wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 01:13 PM EDT

PDB ID	:	2AJF
Title	:	Structure of SARS coronavirus spike receptor-binding domain complexed with its receptor
Authors	:	Li, F.; Li, W.; Farzan, M.; Harrison, S.C.
Deposited on	:	2005-08-01
Resolution	:	2.90 Å(reported)

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

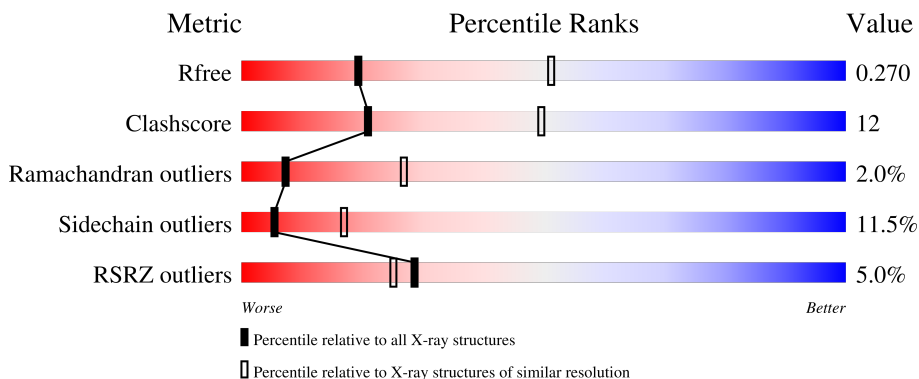|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.90 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		12
Ramachandran outliers		2.0%
Sidechain outliers		11.5%
RSRZ outliers		5.0%

■ Percentile relative to all X-ray structures
⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	597	3% / 66% / 30% / •
1	B	597	5% / 67% / 28% / 5%
2	E	180	8% / 72% / 21% / • • •
2	F	180	8% / 67% / 24% / 5% • •
3	C	3	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	3	33%　　　　　　33%　　　　　　33%

wwPDB X-ray Structure Validation Summary Report

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 12777 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 Angiotensin-converting enzyme-Related Carboxypeptidase (Ace2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			
1	B	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			

- Molecule 2 is a protein called SARS-coronavirus spike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	174	Total	C	N	O	S	0	0	0
			1403	909	228	259	7			
2	F	174	Total	C	N	O	S	0	0	0
			1403	909	228	259	7			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
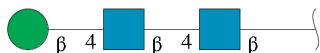
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Cl 1	0	0

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0

- Molecule 7 is water.

