



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 02:21 AM JST

PDB ID : 7EAM
Title : immune complex of SARS-CoV-2 RBD and cross-neutralizing antibody 7D6
Authors : Li, T.T.; Gu, Y.; Li, S.W.
Deposited on : 2021-03-07
Resolution : 1.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

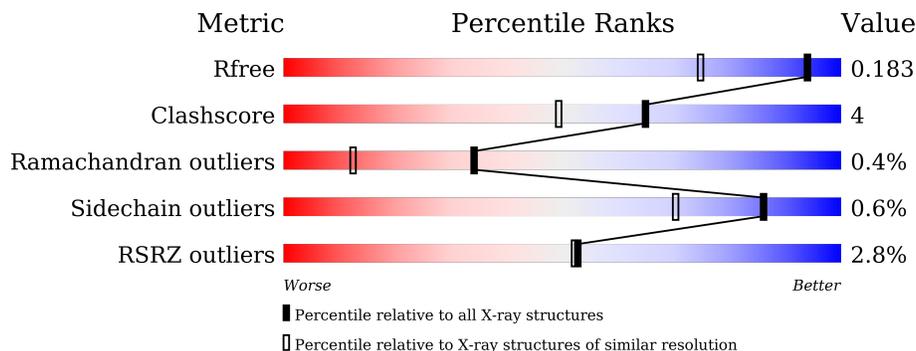
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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.



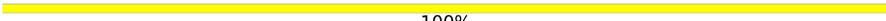
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	233	 5% 79% 9% 12%
1	B	233	 9% 78% 9% 12%
2	C	220	 % 90% 7% •
2	H	220	 % 90% 7% •
3	D	214	 95% 5%
3	L	214	 93% 7%

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	F	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11106 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	204	1618	1038	270	302	8	0	0	0
1	B	204	1618	1038	270	302	8	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	HIS	-	expression tag	UNP P0DTC2
A	543	HIS	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2
A	550	HIS	-	expression tag	UNP P0DTC2
A	551	HIS	-	expression tag	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
B	548	HIS	-	expression tag	UNP P0DTC2
B	549	HIS	-	expression tag	UNP P0DTC2
B	550	HIS	-	expression tag	UNP P0DTC2
B	551	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called the heavy chain of Fab fragment of antibody 7D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	215	Total 1638	C 1033	N 263	O 336	S 6	0	0	0
2	C	215	Total 1638	C 1033	N 263	O 336	S 6	0	0	0

- Molecule 3 is a protein called the light chain of Fab fragment of antibody 7D6.

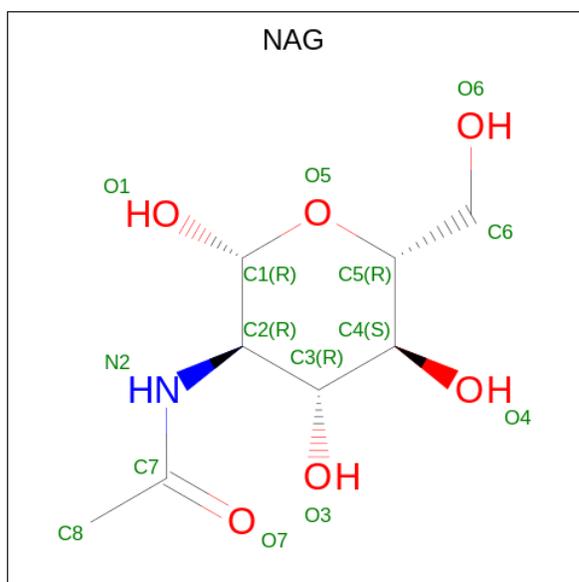
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	Total 1662	C 1038	N 283	O 335	S 6	0	0	0
3	D	214	Total 1662	C 1038	N 283	O 335	S 6	0	0	0

- 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
			Total	C	N	O			
4	E	2	Total 28	C 16	N 2	O 10	0	0	0
4	F	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 water.

