:54:LEU:O	1.95	0.67
5:B:8:PRO:O	5:B:102:THR:HG23	1.95	0.67
5:B:16:GLY:O	5:B:77:SER:HA	1.94	0.67
3:C:412:PRO:HG3	3:C:429:PHE:HB3	1.76	0.66
5:B:4:MET:HE2	5:B:90:GLN:HB3	1.76	0.66
5:B:29:ILE:HG22	5:B:29:ILE:O	1.96	0.66
4:A:37:VAL:HG21	4:A:109:TRP:CZ3	2.30	0.66
2:L:78:LEU:C	2:L:78:LEU:HD12	2.16	0.65
4:A:151:TYR:HH	4:A:174:ALA:HB1	1.61	0.64
1:H:9:GLY:HA3	1:H:114:THR:HG22	1.78	0.64
4:A:106:MET:HG3	5:B:89:GLN:NE2	2.13	0.64
4:A:37:VAL:HB	4:A:95:TYR:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:VAL:HG22	1:H:189:VAL:HG22	1.80	0.64
2:L:181:LEU:HD23	2:L:181:LEU:O	1.98	0.64
1:H:105:PHE:CZ	3:C:378:LYS:HB3	2.33	0.64
3:C:438:SER:OG	3:C:507:PRO:C	2.37	0.63
5:B:29:ILE:HD13	5:B:90:GLN:CB	2.26	0.63
1:H:159:VAL:HG22	1:H:205:VAL:HG22	1.81	0.63
3:C:403:ARG:HD2	3:C:505:TYR:HA	1.79	0.63
2:L:37:GLN:HB2	2:L:86:TYR:CE1	2.34	0.63
1:H:34:MET:SD	1:H:100:ARG:CB	2.89	0.61
5:B:6:GLN:OE1	5:B:87:TYR:HA	2.00	0.61
2:L:96:VAL:HG12	2:L:96:VAL:O	2.02	0.60
3:C:357:ARG:NH2	3:C:396:TYR:OH	2.35	0.60
1:H:16:GLY:O	1:H:88:LEU:HD12	2.02	0.60
1:H:34:MET:HB3	1:H:81:LEU:HD22	1.84	0.60
2:L:21:ILE:HG23	2:L:102:THR:HG21	1.84	0.60
1:H:9:GLY:H	1:H:114:THR:CG2	2.14	0.59
5:B:3:GLN:O	5:B:26:SER:CB	2.49	0.59
1:H:91:GLU:OE2	1:H:91:GLU:N	2.32	0.59
4:A:36:TRP:CZ3	4:A:96:CYS:HB3	2.38	0.59
5:B:28:SER:HA	5:B:69:THR:HG22	1.85	0.59
1:H:161:TRP:CH2	1:H:203:CYS:HB3	2.38	0.58
2:L:150:VAL:CG2	2:L:155:GLN:HG3	2.32	0.58
4:A:142:ALA:HB3	4:A:195:LEU:HD11	1.84	0.58
4:A:106:MET:O	5:B:46:LEU:HD22	2.03	0.58
2:L:13:ALA:O	2:L:106:ILE:HA	2.04	0.58
2:L:79:GLN:CB	2:L:80:PRO:HD2	2.27	0.57
5:B:85:THR:CA	5:B:102:THR:O	2.51	0.57
3:C:475:ALA:HB1	5:B:31:SER:HB2	1.85	0.57
4:A:4:LEU:HD23	4:A:24:GLY:HA3	1.86	0.56
4:A:106:MET:HG3	5:B:89:GLN:HE22	1.70	0.56
5:B:144:ALA:HB2	5:B:198:HIS:CD2	2.41	0.56