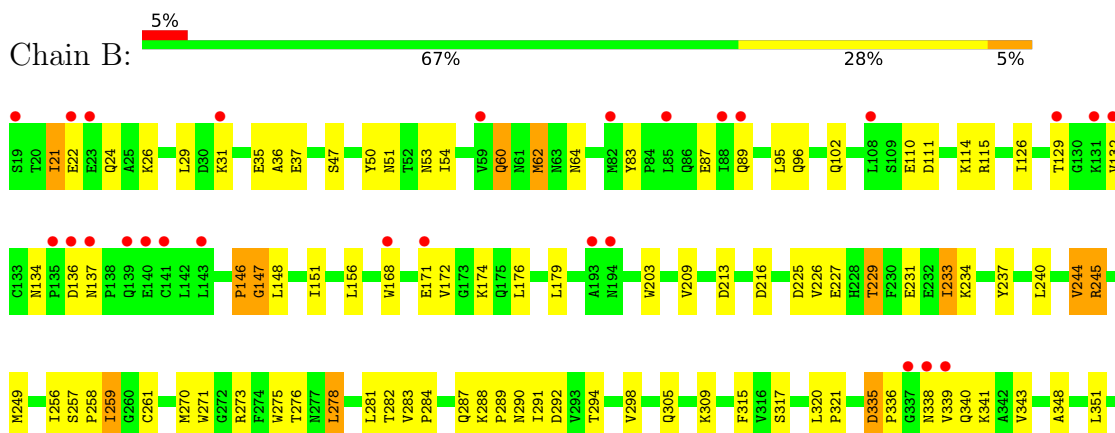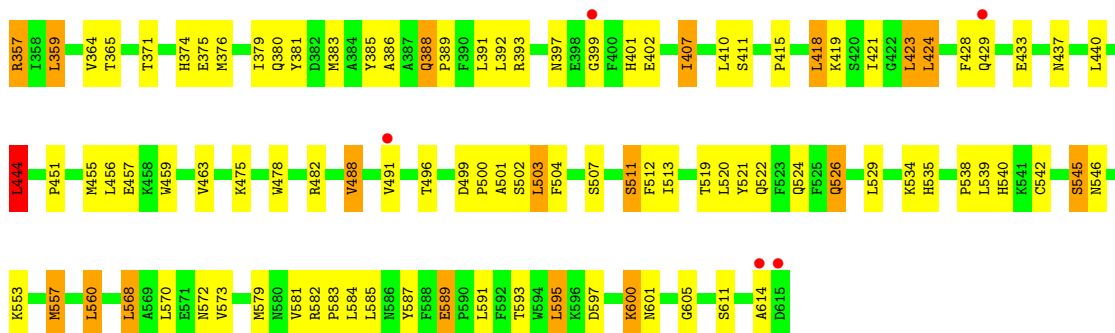| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total 36	O 36	0	0
7	B	24	Total 24	O 24	0	0
7	E	4	Total 4	O 4	0	0
7	F	1	Total 1	O 1	0	0

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.

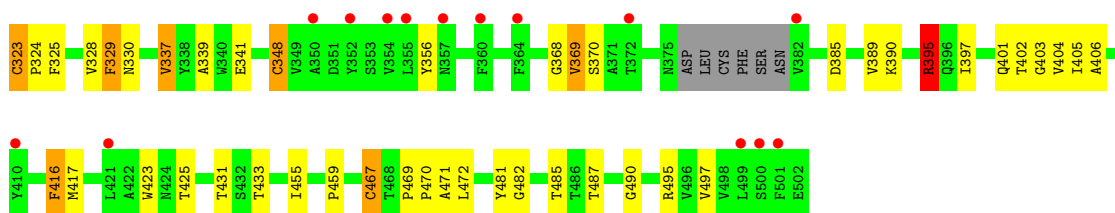- Molecule 1: Angiotensin-converting enzyme-Related Carboxypeptidase (Ace2)

Chain A:

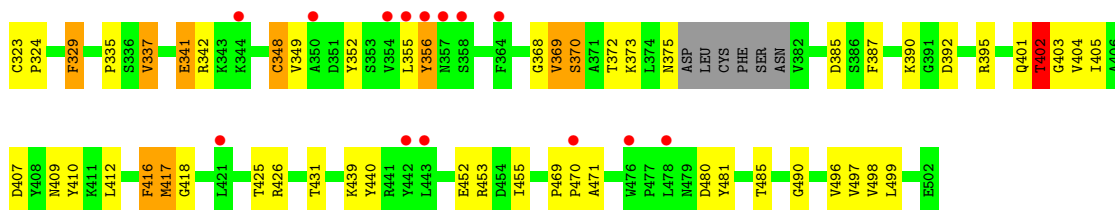- Molecule 1: Angiotensin-converting enzyme-Related Carboxypeptidase (Ace2)

Chain B:

R357 I358 L359 V364 T365 T371 H374 E375 M376 I379 Q380 Y381 D382 M383 A384 Y385 A386 A387 Q388 P389 F390 L391 L392 R393 N397 E398 G399 F400 H401 E402 I407 L410 S411 P415 L418 K419 S420 I421 G422 L423 L424 F428 Q429 E433 N437 L440

