



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:50 PM UTC

PDB ID : 9O5T / pdb_00009o5t
Title : Crystal structure of chimeric SARS-CoV-2 RBD complexed with chimeric Rhinolophus sinicus ACE2
Authors : Hsueh, F.-C.; Shi, K.; Aihara, H.; Li, F.
Deposited on : 2025-04-10
Resolution : 2.90 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

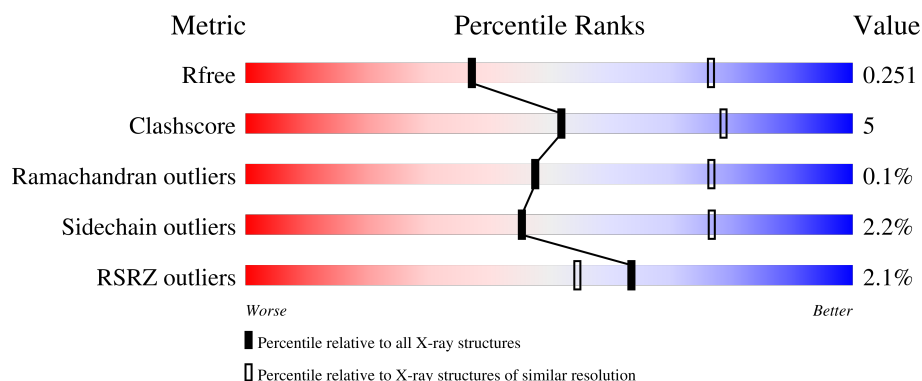
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	603	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	603	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
2	E	232	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>7%</div> <div>19%</div> </div> </div>
2	F	232	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>19%</div> </div> </div>
3	C	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	3	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12865 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 ACE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4847	3095	808	915	29			
1	B	595	Total	C	N	O	S	0	0	0
			4847	3095	808	915	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	188	Total	C	N	O	S	0	1	0
			1498	963	242	283	10			
2	F	188	Total	C	N	O	S	0	0	0
			1495	961	242	283	9			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	321	VAL	GLN	conflict	UNP P0DTC2
E	323	SER	THR	conflict	UNP P0DTC2
E	324	GLY	GLU	conflict	UNP P0DTC2
E	325	ASP	SER	conflict	UNP P0DTC2
E	326	VAL	ILE	conflict	UNP P0DTC2
E	346	LYS	ARG	conflict	UNP P0DTC2
E	348	PRO	ALA	conflict	UNP P0DTC2
E	354	GLU	ASN	conflict	UNP P0DTC2
E	357	LYS	ARG	conflict	UNP P0DTC2
E	372	THR	ALA	conflict	UNP P0DTC2
E	373	PHE	SER	conflict	UNP P0DTC2
E	384	ALA	PRO	conflict	UNP P0DTC2
E	393	SER	THR	conflict	UNP P0DTC2
E	402	VAL	ILE	conflict	UNP P0DTC2
E	403	LYS	ARG	conflict	UNP P0DTC2
E	406	ASP	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	417	VAL	LYS	conflict	UNP P0DTC2
E	430	MET	THR	conflict	UNP P0DTC2
E	434	LEU	ILE	conflict	UNP P0DTC2
E	438	THR	SER	conflict	UNP P0DTC2
E	439	ARG	ASN	conflict	UNP P0DTC2
E	441	ILE	LEU	conflict	UNP P0DTC2
E	443	ALA	SER	conflict	UNP P0DTC2
E	444	THR	LYS	conflict	UNP P0DTC2
E	445	SER	VAL	conflict	UNP P0DTC2
E	446	THR	GLY	conflict	UNP P0DTC2
E	452	LYS	LEU	conflict	UNP P0DTC2
E	519	ASN	HIS	conflict	UNP P0DTC2
E	529	LEU	LYS	conflict	UNP P0DTC2
E	532	ASP	ASN	conflict	UNP P0DTC2
E	534	ILE	VAL	conflict	UNP P0DTC2
E	536	SER	ASN	conflict	UNP P0DTC2
E	537	GLY	-	expression tag	UNP P0DTC2
E	538	GLU	-	expression tag	UNP P0DTC2
E	539	ASN	-	expression tag	UNP P0DTC2
E	540	LEU	-	expression tag	UNP P0DTC2
E	541	TYR	-	expression tag	UNP P0DTC2
E	542	PHE	-	expression tag	UNP P0DTC2
E	543	GLN	-	expression tag	UNP P0DTC2
E	544	GLY	-	expression tag	UNP P0DTC2
E	545	HIS	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	HIS	-	expression tag	UNP P0DTC2
E	548	HIS	-	expression tag	UNP P0DTC2
E	549	HIS	-	expression tag	UNP P0DTC2
E	550	HIS	-	expression tag	UNP P0DTC2
F	321	VAL	GLN	conflict	UNP P0DTC2
F	323	SER	THR	conflict	UNP P0DTC2
F	324	GLY	GLU	conflict	UNP P0DTC2
F	325	ASP	SER	conflict	UNP P0DTC2
F	326	VAL	ILE	conflict	UNP P0DTC2
F	346	LYS	ARG	conflict	UNP P0DTC2
F	348	PRO	ALA	conflict	UNP P0DTC2
F	354	GLU	ASN	conflict	UNP P0DTC2
F	357	LYS	ARG	conflict	UNP P0DTC2
F	372	THR	ALA	conflict	UNP P0DTC2
F	373	PHE	SER	conflict	UNP P0DTC2
F	384	ALA	PRO	conflict	UNP P0DTC2