5:B:85:THR:HA	5:B:103:LYS:HA	1.88	0.56
1:H:6:GLU:OE2	1:H:111:GLY:HA3	2.06	0.55
1:H:29:PHE:O	1:H:74:ARG:NH2	2.40	0.55
1:H:208:LYS:N	1:H:209:PRO:CD	2.69	0.55
4:A:175:VAL:O	4:A:182:TYR:CA	2.54	0.55
1:H:51:THR:HG23	1:H:72:ILE:HG21	1.89	0.54
5:B:79:GLN:OE1	5:B:79:GLN:HA	2.07	0.54
1:H:6:GLU:HB3	1:H:114:THR:OG1	2.07	0.54
1:H:210:SER:OG	1:H:212:THR:OG1	2.15	0.54
5:B:12:SER:HA	5:B:105:GLU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:4:MET:HE1	5:B:90:GLN:HB3	1.87	0.54
1:H:47:TRP:CD2	2:L:96:VAL:HB	2.44	0.53
4:A:184:LEU:HD23	4:A:184:LEU:O	2.07	0.53
2:L:6:GLN:NE2	2:L:102:THR:CG2	2.54	0.53
5:B:29:ILE:CD1	5:B:90:GLN:HB2	2.32	0.53
2:L:110:VAL:CG1	2:L:199:GLN:OE1	2.56	0.53
3:C:337:PRO:HD2	3:C:358:ILE:CG2	2.39	0.53
4:A:94:TYR:N	4:A:113:THR:O	2.42	0.52
1:H:17:SER:OG	1:H:86:ASN:HA	2.10	0.52
6:D:1:NAG:C8	6:D:1:NAG:C1	2.88	0.52
2:L:8:PRO:HG2	2:L:11:LEU:HB2	1.91	0.52
5:B:112:ALA:HB2	5:B:200:GLY:O	2.09	0.52
2:L:79:GLN:HB3	2:L:80:PRO:CD	2.21	0.52
3:C:404:GLY:HA2	3:C:508:TYR:CD1	2.44	0.52
5:B:86:TYR:N	5:B:102:THR:O	2.42	0.51
1:H:93:THR:O	1:H:94:ALA:HB2	2.09	0.51
5:B:112:ALA:HA	5:B:200:GLY:HA3	1.91	0.51
1:H:62:TYR:CE1	1:H:72:ILE:HG13	2.46	0.51
4:A:37:VAL:N	4:A:95:TYR:O	2.30	0.51
3:C:350:VAL:HG22	3:C:422:ASN:HB3	1.92	0.51
2:L:54:LEU:HD23	2:L:54:LEU:C	2.32	0.50
4:A:20:ILE:HD12	4:A:113:THR:CG2	2.39	0.50
3:C:487:ASN:N	3:C:487:ASN:HD22	2.10	0.50
1:H:9:GLY:N	1:H:114:THR:HG21	2.26	0.50
5:B:15:VAL:HG13	5:B:78:LEU:O	2.11	0.50
1:H:19:ARG:O	1:H:19:ARG:HG3	2.12	0.49
1:H:58:TYR:CD1	1:H:74:ARG:HD3	2.47	0.49
6:D:2:NAG:H83	6:D:2:NAG:C3	2.41	0.49
5:B:108:ARG:HB2	5:B:108:ARG:CZ	2.43	0.49
5:B:6:GLN:HE21	5:B:102:THR:HB	1.77	0.49
5:B:29:ILE:HG23	5:B:92:ASP:CG	2.32	0.49
6:D:2:NAG:C8	6:D:2:NAG:C3	2.90	0.49
4:A:106:MET:HG3	5:B:36:TYR:OH	2.13	0.49