L444 P451 M455 L456 E457 K458 W459 V463 K475 W478 R482 V488 V491 T496 D499 P500 A501 S502 L503 F504 S507 S511 F512 I513 T519 L520 Y521 Q522 F523 Q524 F525 Q526 L529 K534 H535 P538 L539 H540 K541 C542 S545 N546

K553 M557 L560 L568 A569 L570 E571 N572 V573 M579 N580 V581 R582 P583 L584 L585 N586 Y587 F588 E589 P590 L591 F592 T593 W594 L595 K596 D597 K600 N601 G605 S611 A614 D615

• Molecule 2: SARS-coronavirus spike protein

Chain E:

C323 P324 F325 V328 F329 N330 V337 Y338 A339 W340 E341 C348 V349 A350 D351 Y352 S353 V354 L355 Y356 N357 F360 F364 G368 G369 S370 A371 T372 N375 ASP LEU CYS PHE SER ASN V382 D385 V389 K390 R395 Q396 I397 Q401 T402 G403 V404 I405 A406

Y410 F416 M417 L421 A422 W423 N424 T425 T431 S432 T433 I455 P459 C467 T468 P469 P470 A471 L472 Y481 G482 T485 T486 T487 G490 R495 V496 V497 V498 L499 S500 F501 E502

• Molecule 2: SARS-coronavirus spike protein

Chain F:

C323 P324 F329 P335 S336 V337 E341 R342 K343 K344 C348 V349 A350 D351 Y352 S353 V354 L355 Y356 N357 S358 F364 G368 G369 S370 A371 T372 K373 L374 N375 ASP LEU CYS PHE SER ASN V382 D385 S386 F387 K390 G391 D392 R395 Q401 T402 G403 V404 I405 A406

D407 Y408 N409 Y410 K411 L412 F416 M417 G418 L421 T425 R426 T431 K439 V440 R441 Y442 L443 E452 R453 D454 I455 P469 P470 A471 W476 P477 L478 N479 D480 Y481 T485 G490 V496 V497 V498 L499 E502

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

NAG1 NAG2 BMA3

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

NAG1 NAG2 BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.30Å 119.43Å 113.24Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	47.40 – 2.90 47.39 – 2.81	Depositor EDS
% Data completeness (in resolution range)	92.4 (47.40-2.90) 85.9 (47.39-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.218 , 0.275 0.213 , 0.270	Depositor DCC
R_{free} test set	2449 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	73.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 80.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, BMA, NAG, ZN

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	0.47	0/5007	0.62	0/6803
1	B	0.45	0/5007	0.58	2/6803 (0.0%)
2	E	0.47	0/1448	0.62	0/1972
2	F	0.44	0/1448	0.60	0/1972
All	All	0.46	0/12910	0.60	2/17550 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	444	LEU	CA-CB-CG	5.95	128.99	115.30
1	B	423	LEU	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4870	0	4639	124	0
1	B	4870	0	4641	124	0
2	E	1403	0	1326	24	0
2	F	1403	0	1325	31	0
3	C	39	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	39	0	34	1	0
4	A	42	0	39	2	0
4	B	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	A	36	0	0	3	0
7	B	24	0	0	3	0
7	E	4	0	0	0	0
7	F	1	0	0	0	0
All	All	12777	0	12077	302	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 302 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:320:LEU:HD13	1:A:380:GLN:HG2	1.36	1.05
1:A:261:CYS:HB2	1:A:488:VAL:CG2	1.93	0.97
1:B:245:ARG:HG2	1:B:245:ARG:HH21	1.32	0.94
1:A:261:CYS:HB2	1:A:488:VAL:HG22	1.48	0.94
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.49	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	595/597 (100%)	536 (90%)	55 (9%)	4 (1%)	22	54
1	B	595/597 (100%)	529 (89%)	56 (9%)	10 (2%)	9	31
2	E	170/180 (94%)	137 (81%)	24 (14%)	9 (5%)	2	6
2	F	170/180 (94%)	143 (84%)	19 (11%)	8 (5%)	2	8
All	All	1530/1554 (98%)	1345 (88%)	154 (10%)	31 (2%)	7	27