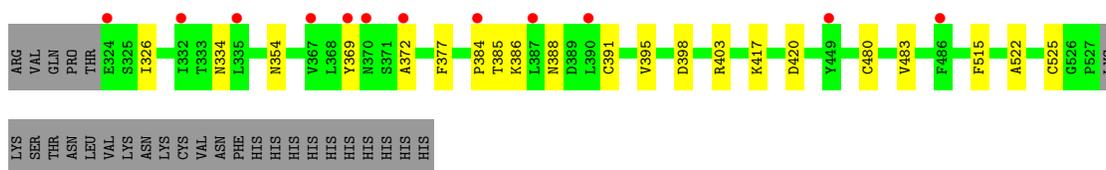
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	141	Total	O	0	0
			141	141		
6	H	243	Total	O	0	0
			243	243		
6	L	213	Total	O	0	0
			213	213		
6	B	142	Total	O	0	0
			142	142		
6	C	228	Total	O	0	0
			228	228		
6	D	219	Total	O	0	0
			219	219		

3 Residue-property plots

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

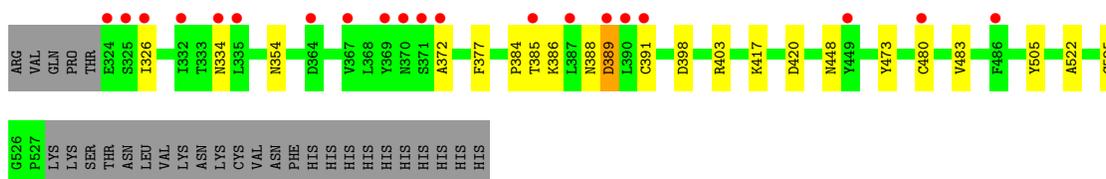
- Molecule 1: Spike protein S1

Chain A: 

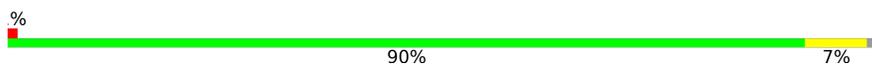


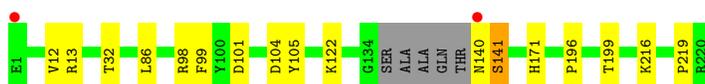
- Molecule 1: Spike protein S1

Chain B: 

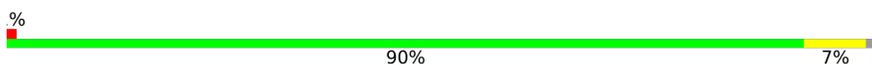


- Molecule 2: the heavy chain of Fab fragment of antibody 7D6

Chain H: 



- Molecule 2: the heavy chain of Fab fragment of antibody 7D6

Chain C: 



- Molecule 3: the light chain of Fab fragment of antibody 7D6

Chain L: 



- Molecule 3: the light chain of Fab fragment of antibody 7D6

Chain D: 95% 5%



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

Chain E: 100%



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

Chain F: 100%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.44Å 87.97Å 102.72Å 89.96° 87.05° 89.98°	Depositor
Resolution (Å)	22.32 – 1.40 29.32 – 1.40	Depositor EDS
% Data completeness (in resolution range)	92.3 (22.32-1.40) 83.2 (29.32-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 1.40Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.174 , 0.181 0.182 , 0.183	Depositor DCC
R_{free} test set	1952 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtrriage
Anisotropy	0.501	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-l 0.460 for -h,k,-l 0.027 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11106	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.46	0/1664	0.64	0/2266
1	B	0.46	0/1664	0.64	0/2266
2	C	0.53	0/1681	0.72	0/2302
2	H	0.52	0/1681	0.74	0/2302
3	D	0.50	0/1704	0.68	0/2317
3	L	0.50	0/1704	0.67	0/2317
All	All	0.50	0/10098	0.68	0/13770

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1618	0	1535	16	0
1	B	1618	0	1535	20	0
2	C	1638	0	1564	14	0
2	H	1638	0	1564	14	0
3	D	1662	0	1582	7	0
3	L	1662	0	1582	11	0
4	E	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	28	0	25	1	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	141	0	0	8	1
6	B	142	0	0	12	1
6	C	228	0	0	2	0
6	D	219	0	0	5	0
6	H	243	0	0	2	0
6	L	213	0	0	8	0
All	All	11106	0	9438	80	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 4.