5:B:16:GLY:C	5:B:77:SER:HA	2.32	0.49
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.48	0.48
5:B:19:VAL:O	5:B:74:THR:HA	2.13	0.48
5:B:29:ILE:CG2	5:B:29:ILE:O	2.60	0.48
4:A:36:TRP:HB2	4:A:48:MET:CB	2.43	0.48
5:B:29:ILE:CD1	5:B:90:GLN:CB	2.91	0.48
5:B:146:VAL:HG11	5:B:177:SER:HB2	1.95	0.48
4:A:132:PRO:HG3	4:A:195:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:107:ASP:OD1	5:B:55:GLN:NE2	2.47	0.48
5:B:144:ALA:HB2	5:B:198:HIS:HD2	1.76	0.48
5:B:25:ALA:HB3	5:B:69:THR:HA	1.96	0.47
4:A:142:ALA:CB	4:A:195:LEU:HD11	2.44	0.47
2:L:48:ILE:HD13	2:L:64:GLY:N	2.29	0.47
1:H:12:VAL:HG21	1:H:18:LEU:HB2	1.96	0.47
2:L:11:LEU:C	2:L:11:LEU:HD23	2.35	0.47
2:L:161:GLU:HA	2:L:176:SER:O	2.14	0.47
4:A:38:ARG:HD3	4:A:64:PHE:CZ	2.49	0.47
5:B:16:GLY:HA2	5:B:77:SER:CB	2.44	0.47
1:H:51:THR:HG23	1:H:72:ILE:CG2	2.45	0.47
2:L:16:GLY:O	2:L:77:SER:HA	2.14	0.47
4:A:37:VAL:HG11	4:A:109:TRP:HZ3	1.80	0.47
5:B:115:VAL:HA	5:B:135:LEU:O	2.14	0.47
3:C:440:ASN:ND2	3:C:441:LEU:HD13	2.29	0.46
2:L:21:ILE:CG2	2:L:102:THR:HG21	2.45	0.46
5:B:143:GLU:O	5:B:198:HIS:CD2	2.69	0.46
4:A:33:TRP:CH2	4:A:106:MET:SD	3.09	0.46
4:A:132:PRO:HD3	4:A:144:LEU:HB3	1.98	0.46
3:C:487:ASN:N	3:C:487:ASN:ND2	2.63	0.46
1:H:204:ASN:ND2	1:H:215:ASP:OD1	2.47	0.46
2:L:171:SER:O	2:L:171:SER:OG	2.34	0.46
1:H:47:TRP:CG	2:L:96:VAL:HB	2.50	0.46
1:H:161:TRP:CZ3	1:H:203:CYS:HB3	2.52	0.45
1:H:160:SER:OG	1:H:204:ASN:OD1	2.35	0.45
4:A:93:ILE:HG21	4:A:95:TYR:CE2	2.52	0.45
5:B:94:HIS:ND1	5:B:95:PRO:HA	2.30	0.45
2:L:150:VAL:HG23	2:L:155:GLN:HG3	1.98	0.45
4:A:172:PHE:CE2	5:B:176:SER:HB2	2.52	0.45
5:B:66:GLY:HA3	5:B:71:PHE:HA	1.99	0.45
1:H:40:ALA:HA	1:H:94:ALA:HA	1.98	0.45
3:C:357:ARG:HG3	3:C:396:TYR:CE1	2.52	0.45
5:B:143:GLU:O	5:B:198:HIS:HD2	2.00	0.45
1:H:22:CYS:O	1:H:80:SER:HA	2.17	0.44