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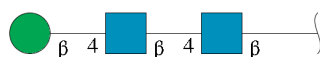
Chain	Residue	Modelled	Actual	Comment	Reference
F	393	SER	THR	conflict	UNP P0DTC2
F	402	VAL	ILE	conflict	UNP P0DTC2
F	403	LYS	ARG	conflict	UNP P0DTC2
F	406	ASP	GLU	conflict	UNP P0DTC2
F	417	VAL	LYS	conflict	UNP P0DTC2
F	430	MET	THR	conflict	UNP P0DTC2
F	434	LEU	ILE	conflict	UNP P0DTC2
F	438	THR	SER	conflict	UNP P0DTC2
F	439	ARG	ASN	conflict	UNP P0DTC2
F	441	ILE	LEU	conflict	UNP P0DTC2
F	443	ALA	SER	conflict	UNP P0DTC2
F	444	THR	LYS	conflict	UNP P0DTC2
F	445	SER	VAL	conflict	UNP P0DTC2
F	446	THR	GLY	conflict	UNP P0DTC2
F	452	LYS	LEU	conflict	UNP P0DTC2
F	519	ASN	HIS	conflict	UNP P0DTC2
F	529	LEU	LYS	conflict	UNP P0DTC2
F	532	ASP	ASN	conflict	UNP P0DTC2
F	534	ILE	VAL	conflict	UNP P0DTC2
F	536	SER	ASN	conflict	UNP P0DTC2
F	537	GLY	-	expression tag	UNP P0DTC2
F	538	GLU	-	expression tag	UNP P0DTC2
F	539	ASN	-	expression tag	UNP P0DTC2
F	540	LEU	-	expression tag	UNP P0DTC2
F	541	TYR	-	expression tag	UNP P0DTC2
F	542	PHE	-	expression tag	UNP P0DTC2
F	543	GLN	-	expression tag	UNP P0DTC2
F	544	GLY	-	expression tag	UNP P0DTC2
F	545	HIS	-	expression tag	UNP P0DTC2
F	546	HIS	-	expression tag	UNP P0DTC2
F	547	HIS	-	expression tag	UNP P0DTC2
F	548	HIS	-	expression tag	UNP P0DTC2
F	549	HIS	-	expression tag	UNP P0DTC2
F	550	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.

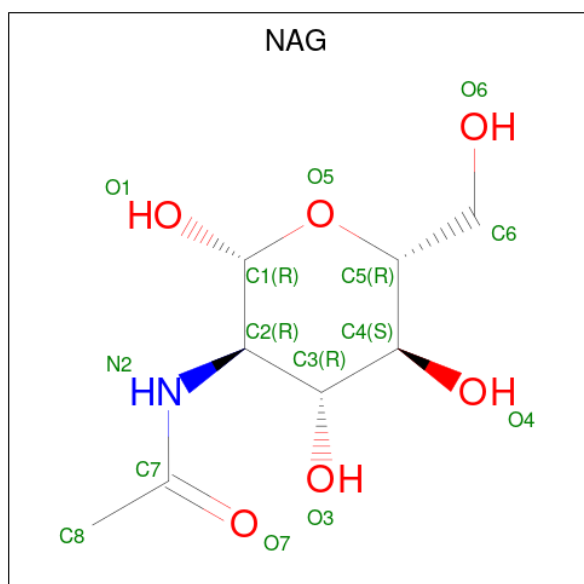


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

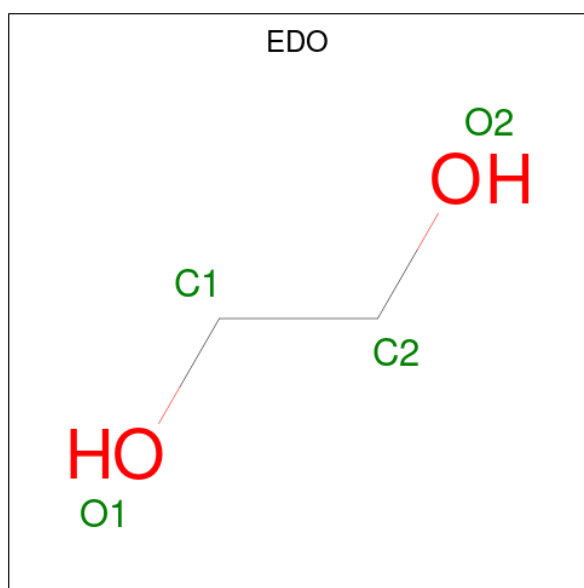
- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

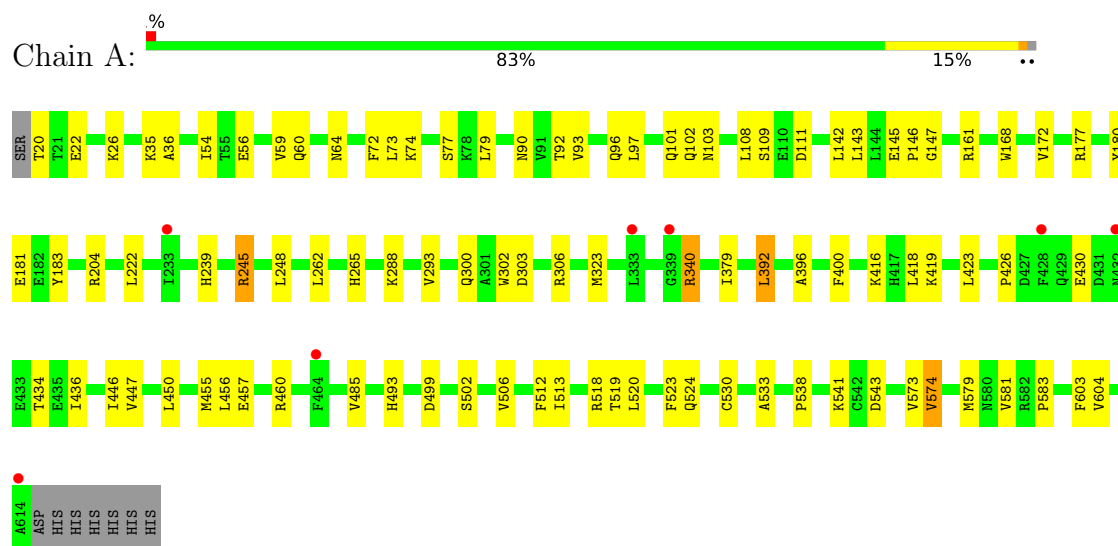
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total O 4 4	0	0
10	B	6	Total O 6 6	0	0
10	F	1	Total O 1 1	0	0