All (80) 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:A:417:LYS:NZ	6:A:701:HOH:O	1.97	0.98
3:D:79:GLN:OE1	6:D:301:HOH:O	1.86	0.93
1:B:417:LYS:NZ	6:B:703:HOH:O	2.03	0.90
2:H:104:ASP:OD1	6:H:301:HOH:O	1.91	0.89
1:B:334:ASN:OD1	6:B:701:HOH:O	1.95	0.84
1:A:384:PRO:O	1:A:385:THR:OG1	1.99	0.80
1:B:384:PRO:O	1:B:385:THR:OG1	2.00	0.79
1:A:334:ASN:OD1	6:A:703:HOH:O	2.01	0.78
1:A:372:ALA:O	6:A:702:HOH:O	2.00	0.78
1:B:372:ALA:O	6:B:702:HOH:O	2.02	0.77
3:L:79:GLN:NE2	6:L:302:HOH:O	2.15	0.74
3:L:56:ASP:O	6:L:301:HOH:O	2.05	0.73
1:A:386:LYS:NZ	6:A:705:HOH:O	2.17	0.73
1:A:420:ASP:OD1	6:A:704:HOH:O	2.06	0.72
1:B:403:ARG:NH1	6:B:707:HOH:O	2.18	0.72
1:B:386:LYS:NZ	6:B:704:HOH:O	2.11	0.68
2:C:101:ASP:OD2	6:C:301:HOH:O	2.12	0.67
1:A:403:ARG:HD2	6:A:710:HOH:O	1.96	0.66
1:B:505:TYR:OH	6:B:705:HOH:O	2.13	0.63
2:H:140:ASN:HA	2:H:141:SER:CB	2.30	0.61
2:C:140:ASN:HA	2:C:141:SER:CB	2.31	0.61
3:L:186:GLU:OE2	6:L:303:HOH:O	2.16	0.60
2:C:12:VAL:HG21	2:C:86:LEU:HD13	1.84	0.60
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:TYR:OH	6:B:706:HOH:O	2.18	0.56
1:B:403:ARG:HD2	6:B:707:HOH:O	2.05	0.56
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.87	0.55
2:H:122:LYS:NZ	6:H:308:HOH:O	2.39	0.55
1:A:391:CYS:HB3	1:A:522:ALA:HB1	1.88	0.55
1:A:525:CYS:HB2	4:E:2:NAG:H83	1.87	0.54
3:L:148:LYS:HE2	6:L:337:HOH:O	2.07	0.54
3:D:148:LYS:HE2	6:D:356:HOH:O	2.07	0.54
3:D:169:SER:HA	6:D:475:HOH:O	2.07	0.53
2:H:171:HIS:HD2	6:L:475:HOH:O	1.92	0.52
3:L:1:ASP:OD2	6:L:304:HOH:O	2.19	0.52
2:C:171:HIS:HD2	6:D:483:HOH:O	1.92	0.52
2:H:32:THR:HG21	2:H:98:ARG:HG3	1.93	0.51
1:B:525:CYS:HB2	4:F:2:NAG:H83	1.93	0.51
3:D:30:HIS:HE1	6:D:495:HOH:O	1.93	0.51
3:L:143:LYS:NZ	6:L:309:HOH:O	2.43	0.51
2:C:140:ASN:HA	2:C:141:SER:HB3	1.92	0.51
2:H:140:ASN:HA	2:H:141:SER:HB3	1.91	0.50
1:A:403:ARG:NH1	6:A:710:HOH:O	2.37	0.49
2:C:105:TYR:HB3	3:D:49:TYR:CG	2.48	0.49
1:A:354:ASN:O	1:A:398:ASP:HA	2.13	0.49
1:B:354:ASN:O	1:B:398:ASP:HA	2.12	0.48
2:H:105:TYR:HB3	3:L:49:TYR:CG	2.49	0.47
3:L:186:GLU:CG	6:L:303:HOH:O	2.61	0.47
2:H:140:ASN:CA	2:H:141:SER:CB	2.93	0.46
2:C:140:ASN:CA	2:C:141:SER:CB	2.93	0.46
1:B:420:ASP:OD1	6:B:708:HOH:O	2.21	0.46
2:C:196:PRO:HB3	2:C:219:PRO:HG3	1.98	0.46
1:A:384:PRO:O	1:A:385:THR:CB	2.64	0.46
1:B:389:ASP:N	1:B:389:ASP:OD1	2.49	0.46
1:B:480:CYS:O	1:B:483:VAL:HG12	2.16	0.45
3:D:33:LEU:HD22	3:D:71:TYR:CG	2.51	0.45
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.81	0.45
3:D:48:VAL:HG22	3:D:54:LEU:HD23	1.99	0.45
2:H:140:ASN:CA	2:H:141:SER:HB3	2.47	0.45
1:B:448:ASN:O	6:B:709:HOH:O	2.21	0.44
2:H:199:THR:HG22	2:H:216:LYS:HE3	1.98	0.44
2:C:41:PRO:HG3	6:C:500:HOH:O	2.18	0.44
2:H:140:ASN:HA	2:H:141:SER:OG	2.17	0.44
1:B:384:PRO:O	1:B:385:THR:CB	2.66	0.44
2:C:140:ASN:HA	2:C:141:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:48:VAL:HG22	3:L:54:LEU:HD23	2.01	0.43
3:L:33:LEU:HD22	3:L:71:TYR:CG	2.53	0.43
2:C:140:ASN:CA	2:C:141:SER:HB3	2.48	0.43
1:B:326:ILE:O	1:B:326:ILE:HG23	2.19	0.43
1:A:480:CYS:O	1:A:483:VAL:HG12	2.19	0.43
2:C:32:THR:HG21	2:C:98:ARG:HG3	2.02	0.42
2:C:157:VAL:CG2	2:C:184:LEU:HD21	2.49	0.42
2:H:196:PRO:HB3	2:H:219:PRO:HG3	2.02	0.42
2:H:99:PHE:CE2	2:H:101:ASP:HA	2.55	0.41
1:A:372:ALA:CA	6:A:723:HOH:O	2.69	0.41
3:L:17:GLU:HG2	3:L:18:THR:N	2.35	0.41
1:B:372:ALA:HA	6:B:730:HOH:O	2.21	0.41
2:C:99:PHE:CE2	2:C:101:ASP:HA	2.56	0.41
1:A:326:ILE:O	1:A:326:ILE:HG23	2.21	0.40
1:B:372:ALA:CA	6:B:730:HOH:O	2.69	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)
6:A:821:HOH:O	6:B:718:HOH:O[1_564]	1.77	0.43