1:H:33:TYR:CE2	1:H:104:PRO:HB3	2.52	0.44
3:C:410:ILE:O	3:C:433:VAL:HG21	2.17	0.44
5:B:36:TYR:OH	5:B:89:GLN:NE2	2.50	0.44
5:B:31:SER:O	5:B:50:ALA:HA	2.17	0.44
4:A:35:GLY:HA3	4:A:47:TRP:CZ2	2.52	0.44
3:C:438:SER:OG	3:C:507:PRO:O	2.35	0.44
4:A:91:THR:O	4:A:92:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:PRO:CG	2:L:11:LEU:HB2	2.48	0.44
2:L:93:ASP:OD2	3:C:385:THR:CG2	2.66	0.44
4:A:22:CYS:CB	4:A:36:TRP:CH2	3.01	0.44
4:A:38:ARG:HG2	4:A:46:GLU:HB3	2.00	0.44
1:H:73:SER:OG	1:H:82:TYR:HB2	2.18	0.43
3:C:358:ILE:CG1	3:C:395:VAL:HG13	2.48	0.43
5:B:78:LEU:CD1	5:B:82:ASP:HB2	2.48	0.43
3:C:473:TYR:HE1	3:C:475:ALA:HB2	1.83	0.43
1:H:157:VAL:CG2	1:H:185:LEU:HD21	2.49	0.43
4:A:172:PHE:HB3	5:B:162:SER:OG	2.17	0.43
2:L:10:SER:HA	2:L:103:LYS:O	2.19	0.43
2:L:143:GLU:CD	2:L:143:GLU:H	2.20	0.43
3:C:409:GLN:OE1	3:C:418:ILE:HB	2.18	0.43
2:L:80:PRO:C	2:L:81:GLU:HG3	2.39	0.43
5:B:16:GLY:HA2	5:B:77:SER:CA	2.49	0.43
2:L:187:GLU:O	2:L:211:ARG:NH2	2.52	0.43
3:C:520:ALA:HB1	3:C:521:PRO:HD2	2.01	0.43
4:A:151:TYR:CZ	4:A:174:ALA:HB1	2.49	0.43
5:B:146:VAL:HG21	5:B:175:LEU:HD22	2.01	0.43
3:C:455:LEU:HG	3:C:456:PHE:CE2	2.54	0.43
5:B:29:ILE:HG22	5:B:32:ALA:HB3	2.01	0.43
1:H:85:MET:HE1	1:H:116:VAL:HG21	2.01	0.42
2:L:93:ASP:OD1	3:C:383:SER:HB2	2.19	0.42
5:B:155:GLN:HB3	5:B:158:ASN:HD21	1.83	0.42
2:L:181:LEU:HD23	2:L:181:LEU:C	2.38	0.42
2:L:183:LYS:O	2:L:187:GLU:HG3	2.19	0.42
5:B:28:SER:CA	5:B:69:THR:HG22	2.48	0.42
4:A:76:ILE:HG13	4:A:78:THR:HB	2.01	0.42
4:A:64:PHE:HA	4:A:67:GLN:HG3	2.00	0.42
5:B:29:ILE:CG2	5:B:32:ALA:HB3	2.50	0.42
5:B:34:ASN:HB2	5:B:89:GLN:HG2	2.01	0.42
6:D:2:NAG:H82	6:D:3:FUC:C1	2.49	0.42
5:B:83:PHE:CE1	5:B:106:ILE:N	2.88	0.42
3:C:468:ILE:HG22	3:C:468:ILE:O	2.20	0.42
5:B:175:LEU:HD23	5:B:176:SER:N	2.35	0.42