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
1	B	146	PRO
2	E	402	THR
2	E	404	VAL
2	E	416	PHE

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	527/527 (100%)	458 (87%)	69 (13%)	4	12
1	B	527/527 (100%)	473 (90%)	54 (10%)	7	22
2	E	152/158 (96%)	134 (88%)	18 (12%)	5	16
2	F	152/158 (96%)	137 (90%)	15 (10%)	8	24
All	All	1358/1370 (99%)	1202 (88%)	156 (12%)	5	17

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	568	LEU
2	F	341	GLU
1	B	589	GLU
2	E	395	ARG
2	F	417	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	556	ASN
1	B	586	ASN
2	E	473	ASN
1	A	580	ASN
1	A	526	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

6 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	$\#|Z| > 2$
3	NAG	C	1	3,1	14,14,15	0.48	0	17,19,21	2.04	6 (35%)
3	NAG	C	2	3	14,14,15	0.33	0	17,19,21	2.62	3 (17%)
3	BMA	C	3	3	11,11,12	0.62	0	15,15,17	1.12	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.54	0	17,19,21	0.77	0
3	NAG	D	2	3	14,14,15	0.48	0	17,19,21	1.18	2 (11%)
3	BMA	D	3	3	11,11,12	0.63	0	15,15,17	1.44	4 (26%)