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	202/233 (87%)	191 (95%)	10 (5%)	1 (0%)	29 9
1	B	202/233 (87%)	191 (95%)	11 (5%)	0	100 100
2	C	211/220 (96%)	206 (98%)	4 (2%)	1 (0%)	29 9
2	H	211/220 (96%)	207 (98%)	3 (1%)	1 (0%)	29 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	212/214 (99%)	210 (99%)	1 (0%)	1 (0%)	29	9
3	L	212/214 (99%)	208 (98%)	3 (1%)	1 (0%)	29	9
All	All	1250/1334 (94%)	1213 (97%)	32 (3%)	5 (0%)	34	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	141	SER
2	C	141	SER
3	D	93	SER
3	L	93	SER
1	A	369	TYR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/206 (86%)	175 (99%)	2 (1%)	73	50
1	B	177/206 (86%)	174 (98%)	3 (2%)	60	31
2	C	187/190 (98%)	186 (100%)	1 (0%)	88	74
2	H	187/190 (98%)	186 (100%)	1 (0%)	88	74
3	D	188/188 (100%)	188 (100%)	0	100	100
3	L	188/188 (100%)	188 (100%)	0	100	100
All	All	1104/1168 (94%)	1097 (99%)	7 (1%)	86	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	PHE
1	A	388	ASN
2	H	13	ARG
1	B	377	PHE
1	B	388	ASN