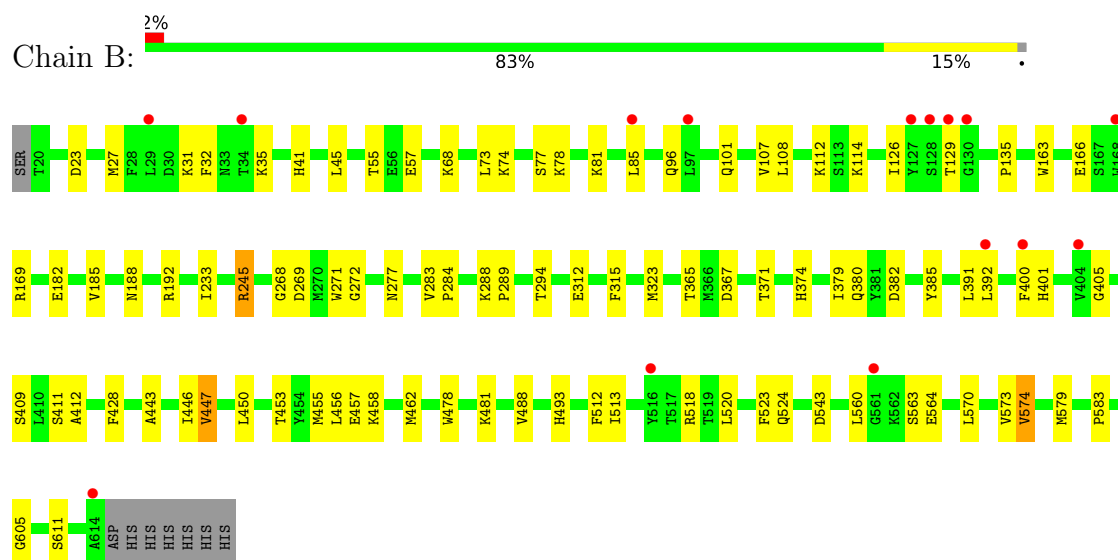
3 Residue-property plots [i](#)

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: ACE2

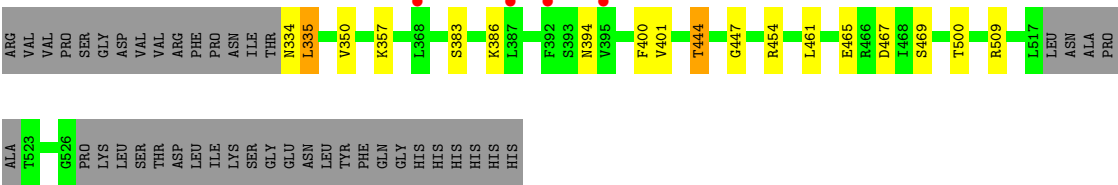


• Molecule 1: ACE2

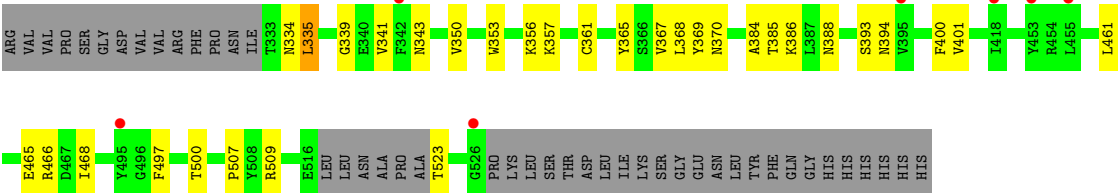


• Molecule 2: Spike protein S1





• Molecule 2: Spike protein S1



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.55Å 120.04Å 112.40Å 90.00° 92.81° 90.00°	Depositor
Resolution (Å)	33.92 – 2.90 33.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	63.0 (33.92-2.90) 58.6 (33.92-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.206 , 0.251 0.206 , 0.251	Depositor DCC
R_{free} test set	1435 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12865	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, ZN, BMA, CL, EDO, NA

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	0.08	0/4981	0.23	0/6761
1	B	0.08	0/4981	0.22	0/6761
2	E	0.08	0/1539	0.25	0/2092
2	F	0.08	0/1536	0.25	0/2087
All	All	0.08	0/13037	0.23	0/17701

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	4847	0	4632	49	0
1	B	4847	0	4632	50	0
2	E	1498	0	1405	9	0
2	F	1495	0	1410	19	0
3	C	28	0	25	0	0
4	D	39	0	34	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	42	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	26	0	0
6	F	14	0	13	3	0
7	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	12	0	16	0	0
10	A	4	0	0	0	0
10	B	6	0	0	0	0
10	F	1	0	0	0	0
All	All	12865	0	12232	127	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 5.