5:B:90:GLN:NE2	5:B:95:PRO:O	2.53	0.42
2:L:181:LEU:HD21	2:L:186:TYR:HB2	2.00	0.41
4:A:22:CYS:HB3	4:A:36:TRP:CH2	2.55	0.41
6:D:1:NAG:C1	6:D:1:NAG:H83	2.50	0.41
3:C:438:SER:OG	3:C:507:PRO:HB2	2.19	0.41
5:B:83:PHE:HE1	5:B:105:GLU:C	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:393:THR:HG21	3:C:518:LEU:CB	2.50	0.41
1:H:38:ARG:HA	1:H:95:VAL:O	2.20	0.41
3:C:419:ALA:HA	3:C:423:TYR:O	2.19	0.41
4:A:145:GLY:HA2	4:A:160:TRP:CZ2	2.56	0.41
5:B:25:ALA:HB3	5:B:69:THR:CA	2.50	0.41
3:C:438:SER:HB3	3:C:509:ARG:HG3	2.02	0.41
4:A:149:LYS:HA	4:A:183:SER:HA	2.03	0.41
1:H:36:TRP:HD1	1:H:72:ILE:HD13	1.85	0.41
1:H:70:PHE:CZ	1:H:85:MET:HB3	2.56	0.41
5:B:136:LEU:HD12	5:B:136:LEU:N	2.35	0.41
4:A:93:ILE:CA	4:A:113:THR:O	2.64	0.41
4:A:181:LEU:HD23	4:A:181:LEU:HA	1.92	0.41
3:C:468:ILE:O	3:C:469:SER:C	2.60	0.40
2:L:6:GLN:HB3	2:L:102:THR:CG2	2.51	0.40
2:L:131:SER:OG	2:L:180:THR:HG23	2.22	0.40
4:A:106:MET:SD	4:A:106:MET:N	2.95	0.40
5:B:3:GLN:H	5:B:26:SER:CB	2.34	0.40
5:B:181:LEU:HD23	5:B:181:LEU:HA	1.96	0.40
1:H:191:VAL:CG1	1:H:201:TYR:OH	2.69	0.40
2:L:6:GLN:N	2:L:100:GLN:OE1	2.50	0.40
2:L:33:LEU:HD13	2:L:33:LEU:C	2.41	0.40
3:C:440:ASN:CG	3:C:441:LEU:HD13	2.42	0.40
3:C:340:GLU:O	3:C:344:ALA:HB2	2.21	0.40
1:H:51:THR:CG2	1:H:72:ILE:CG2	2.99	0.40
1:H:129:PHE:HB3	2:L:121:SER:OG	2.21	0.40

All (1) 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:H:123:THR:OG1	2:L:17:ASP:OD1[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	H	210/231 (91%)	201 (96%)	9 (4%)	0	100	100
2	L	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	C	190/204 (93%)	176 (93%)	14 (7%)	0	100	100
4	A	154/230 (67%)	142 (92%)	10 (6%)	2 (1%)	12	26
5	B	196/214 (92%)	177 (90%)	17 (9%)	2 (1%)	15	31
All	All	962/1093 (88%)	898 (93%)	60 (6%)	4 (0%)	34	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	155	PRO