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Mol	Chain	Res	Type
1	B	389	ASP
2	C	13	ARG

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

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](#)

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	E	1	1,4	14,14,15	1.30	1 (7%)	17,19,21	0.54	0
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	F	1	1,4	14,14,15	1.52	2 (14%)	17,19,21	0.51	0
4	NAG	F	2	4	14,14,15	0.25	0	17,19,21	0.45	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	E	1	1,4	-	0/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O4-C4	5.17	1.55	1.43
4	E	1	NAG	O4-C4	4.45	1.53	1.43
4	F	1	NAG	O5-C1	-2.27	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

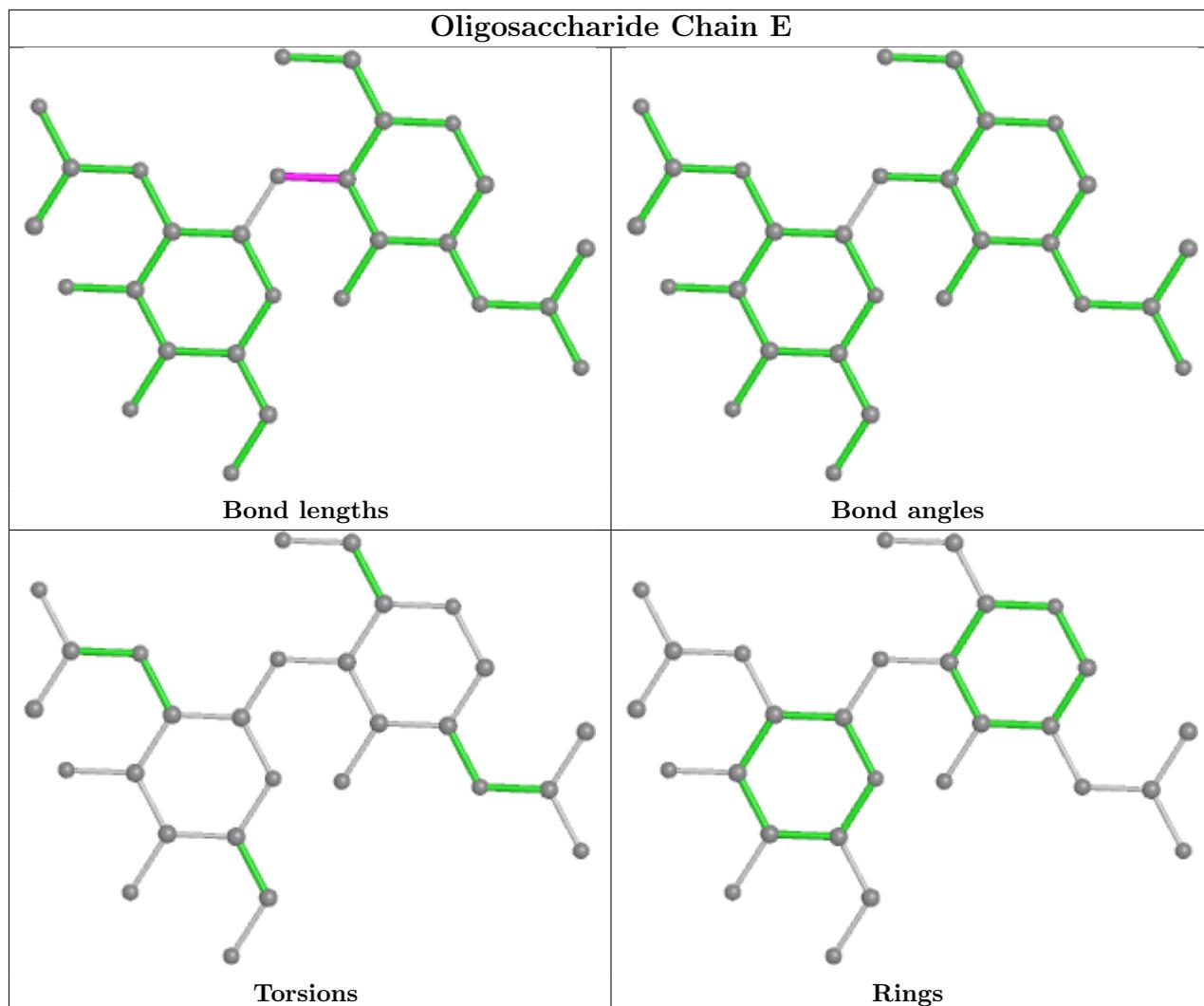
There are no torsion outliers.