All (127) 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:B:560:LEU:HD13	1:B:564:GLU:HG3	1.72	0.71
1:A:418:LEU:HD22	1:A:423:LEU:HD12	1.75	0.67
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.78	0.65
2:F:357:LYS:HE3	2:F:394:ASN:HD22	1.63	0.64
2:E:357:LYS:HE3	2:E:394:ASN:HD22	1.62	0.64
1:B:245:ARG:NH2	1:B:605:GLY:O	2.30	0.64
2:F:341:VAL:HG22	2:F:356:LYS:HD3	1.80	0.63
1:A:245:ARG:NH2	1:A:603:PHE:O	2.32	0.62
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.83	0.61
2:E:444:THR:HG22	2:E:447:GLY:H	1.64	0.60
2:F:343:ASN:ND2	6:F:601:NAG:O7	2.35	0.60
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.83	0.60
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.83	0.59
2:F:497:PHE:CG	2:F:507:PRO:HG3	2.38	0.59
2:F:367:VAL:HG13	2:F:368:LEU:HD13	1.85	0.58
1:A:419:LYS:HE3	1:A:426:PRO:HA	1.86	0.58
1:A:73:LEU:O	1:A:77:SER:N	2.37	0.57
2:E:383:SER:HB2	2:E:386:LYS:HB2	1.86	0.56
1:A:177:ARG:NH1	1:A:181:GLU:OE2	2.38	0.56
1:B:85:LEU:HD22	1:B:101:GLN:HE22	1.72	0.56
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.88	0.55
2:F:339:GLY:HA2	6:F:601:NAG:O7	2.06	0.54
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.88	0.54
1:B:73:LEU:O	1:B:77:SER:N	2.41	0.54
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:461:LEU:HD22	2:F:465:GLU:HB3	1.90	0.53
1:A:416:LYS:HE3	1:A:543:ASP:HB3	1.91	0.52
1:A:20:THR:HG22	1:A:22:GLU:H	1.75	0.52
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.93	0.51
1:A:300:GLN:HE22	1:A:423:LEU:HA	1.75	0.51
1:B:289:PRO:HB2	1:B:428:PHE:HE1	1.74	0.51
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.43	0.51
1:B:312:GLU:HG3	1:B:323:MET:HG2	1.91	0.51
1:B:478:TRP:HA	1:B:481:LYS:HB2	1.93	0.50
1:B:573:VAL:HG13	1:B:574:VAL:HG13	1.94	0.50
2:F:353:TRP:O	2:F:466:ARG:NE	2.42	0.50
1:B:78:LYS:HA	1:B:81:LYS:HD2	1.92	0.50
1:A:248:LEU:HD12	1:A:262:LEU:HD22	1.94	0.50
1:B:32:PHE:HE2	1:B:391:LEU:HD21	1.77	0.50
1:B:23:ASP:O	1:B:27:MET:HG3	2.12	0.49
2:E:454:ARG:NH1	2:E:467:ASP:O	2.40	0.49
1:A:60:GLN:O	1:A:64:ASN:N	2.43	0.49
2:F:384:ALA:O	2:F:386:LYS:N	2.42	0.49
1:A:430:GLU:OE1	1:A:541:LYS:NZ	2.46	0.48
1:B:392:LEU:HD23	1:B:563:SER:HB3	1.95	0.48
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.95	0.48
1:B:409:SER:HA	1:B:412:ALA:HB3	1.95	0.48
1:B:166:GLU:OE1	1:B:493:HIS:NE2	2.36	0.48
1:B:411:SER:HB3	1:B:543:ASP:HA	1.96	0.48
2:F:350:VAL:HA	2:F:400:PHE:HB2	1.96	0.48
1:A:538:PRO:HD2	1:A:541:LYS:HD3	1.95	0.47
2:E:461:LEU:HD22	2:E:465:GLU:HB3	1.95	0.47
1:B:400:PHE:HZ	1:B:570:LEU:HB2	1.80	0.47
1:A:396:ALA:HB3	1:A:400:PHE:CG	2.49	0.47
1:B:108:LEU:HD23	1:B:112:LYS:HB3	1.97	0.47
1:A:450:LEU:HD21	1:A:519:THR:HG21	1.97	0.47
1:B:182:GLU:HA	1:B:185:VAL:HG12	1.97	0.47
2:E:350:VAL:HA	2:E:400:PHE:HB2	1.96	0.46
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.96	0.46
1:B:96:GLN:HB3	1:B:391:LEU:HD12	1.98	0.46
1:A:109:SER:OG	1:A:111:ASP:OD1	2.23	0.46
1:A:303:ASP:OD1	1:A:303:ASP:N	2.43	0.46
2:F:339:GLY:HA2	6:F:601:NAG:C7	2.46	0.46
2:F:365:TYR:HB2	2:F:388:ASN:HA	1.98	0.46
2:F:367:VAL:O	2:F:369:TYR:N	2.42	0.46
1:A:102:GLN:O	1:A:103:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:HD3	1:A:506:VAL:HG13	1.99	0.45
1:B:107:VAL:HG13	1:B:108:LEU:HD12	1.98	0.45
1:B:269:ASP:OD1	1:B:272:GLY:N	2.46	0.45
1:B:488:VAL:HG21	1:B:611:SER:HA	1.97	0.45
1:B:188:ASN:HB3	1:B:192:ARG:HE	1.80	0.45
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.98	0.45
2:F:394:ASN:N	2:F:394:ASN:OD1	2.50	0.45
1:B:455:MET:HE3	1:B:455:MET:HB3	1.84	0.45
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.98	0.45
1:A:90:ASN:O	1:A:92:THR:N	2.45	0.45
1:A:530:CYS:HA	1:A:533:ALA:HB3	1.99	0.45
1:B:374:HIS:HA	1:B:405:GLY:HA3	1.99	0.45
1:B:458:LYS:NZ	1:B:462:MET:HE3	2.32	0.45
1:B:268:GLY:O	1:B:277:ASN:ND2	2.50	0.44
2:E:394:ASN:N	2:E:394:ASN:OD1	2.50	0.44
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.83	0.44
1:B:443:ALA:HA	1:B:447:VAL:HG13	1.99	0.44
1:A:96:GLN:HG2	1:A:392:LEU:HD13	2.00	0.44
1:A:22:GLU:HG2	1:A:26:LYS:HE3	1.99	0.43
1:A:455:MET:HE3	1:A:455:MET:HB3	1.85	0.43
1:B:294:THR:HG23	1:B:365:THR:HA	2.00	0.43
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.53	0.43
1:B:367:ASP:O	1:B:371:THR:OG1	2.23	0.43
1:A:56:GLU:HA	1:A:59:VAL:HG12	2.00	0.43
1:A:340:ARG:HG2	6:A:704:NAG:H82	2.01	0.43
1:B:31:LYS:HE2	1:B:35:LYS:NZ	2.34	0.43
1:B:68:LYS:HE2	1:B:68:LYS:HB2	1.87	0.43
1:A:103:ASN:HD22	1:A:103:ASN:HA	1.66	0.43
2:F:335:LEU:C	2:F:361:CYS:HB2	2.44	0.43
1:A:180:TYR:HA	1:A:183:TYR:HB3	2.01	0.43
1:B:446:ILE:HD13	1:B:523:PHE:HZ	1.83	0.43
1:B:114:LYS:HA	1:B:114:LYS:HD2	1.81	0.43
1:B:315:PHE:CD1	1:B:380:GLN:HG3	2.55	0.42
1:B:135:PRO:HD3	1:B:163:TRP:HE1	1.85	0.42
1:B:382:ASP:HA	1:B:385:TYR:CZ	2.54	0.42
1:B:289:PRO:HB2	1:B:428:PHE:CE1	2.54	0.42
1:B:453:THR:HG23	1:B:512:PHE:CD2	2.55	0.42
2:F:393:SER:O	2:F:523:THR:OG1	2.32	0.42
1:A:573:VAL:HG13	1:A:574:VAL:HG13	2.00	0.42
1:A:524:GLN:HG2	1:A:583:PRO:HG2	2.02	0.42
1:A:143:LEU:H	1:A:143:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HB2	1:A:265:HIS:HD2	1.85	0.42
1:B:169:ARG:HH22	1:B:271:TRP:HA	1.85	0.42
1:A:288:LYS:HD3	1:A:434:THR:HG22	2.01	0.41
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.55	0.41
1:B:74:LYS:HD2	1:B:74:LYS:HA	1.85	0.41
1:B:126:ILE:HA	1:B:129:THR:HG22	2.02	0.41
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.55	0.41
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.93	0.41
2:F:369:TYR:CE1	2:F:385:THR:HG22	2.56	0.41
1:A:302:TRP:CD1	1:A:306:ARG:HG2	2.56	0.41
2:E:334:ASN:HB3	2:E:335:LEU:H	1.65	0.41
1:A:74:LYS:HA	1:A:74:LYS:HD2	1.90	0.41
1:A:97:LEU:O	1:A:101:GLN:N	2.49	0.41
2:F:334:ASN:HB3	2:F:335:LEU:H	1.61	0.41
1:B:41:HIS:O	1:B:45:LEU:HB2	2.21	0.41
1:A:142:LEU:HB3	1:A:147:GLY:HA3	2.03	0.40
1:A:145:GLU:HA	1:A:146:PRO:HA	1.91	0.40
1:A:36:ALA:HB2	1:A:72:PHE:HE2	1.86	0.40
1:A:239:HIS:CE1	1:A:604:VAL:HG21	2.56	0.40
1:A:293:VAL:HG21	1:A:423:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