4	A	51	ILE
5	B	6	GLN
5	B	84	ALA

### 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	H	164/195 (84%)	152 (93%)	12 (7%)	14	29
2	L	173/191 (91%)	155 (90%)	18 (10%)	7	14
3	C	149/176 (85%)	135 (91%)	14 (9%)	8	18
4	A	87/194 (45%)	76 (87%)	11 (13%)	4	8
5	B	130/187 (70%)	116 (89%)	14 (11%)	6	13
All	All	703/943 (74%)	634 (90%)	69 (10%)	8	16

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	19	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	28	THR
1	H	72	ILE
1	H	77	SER
1	H	85	MET
1	H	100	ARG
1	H	108	ASP
1	H	114	THR
1	H	166	LEU
1	H	190	THR
1	H	193	SER
1	H	219	GLU
2	L	1	ASP
2	L	7	SER
2	L	8	PRO
2	L	10	SER
2	L	11	LEU
2	L	22	THR
2	L	26	SER
2	L	54	LEU
2	L	63	SER
2	L	72	THR
2	L	78	LEU
2	L	82	ASP
2	L	100	GLN
2	L	102	THR
2	L	177	SER
2	L	181	LEU
2	L	185	ASP
2	L	214	CYS
3	C	347	PHE
3	C	354	ASN
3	C	358	ILE
3	C	373	SER
3	C	377	PHE
3	C	399	SER
3	C	408	ARG
3	C	441	LEU
3	C	443	SER
3	C	455	LEU
3	C	457	ARG
3	C	458	LYS
3	C	480	CYS

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Mol	Chain	Res	Type
3	C	525	CYS
4	A	20	ILE
4	A	38	ARG
4	A	46	GLU
4	A	63	SER
4	A	70	ILE
4	A	91	THR
4	A	116	THR
4	A	151	TYR
4	A	155	PRO
4	A	184	LEU
4	A	214	ASP
5	B	47	LEU
5	B	54	LEU
5	B	55	GLN
5	B	70	ASP
5	B	75	ILE
5	B	88	CYS
5	B	91	THR
5	B	108	ARG
5	B	159	SER
5	B	162	SER
5	B	176	SER
5	B	177	SER
5	B	199	GLN
5	B	214	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	6	GLN
2	L	138	ASN
3	C	487	ASN
5	B	34	ASN
5	B	89	GLN

### 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](#)

3 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
6	NAG	D	1	6,3	14,14,15	0.94	1 (7%)	17,19,21	2.04	8 (47%)
6	NAG	D	2	6	14,14,15	0.50	0	17,19,21	1.41	3 (17%)
6	FUC	D	3	6	10,10,11	0.55	0	14,14,16	2.05	5 (35%)