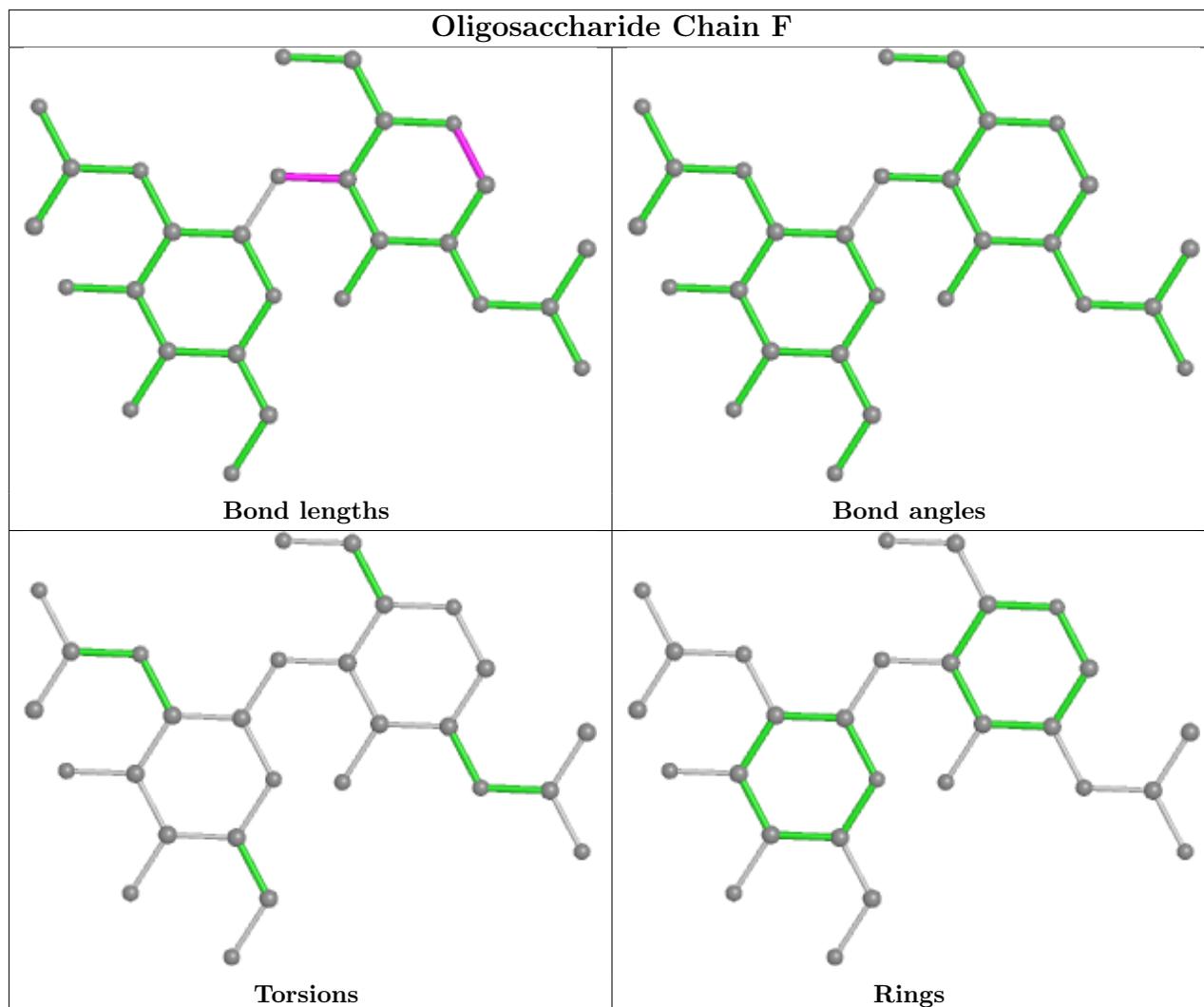
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	E	2	NAG	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	601	1	14,14,15	0.30	0	17,19,21	0.45	0
5	NAG	B	601	1	14,14,15	0.22	0	17,19,21	0.45	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	NAG	O5-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6

