Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:09 AM EDT

PDB ID	:	8DF5
Title	:	SARS-CoV-2 Beta RBD in complex with human ACE2 and S304 Fab and S309 Fab
Authors	:	McCallum, M.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); Snell, G.; Veesler, D.
Deposited on	:	2022-06-21
Resolution	:	2.70 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:

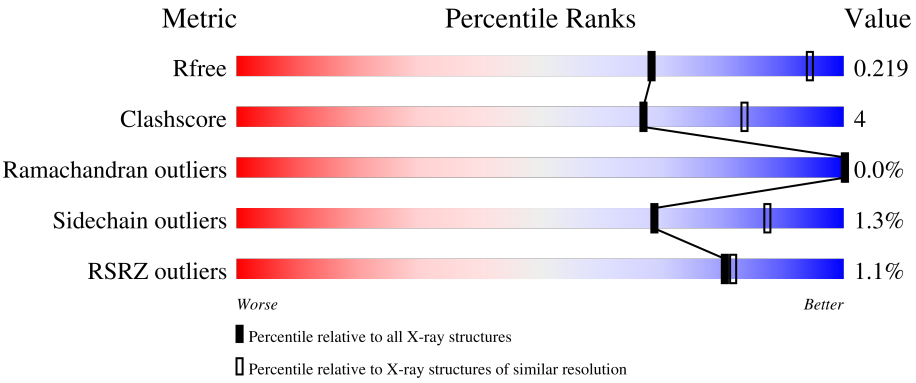
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	230	90% 7% .
1	C	230	% 93% 7%
2	B	214	92% 8%
2	D	214	91% 9%
3	E	805	2% 61% 11% 27%

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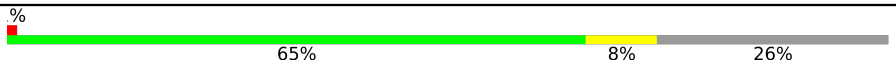
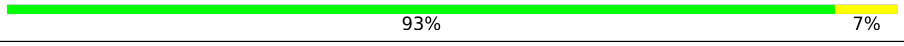
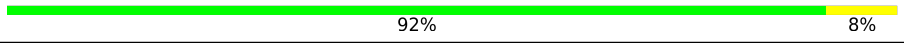
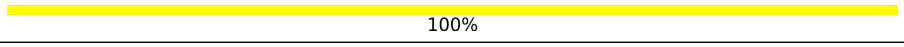
Mol	Chain	Length	Quality of chain
3	F	805	
4	H	223	
4	M	223	
5	L	215	
5	N	215	
6	R	263	
6	S	263	
7	G	2	
7	I	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NAG	E	1105	-	-	-	X
9	CL	C	302	-	-	X	-
9	CL	E	1115	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26905 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 S309 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1661	1050	278	326	7			
1	C	230	Total	C	N	O	S	0	0	0
			1714	1079	289	338	8			

- Molecule 2 is a protein called S309 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1617	1006	276	331	4			
2	D	214	Total	C	N	O	S	0	0	0
			1608	1001	273	329	5			

- Molecule 3 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	587	Total	C	N	O	S	0	0	0
			4580	2918	768	865	29			
3	F	592	Total	C	N	O	S	0	0	0
			4741	3036	786	892	27			

- Molecule 4 is a protein called S304 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	217	Total	C	N	O	S	0	0	0
			1603	1014	263	319	7			
4	M	218	Total	C	N	O	S	0	0	0
			1621	1025	266	324	6			

- Molecule 5 is a protein called S304 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	215	Total	C	N	O	S	0	0	0
			1622	1016	269	331	6			
5	N	215	Total	C	N	O	S	0	0	0
			1615	1011	267	332	5			