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
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C1-O5-C5	8.95	124.32	112.19
3	C	1	NAG	C1-O5-C5	5.90	120.18	112.19
3	C	2	NAG	O5-C1-C2	4.29	118.06	111.29
3	D	3	BMA	C1-C2-C3	3.13	113.52	109.67
3	C	3	BMA	C1-O5-C5	3.10	116.39	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
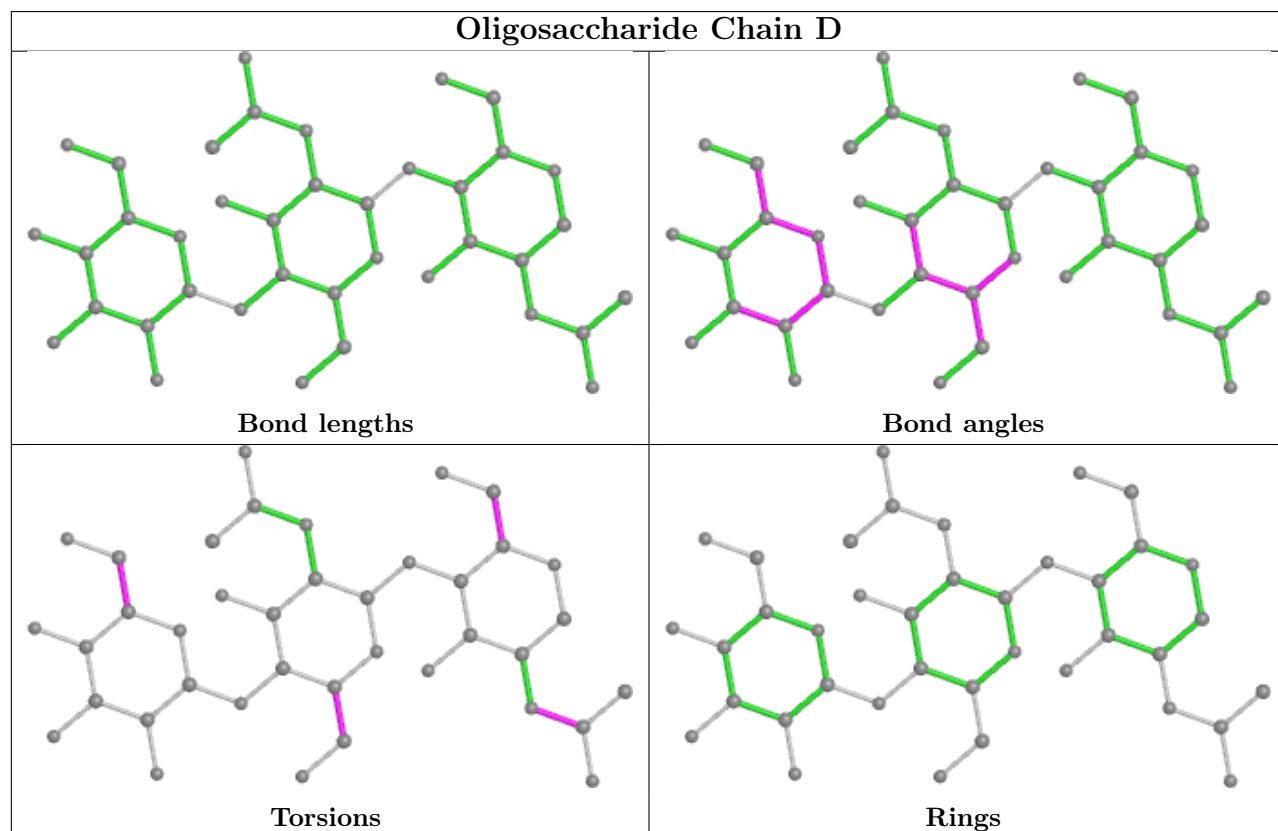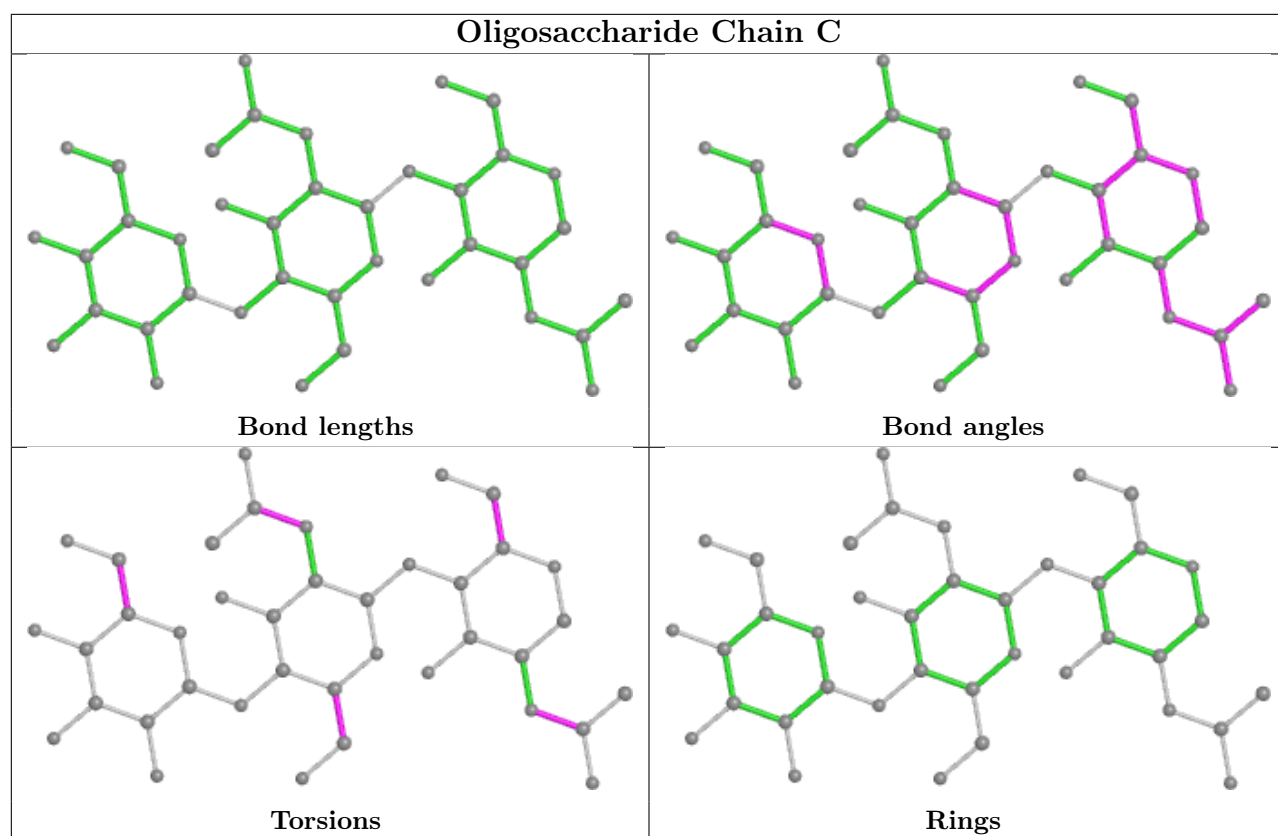
5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	NAG	A	1322	1	14,14,15	0.56	0	17,19,21	1.83	1 (5%)
4	NAG	A	1546	1	14,14,15	0.71	0	17,19,21	1.79	3 (17%)
4	NAG	E	1330	2	14,14,15	0.51	0	17,19,21	1.41	2 (11%)
4	NAG	F	1330	2	14,14,15	0.51	0	17,19,21	2.19	4 (23%)
4	NAG	A	1053	1	14,14,15	0.48	0	17,19,21	1.38	2 (11%)
4	NAG	B	1322	1	14,14,15	0.52	0	17,19,21	1.14	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1322	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1546	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1330	2	-	2/6/23/26	0/1/1/1
4	NAG	F	1330	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1053	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1322	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1322	NAG	C1-O5-C5	6.22	120.62	112.19
4	F	1330	NAG	C1-O5-C5	5.82	120.08	112.19
4	A	1053	NAG	C1-O5-C5	4.34	118.07	112.19
4	F	1330	NAG	C4-C3-C2	-4.33	104.67	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1546	NAG	C4-C3-C2	-3.95	105.23	111.02