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
6	NAG	D	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	4/6/23/26	0/1/1/1
6	FUC	D	3	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1	NAG	O5-C1	-2.52	1.39	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3	FUC	C1-C2-C3	4.11	114.72	109.67
6	D	1	NAG	O5-C1-C2	-3.92	105.10	111.29
6	D	2	NAG	C2-N2-C7	3.79	128.30	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3	FUC	O2-C2-C3	-3.38	103.36	110.14
6	D	1	NAG	O5-C5-C6	-3.30	102.02	107.20
6	D	3	FUC	O5-C1-C2	-3.23	105.79	110.77
6	D	2	NAG	C8-C7-N2	2.88	120.98	116.10
6	D	1	NAG	C1-C2-N2	2.64	115.00	110.49
6	D	3	FUC	O5-C5-C4	2.52	114.04	109.52
6	D	1	NAG	O6-C6-C5	-2.49	102.73	111.29
6	D	2	NAG	O4-C4-C3	-2.38	104.84	110.35
6	D	1	NAG	O7-C7-N2	-2.37	117.59	121.95
6	D	1	NAG	C4-C3-C2	-2.35	107.58	111.02
6	D	1	NAG	C8-C7-N2	2.34	120.07	116.10
6	D	1	NAG	C1-O5-C5	2.30	115.31	112.19
6	D	3	FUC	O3-C3-C2	-2.23	105.72	109.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

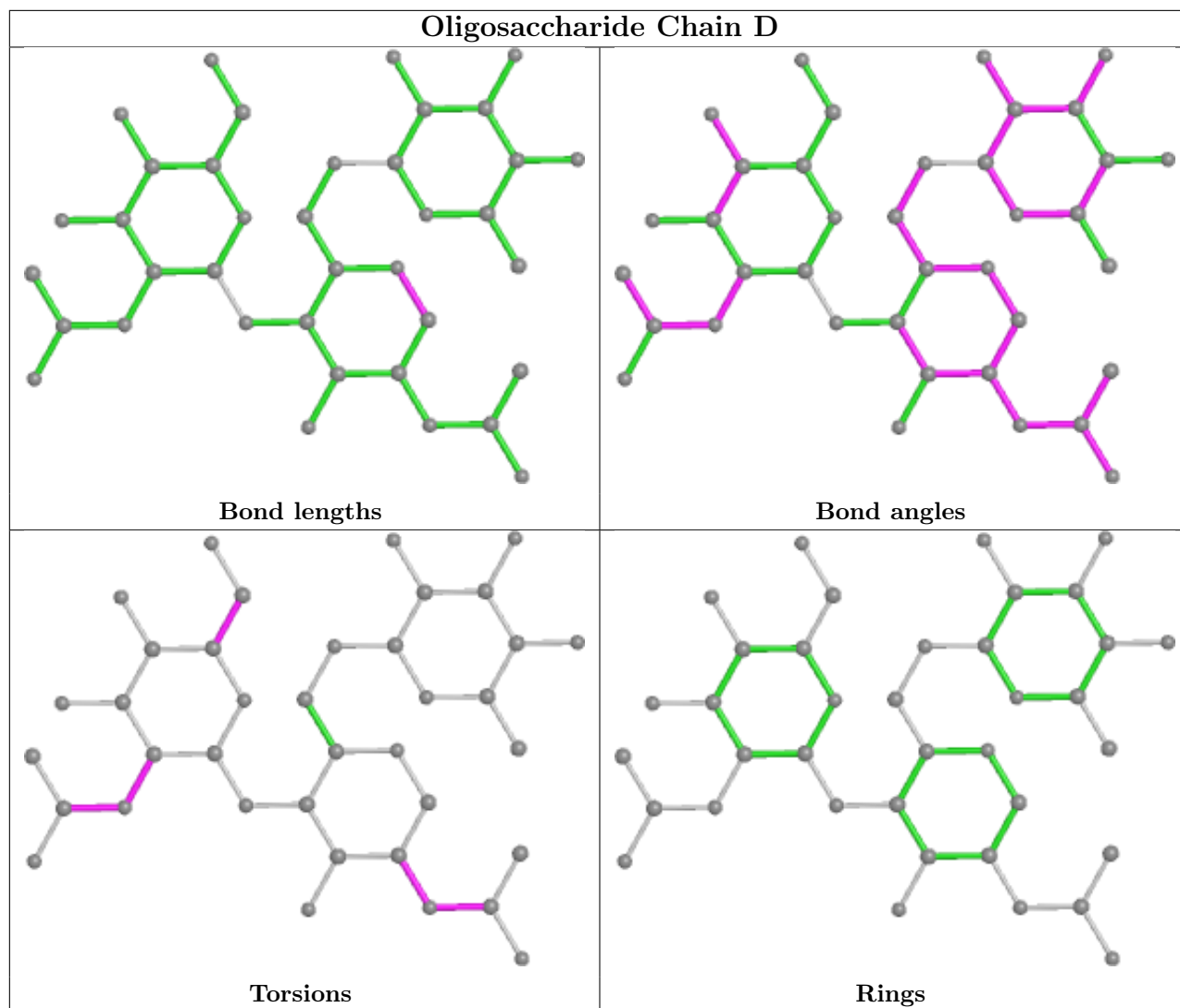
Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2
6	D	2	NAG	C3-C2-N2-C7
6	D	2	NAG	C8-C7-N2-C2
6	D	2	NAG	O7-C7-N2-C2
6	D	1	NAG	C3-C2-N2-C7
6	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2	NAG	5	0
6	D	1	NAG	2	0
6	D	3	FUC	1	0

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



## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	214/231 (92%)	-0.10	3 (1%) 75 71	42, 67, 120, 149	0
2	L	214/214 (100%)	-0.19	0 100 100	46, 67, 102, 137	0
3	C	192/204 (94%)	0.02	4 (2%) 63 58	39, 66, 124, 145	0
4	A	170/230 (73%)	0.82	26 (15%) 2 1	111, 149, 195, 209	0
5	B	202/214 (94%)	0.97	44 (21%) 0 0	81, 123, 148, 155	0
All	All	992/1093 (90%)	0.28	77 (7%) 13 8	39, 88, 162, 209	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	87	TYR	8.1