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	204/233 (87%)	0.04	12 (5%) 22 20	19, 36, 89, 126	0
1	B	204/233 (87%)	0.11	20 (9%) 7 7	18, 36, 85, 124	0
2	C	215/220 (97%)	-0.52	2 (0%) 84 82	18, 26, 62, 130	0
2	H	215/220 (97%)	-0.47	2 (0%) 84 82	18, 26, 58, 138	0
3	D	214/214 (100%)	-0.51	0 100 100	19, 30, 63, 90	0
3	L	214/214 (100%)	-0.49	0 100 100	20, 30, 62, 85	0
All	All	1266/1334 (94%)	-0.31	36 (2%) 53 52	18, 30, 76, 138	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	LEU	13.0
2	H	140	ASN	11.0
2	C	140	ASN	10.6
1	B	369	TYR	10.2
1	B	387	LEU	9.6
1	A	369	TYR	9.5
1	B	390	LEU	7.2
1	B	324	GLU	6.1
1	B	370	ASN	5.1
1	A	370	ASN	5.1
1	A	390	LEU	4.6
1	A	324	GLU	4.1
1	B	372	ALA	4.0
1	B	449	TYR	4.0
1	A	384	PRO	3.9
1	B	326	ILE	3.9
1	A	332	ILE	3.8
1	B	325	SER	3.6
1	A	335	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	367	VAL	3.2
1	A	372	ALA	3.0
1	B	364	ASP	3.0
2	H	1	GLU	2.9
1	B	391	CYS	2.9
1	A	367	VAL	2.9
1	B	371	SER	2.7
1	B	332	ILE	2.7
1	B	335	LEU	2.6
1	B	486	PHE	2.5
2	C	105	TYR	2.3
1	B	480	CYS	2.2
1	B	334	ASN	2.2
1	B	389	ASP	2.2
1	A	449	TYR	2.1
1	B	385	THR	2.1
1	A	486	PHE	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](#)