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1053	NAG	O7-C7-N2-C2
4	A	1322	NAG	C8-C7-N2-C2
4	A	1322	NAG	O7-C7-N2-C2
4	A	1053	NAG	C8-C7-N2-C2
4	B	1322	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1546	NAG	2	0

5.7 Other polymers ⓘ

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 ⓘ

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	597/597 (100%)	0.14	17 (2%)	53	49	56, 82, 123, 147	0
1	B	597/597 (100%)	0.38	32 (5%)	25	22	56, 82, 123, 148	0
2	E	174/180 (96%)	0.45	14 (8%)	12	9	75, 96, 142, 153	0
2	F	174/180 (96%)	0.43	14 (8%)	12	9	76, 96, 142, 152	0
All	All	1542/1554 (99%)	0.30	77 (4%)	28	25	56, 88, 131, 153	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	ASP	6.7
1	B	615	ASP	6.5
1	B	140	GLU	5.4
2	E	501	PHE	5.2
2	F	354	VAL	5.1

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

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

6.3 Carbohydrates ⓘ

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.
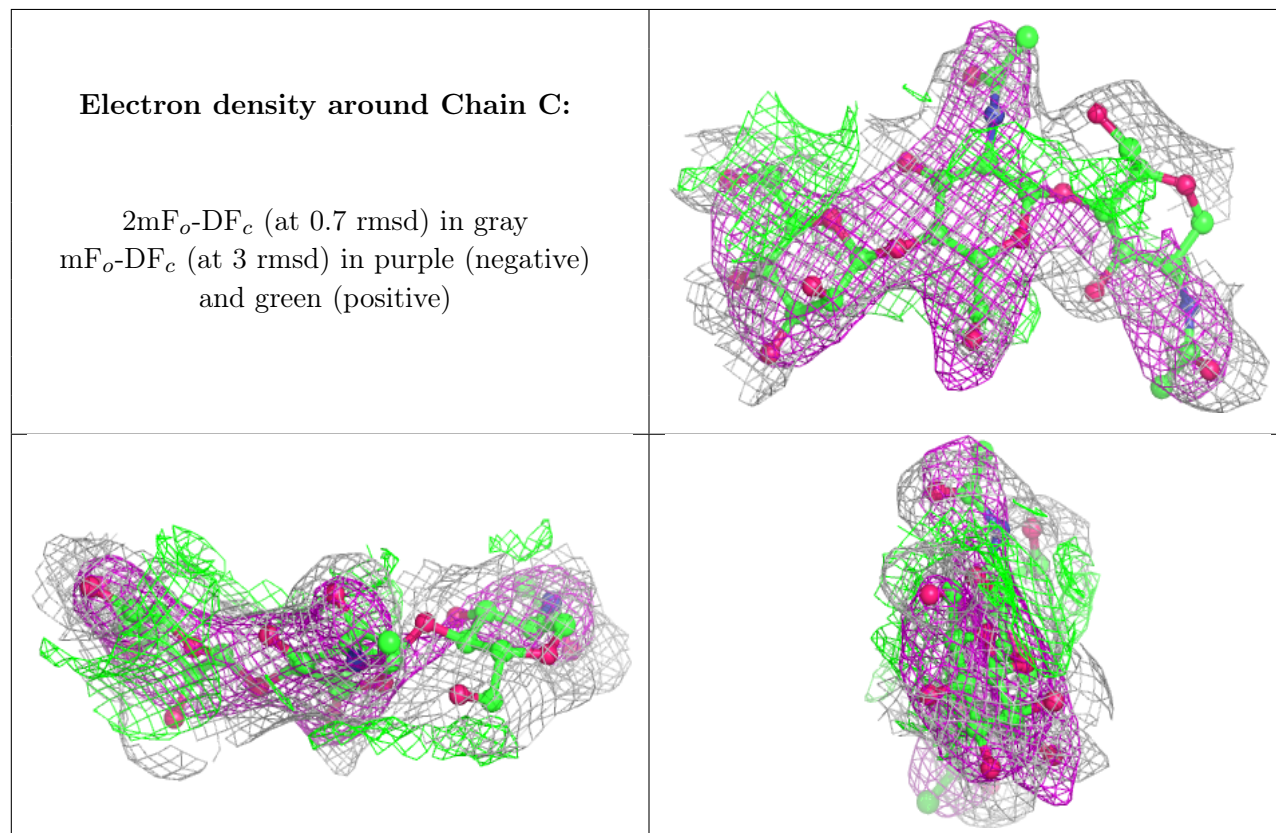
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	C	3	11/12	0.58	0.40	79,80,81,81	0