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	593/603 (98%)	564 (95%)	28 (5%)	1 (0%)	43	72
1	B	593/603 (98%)	572 (96%)	20 (3%)	1 (0%)	43	72
2	E	185/232 (80%)	169 (91%)	16 (9%)	0	100	100
2	F	184/232 (79%)	164 (89%)	20 (11%)	0	100	100
All	All	1555/1670 (93%)	1469 (94%)	84 (5%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	B	284	PRO

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	525/533 (98%)	512 (98%)	13 (2%)	42	74
1	B	525/533 (98%)	516 (98%)	9 (2%)	53	82
2	E	164/203 (81%)	160 (98%)	4 (2%)	43	75
2	F	164/203 (81%)	160 (98%)	4 (2%)	43	75
All	All	1378/1472 (94%)	1348 (98%)	30 (2%)	45	77

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	79	LEU
1	A	108	LEU
1	A	172	VAL
1	A	245	ARG
1	A	340	ARG
1	A	392	LEU
1	A	436	ILE
1	A	447	VAL
1	A	485	VAL
1	A	518	ARG
1	A	574	VAL
1	A	581	VAL
1	B	55	THR
1	B	57	GLU
1	B	245	ARG
1	B	283	VAL
1	B	288	LYS

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Mol	Chain	Res	Type
1	B	401	HIS
1	B	447	VAL
1	B	518	ARG
1	B	574	VAL
2	E	335	LEU
2	E	444	THR
2	E	469	SER
2	E	500	THR
2	F	335	LEU
2	F	370	ASN
2	F	468	ILE
2	F	500	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	194	ASN
1	A	239	HIS
1	A	508	ASN
1	A	599	ASN
1	B	58	ASN
1	B	98	GLN
1	B	101	GLN
2	E	437	ASN
2	F	394	ASN

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](#)

5 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	0.32	0	17,19,21	0.46	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.58	0
4	NAG	D	1	4,1	14,14,15	0.23	0	17,19,21	0.57	0
4	NAG	D	2	4	14,14,15	0.19	0	17,19,21	0.43	0
4	BMA	D	3	4	11,11,12	0.62	0	15,15,17	0.88	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
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2