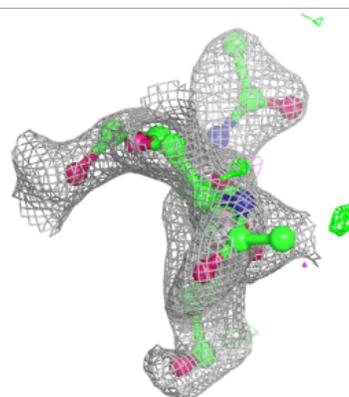
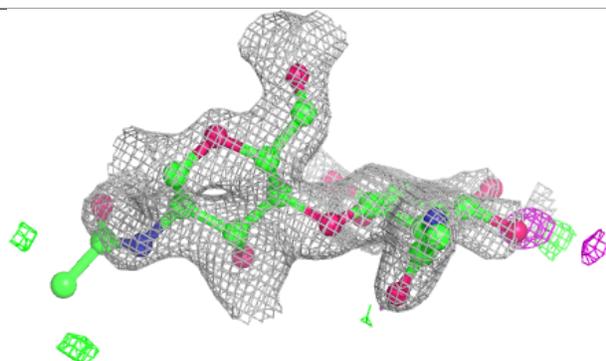
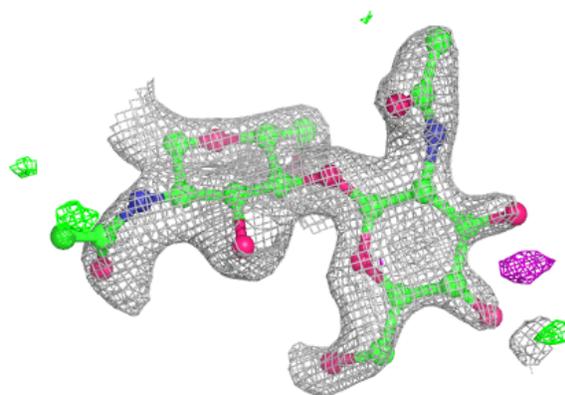
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	F	1	14/15	0.56	0.25	116,128,132,142	0
4	NAG	E	1	14/15	0.65	0.18	77,82,85,87	0
4	NAG	F	2	14/15	0.65	0.24	127,136,141,141	0
4	NAG	E	2	14/15	0.74	0.16	75,89,91,93	0

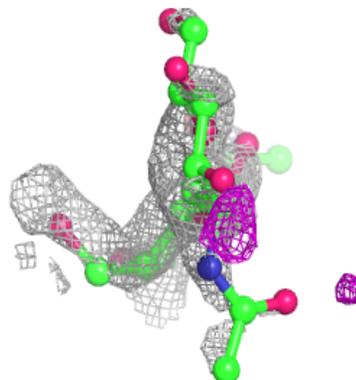
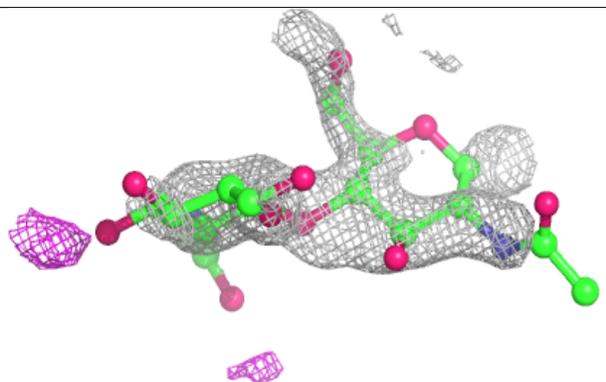
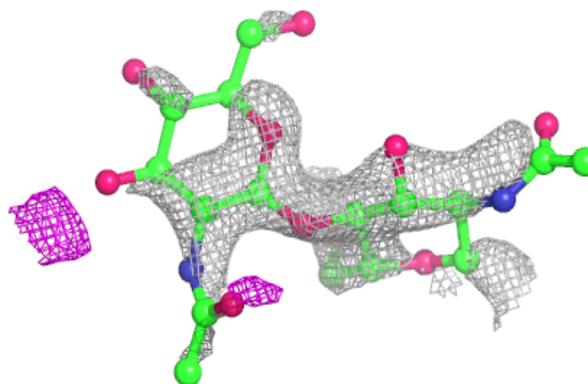
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
5	NAG	B	601	14/15	0.78	0.14	90,107,126,132	0
5	NAG	A	601	14/15	0.87	0.09	49,65,78,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.