3	NAG	C	1	14/15	0.82	0.19	79,86,89,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	BMA	D	3	11/12	0.87	0.28	83,84,84,85	0
3	NAG	C	2	14/15	0.88	0.28	70,75,77,79	0
3	NAG	D	1	14/15	0.89	0.26	93,99,100,102	0
3	NAG	D	2	14/15	0.91	0.28	87,90,91,91	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.
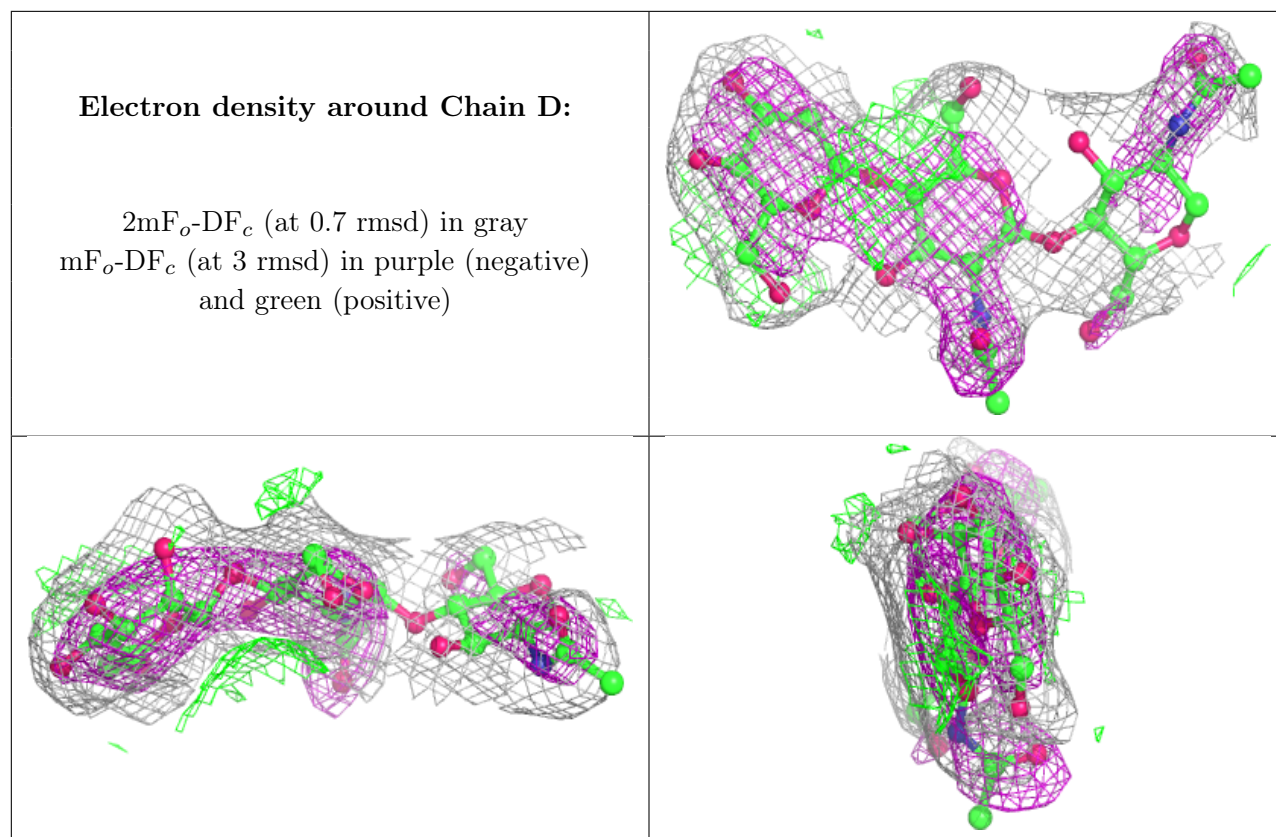
Electron density around Chain C:

$2mF_o$-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 D:

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

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	NAG	E	1330	14/15	0.52	0.28	108,109,112,113	0
4	NAG	F	1330	14/15	0.66	0.28	106,107,108,108	0
4	NAG	A	1053	14/15	0.75	0.29	88,89,90,90	0
4	NAG	A	1546	14/15	0.77	0.27	72,74,77,78	0
4	NAG	B	1322	14/15	0.83	0.16	72,74,76,77	0
4	NAG	A	1322	14/15	0.86	0.12	75,77,78,78	0
6	CL	B	1902	1/1	0.86	0.29	115,115,115,115	0
6	CL	A	902	1/1	0.94	0.13	74,74,74,74	0
5	ZN	B	901	1/1	0.98	0.13	84,84,84,84	0
5	ZN	A	901	1/1	0.99	0.12	74,74,74,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.