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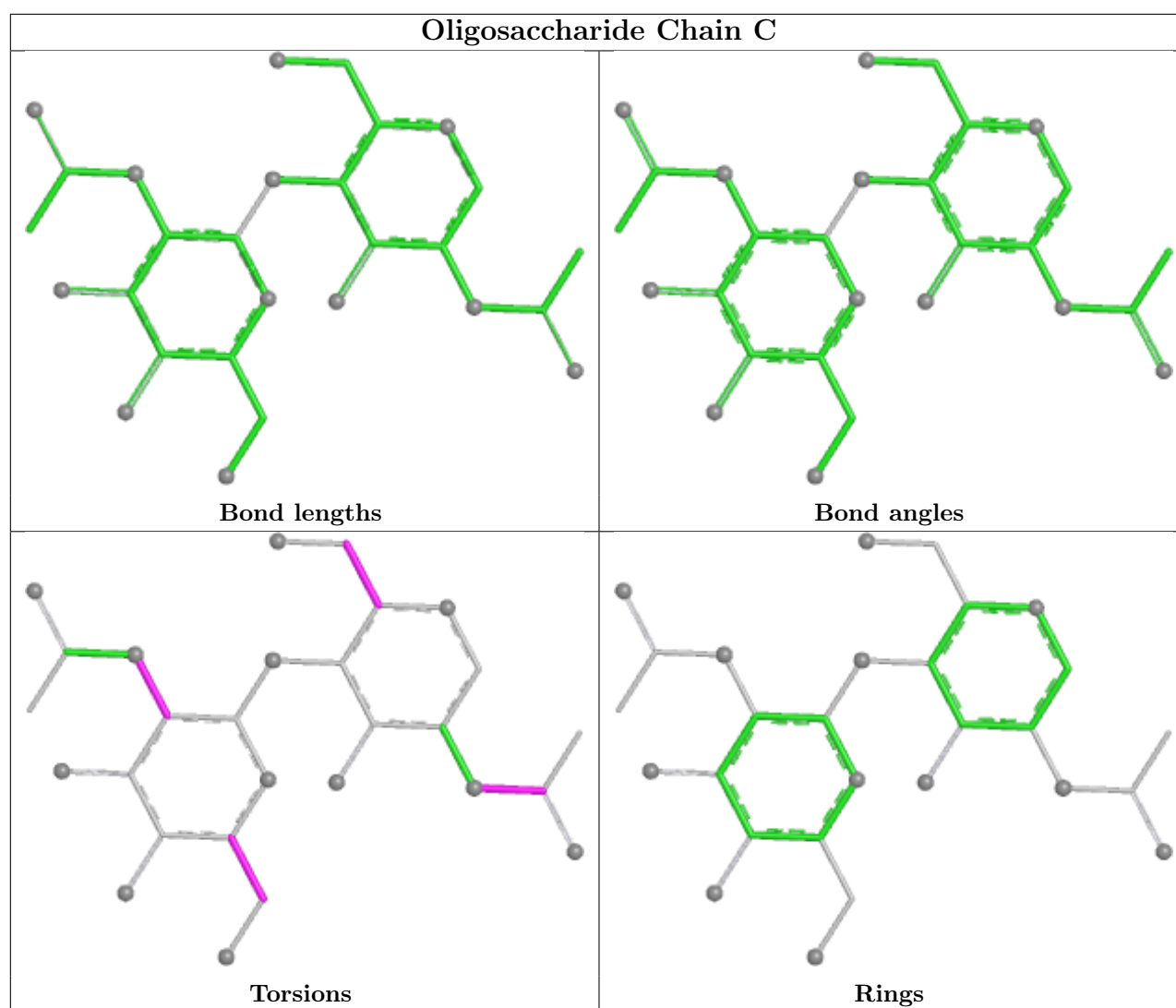
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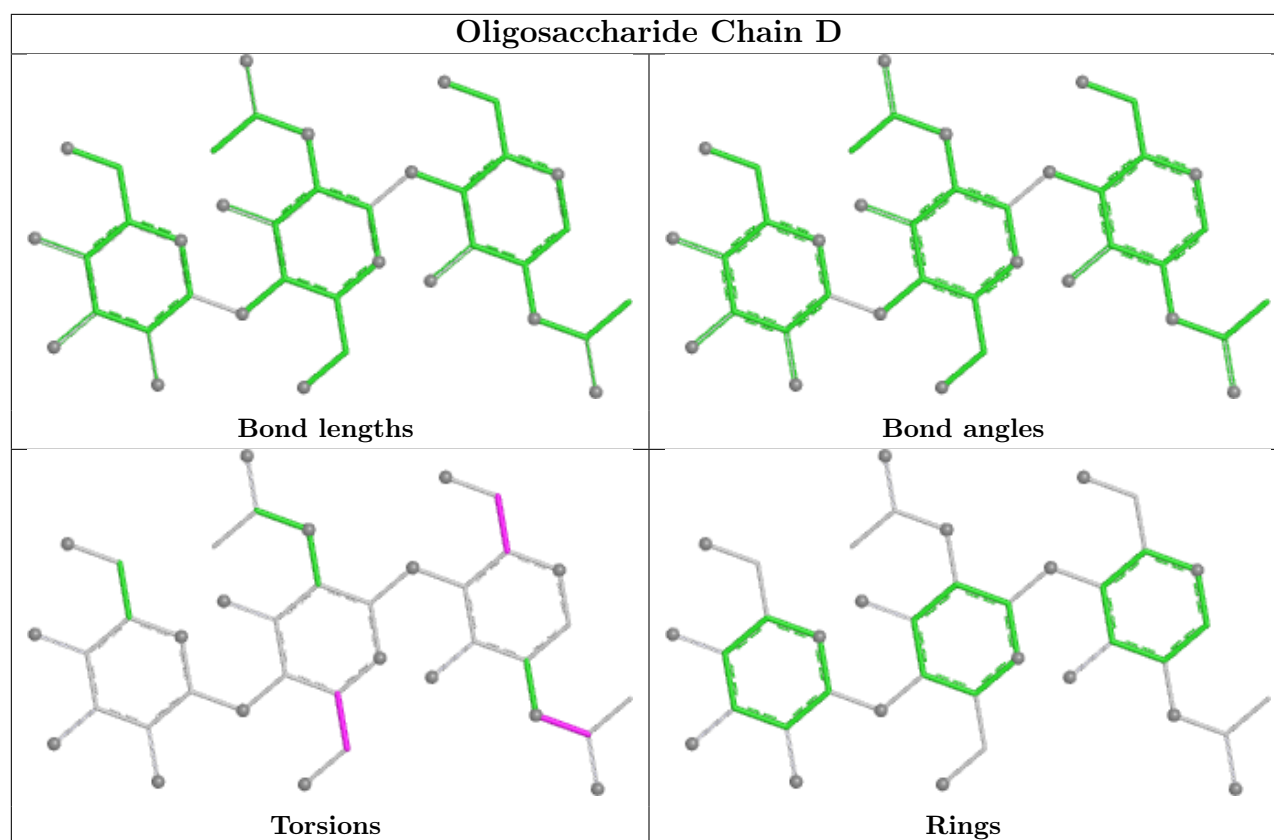
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\# Z > 2$
6	NAG	B	706	1	14,14,15	0.23	0	17,19,21	0.47	0
9	EDO	B	704	-	3,3,3	0.45	0	2,2,2	0.32	0
6	NAG	A	705	1	14,14,15	0.38	0	17,19,21	0.52	0
9	EDO	B	705	-	3,3,3	0.42	0	2,2,2	0.40	0
6	NAG	A	702	1	14,14,15	0.34	0	17,19,21	0.51	0
9	EDO	B	703	-	3,3,3	0.43	0	2,2,2	0.39	0
6	NAG	B	707	1	14,14,15	0.32	0	17,19,21	0.54	0
6	NAG	F	601	2	14,14,15	0.58	1 (7%)	17,19,21	0.87	1 (5%)
6	NAG	A	704	1	14,14,15	0.22	0	17,19,21	0.50	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
6	NAG	B	706	1	-	4/6/23/26	0/1/1/1
9	EDO	B	704	-	-	0/1/1/1	-
6	NAG	A	705	1	-	1/6/23/26	0/1/1/1
9	EDO	B	705	-	-	0/1/1/1	-
6	NAG	A	702	1	-	0/6/23/26	0/1/1/1
9	EDO	B	703	-	-	0/1/1/1	-
6	NAG	B	707	1	-	2/6/23/26	0/1/1/1
6	NAG	F	601	2	-	4/6/23/26	0/1/1/1
6	NAG	A	704	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	601	NAG	C1-C2	2.06	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	601	NAG	C1-O5-C5	2.44	115.45	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	601	NAG	C1-C2-N2-C7
6	F	601	NAG	O5-C5-C6-O6