4	A	187	VAL	5.5
5	B	100	GLN	5.3
5	B	193	ALA	5.3
5	B	71	PHE	5.1
5	B	86	TYR	4.9
5	B	23	CYS	4.9
5	B	96	TYR	4.9
4	A	41	PRO	4.8
4	A	49	GLY	4.7
5	B	132	VAL	4.7
5	B	160	GLN	4.6
5	B	25	ALA	4.6
4	A	148	VAL	4.5
5	B	88	CYS	4.4
5	B	192	TYR	4.4
4	A	167	SER	4.3
5	B	180	THR	4.2
5	B	89	GLN	4.2
5	B	179	LEU	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	B	178	THR	4.1
4	A	175	VAL	3.9
5	B	2	ILE	3.8
5	B	130	ALA	3.5
5	B	148	TRP	3.5
4	A	62	PRO	3.4
5	B	149	LYS	3.4
5	B	26	SER	3.4
1	H	201	TYR	3.3
4	A	61	SER	3.3
5	B	3	GLN	3.2
4	A	71	SER	3.2
5	B	131	SER	3.0
5	B	136	LEU	3.0
5	B	27	GLN	3.0
4	A	162	SER	3.0
3	C	338	PHE	2.9
4	A	147	LEU	2.9
5	B	35	TRP	2.8
5	B	66	GLY	2.8
3	C	365	TYR	2.8
5	B	124	GLN	2.7
4	A	222	CYS	2.7
3	C	368	LEU	2.7
4	A	42	GLY	2.7
4	A	188	VAL	2.6
4	A	97	ALA	2.6
4	A	163	GLY	2.6
5	B	6	GLN	2.6
4	A	185	SER	2.6
5	B	181	LEU	2.5
4	A	193	SER	2.5
5	B	159	SER	2.4
5	B	101	GLY	2.4
5	B	185	ASP	2.4
4	A	168	GLY	2.4
5	B	33	LEU	2.4
1	H	131	LEU	2.3
5	B	91	THR	2.3
4	A	202	CYS	2.3
4	A	184	LEU	2.3
4	A	29	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	142	ALA	2.3
4	A	150	ASP	2.2
1	H	161	TRP	2.2
5	B	135	LEU	2.2
5	B	104	VAL	2.2
5	B	209	PHE	2.1
5	B	29	ILE	2.1
4	A	153	PRO	2.1
5	B	125	LEU	2.1
5	B	164	THR	2.1
3	C	363	ALA	2.1
5	B	57	GLY	2.0
5	B	176	SER	2.0
4	A	183	SER	2.0
5	B	90	GLN	2.0

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

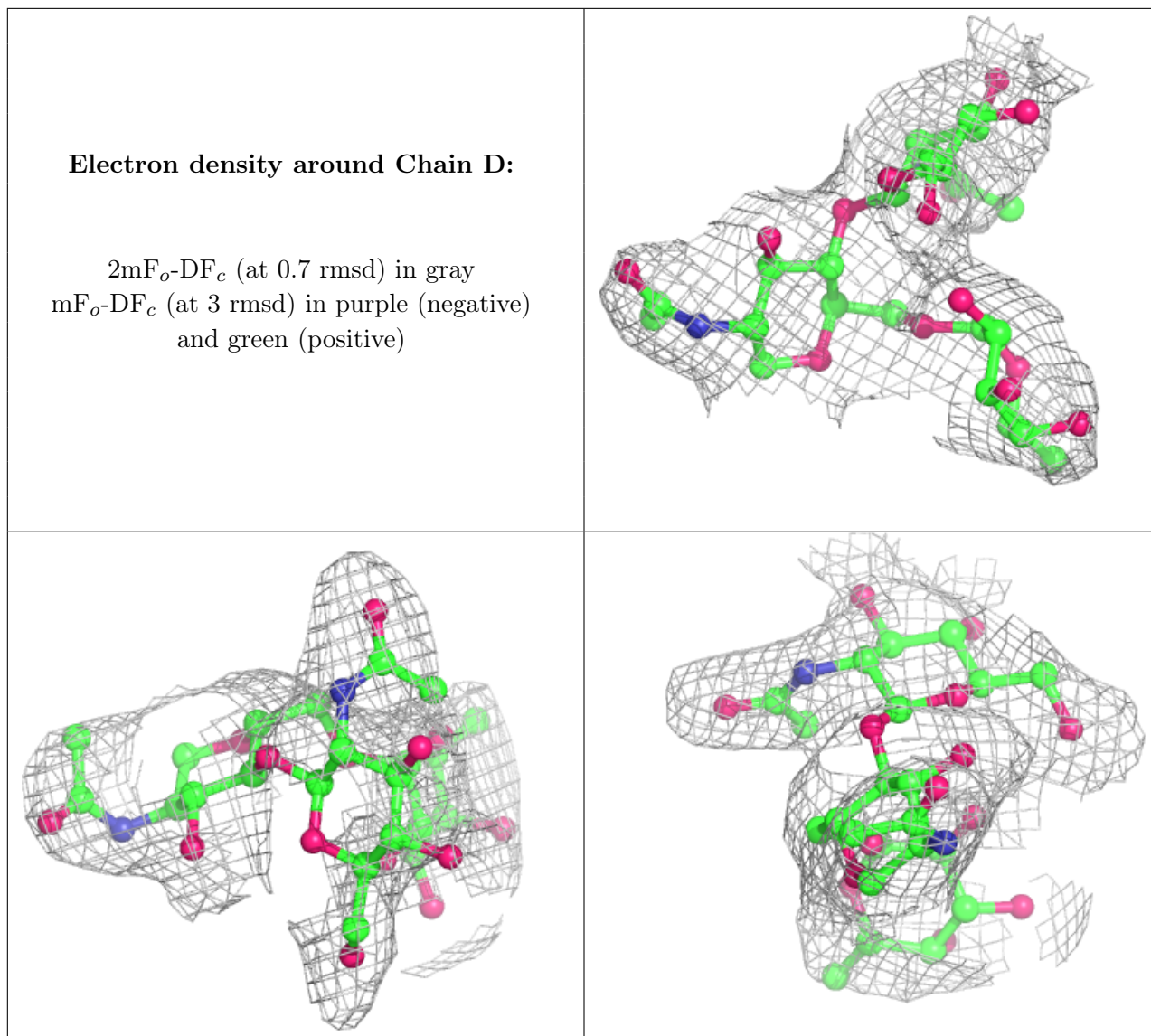
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	FUC	D	3	10/11	0.70	0.21	113,115,116,118	0
6	NAG	D	2	14/15	0.87	0.18	78,107,114,116	0
6	NAG	D	1	14/15	0.93	0.14	79,94,104,109	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	CL	L	301	1/1	0.83	0.19	98,98,98,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.