6	B	707	NAG	O5-C5-C6-O6
6	F	601	NAG	C4-C5-C6-O6
6	B	707	NAG	C4-C5-C6-O6
6	B	706	NAG	C8-C7-N2-C2
6	B	706	NAG	O7-C7-N2-C2
6	F	601	NAG	C3-C2-N2-C7
6	A	705	NAG	O5-C5-C6-O6
6	B	706	NAG	C4-C5-C6-O6
6	B	706	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	601	NAG	3	0
6	A	704	NAG	1	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	595/603 (98%)	0.14	7 (1%) 76 69	40, 84, 138, 225	0
1	B	595/603 (98%)	0.04	15 (2%) 58 48	36, 76, 147, 201	0
2	E	188/232 (81%)	0.11	4 (2%) 63 54	42, 76, 151, 225	1 (0%)
2	F	188/232 (81%)	0.31	7 (3%) 45 37	73, 120, 189, 214	0
All	All	1566/1670 (93%)	0.12	33 (2%) 63 54	36, 84, 158, 225	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	THR	4.3
1	B	168	TRP	3.7
1	B	34	THR	3.4
2	F	395	VAL	3.0
2	F	495	TYR	3.0
1	B	614	ALA	3.0
2	E	387	LEU	3.0
2	F	455	LEU	2.9
2	F	342	PHE	2.9
1	B	404	VAL	2.8
2	E	368	LEU	2.8
2	F	418	ILE	2.8
1	A	233	ILE	2.7
1	B	97	LEU	2.6
1	A	614	ALA	2.6
1	B	128	SER	2.5
1	A	333	LEU	2.5
1	B	127	TYR	2.5
2	F	453	TYR	2.4
1	B	392	LEU	2.4
1	B	130	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	526	GLY	2.3
1	A	464	PHE	2.3
2	E	392	PHE	2.2
1	A	339	GLY	2.2
1	B	516	TYR	2.2
1	B	29	LEU	2.2
1	A	428	PHE	2.1
1	B	400	PHE	2.1
1	A	432	ASN	2.1
2	E	395	VAL	2.1
1	B	561	GLY	2.1
1	B	85	LEU	2.0

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 ⓘ

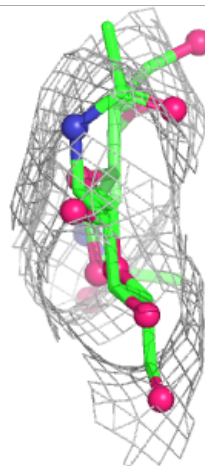
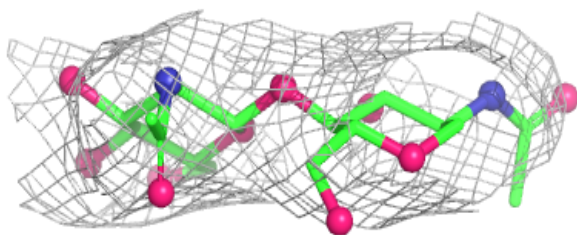
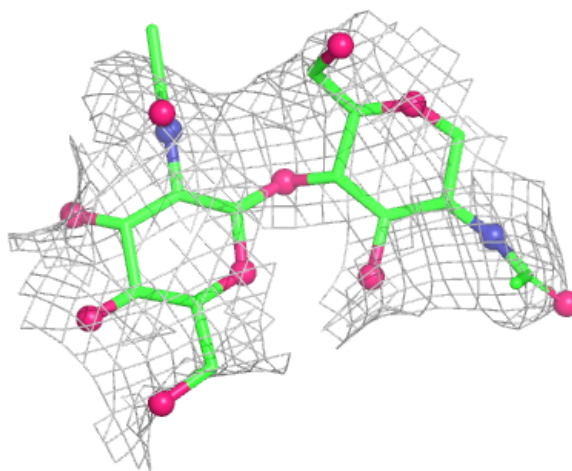
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

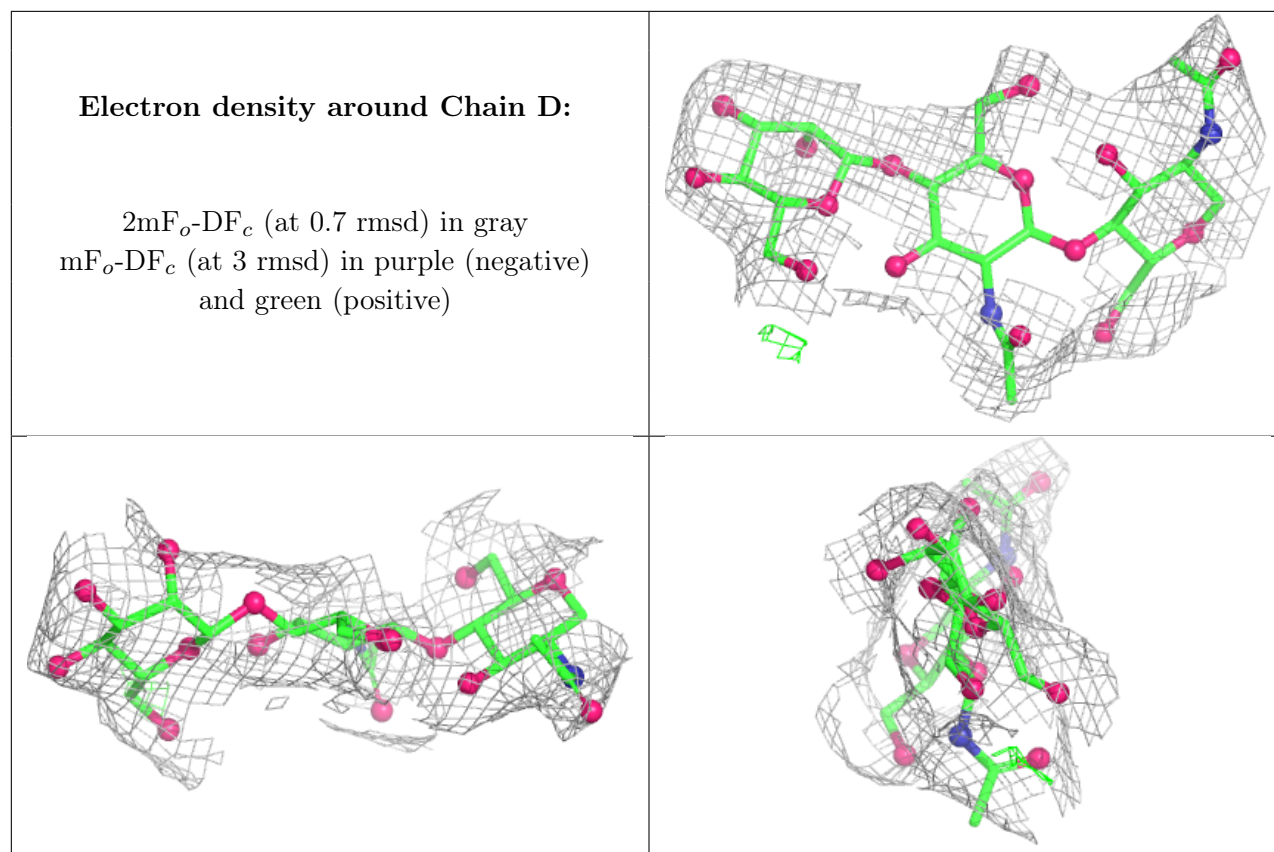
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	100,103,106,108	0
3	NAG	C	2	14/15	-	-	95,108,114,115	0
4	NAG	D	1	14/15	-	-	67,85,93,93	0
4	NAG	D	2	14/15	-	-	89,98,104,106	0
4	BMA	D	3	11/12	-	-	102,107,117,117	0

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)





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
9	EDO	B	704	4/4	0.60	0.19	72,73,79,86	0
6	NAG	A	702	14/15	0.63	0.11	107,123,128,128	0
6	NAG	A	704	14/15	0.66	0.11	92,98,117,123	0
6	NAG	B	707	14/15	0.75	0.09	64,82,95,95	0
6	NAG	B	706	14/15	0.76	0.09	70,99,118,121	0
6	NAG	F	601	14/15	0.80	0.09	119,130,146,147	0
9	EDO	B	705	4/4	0.83	0.29	52,73,77,88	0
7	NA	A	703	1/1	0.85	0.10	66,66,66,66	0
6	NAG	A	705	14/15	0.88	0.08	66,89,97,98	0
9	EDO	B	703	4/4	0.89	0.19	56,65,73,83	0
8	CL	B	702	1/1	0.93	0.23	84,84,84,84	0
5	ZN	B	701	1/1	0.96	0.07	53,53,53,53	0
5	ZN	A	701	1/1	0.99	0.03	96,96,96,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.