- Molecule 6 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	200	Total	C	N	O	S	0	0	0
			1576	1011	263	294	8			
6	S	198	Total	C	N	O	S	0	0	0
			1548	994	255	291	8			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	296	MET	-	expression tag	UNP P0DTC2
R	297	GLY	-	expression tag	UNP P0DTC2
R	298	ILE	-	expression tag	UNP P0DTC2
R	299	LEU	-	expression tag	UNP P0DTC2
R	300	PRO	-	expression tag	UNP P0DTC2
R	301	SER	-	expression tag	UNP P0DTC2
R	302	PRO	-	expression tag	UNP P0DTC2
R	303	GLY	-	expression tag	UNP P0DTC2
R	304	MET	-	expression tag	UNP P0DTC2
R	305	PRO	-	expression tag	UNP P0DTC2
R	306	ALA	-	expression tag	UNP P0DTC2
R	307	LEU	-	expression tag	UNP P0DTC2
R	308	LEU	-	expression tag	UNP P0DTC2
R	309	SER	-	expression tag	UNP P0DTC2
R	310	LEU	-	expression tag	UNP P0DTC2
R	311	VAL	-	expression tag	UNP P0DTC2
R	312	SER	-	expression tag	UNP P0DTC2
R	313	LEU	-	expression tag	UNP P0DTC2
R	314	LEU	-	expression tag	UNP P0DTC2
R	315	SER	-	expression tag	UNP P0DTC2
R	316	VAL	-	expression tag	UNP P0DTC2
R	317	LEU	-	expression tag	UNP P0DTC2
R	318	LEU	-	expression tag	UNP P0DTC2
R	319	MET	-	expression tag	UNP P0DTC2
R	320	GLY	-	expression tag	UNP P0DTC2
R	321	CYS	-	expression tag	UNP P0DTC2
R	322	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	323	ALA	-	expression tag	UNP P0DTC2
R	324	GLU	-	expression tag	UNP P0DTC2
R	325	THR	-	expression tag	UNP P0DTC2
R	326	GLY	-	expression tag	UNP P0DTC2
R	327	THR	-	expression tag	UNP P0DTC2
R	417	ASN	LYS	conflict	UNP P0DTC2
R	484	LYS	GLU	conflict	UNP P0DTC2
R	501	TYR	ASN	conflict	UNP P0DTC2
R	530	SER	-	expression tag	UNP P0DTC2
R	531	THR	-	expression tag	UNP P0DTC2
R	532	HIS	-	expression tag	UNP P0DTC2
R	533	HIS	-	expression tag	UNP P0DTC2
R	534	HIS	-	expression tag	UNP P0DTC2
R	535	HIS	-	expression tag	UNP P0DTC2
R	536	HIS	-	expression tag	UNP P0DTC2
R	537	HIS	-	expression tag	UNP P0DTC2
R	538	HIS	-	expression tag	UNP P0DTC2
R	539	HIS	-	expression tag	UNP P0DTC2
R	540	GLY	-	expression tag	UNP P0DTC2
R	541	GLY	-	expression tag	UNP P0DTC2
R	542	SER	-	expression tag	UNP P0DTC2
R	543	SER	-	expression tag	UNP P0DTC2
R	544	GLY	-	expression tag	UNP P0DTC2
R	545	LEU	-	expression tag	UNP P0DTC2
R	546	ASN	-	expression tag	UNP P0DTC2
R	547	ASP	-	expression tag	UNP P0DTC2
R	548	ILE	-	expression tag	UNP P0DTC2
R	549	PHE	-	expression tag	UNP P0DTC2
R	550	GLU	-	expression tag	UNP P0DTC2
R	551	ALA	-	expression tag	UNP P0DTC2
R	552	GLN	-	expression tag	UNP P0DTC2
R	553	LYS	-	expression tag	UNP P0DTC2
R	554	ILE	-	expression tag	UNP P0DTC2
R	555	GLU	-	expression tag	UNP P0DTC2
R	556	TRP	-	expression tag	UNP P0DTC2
R	557	HIS	-	expression tag	UNP P0DTC2
R	558	GLU	-	expression tag	UNP P0DTC2
S	296	MET	-	expression tag	UNP P0DTC2
S	297	GLY	-	expression tag	UNP P0DTC2
S	298	ILE	-	expression tag	UNP P0DTC2
S	299	LEU	-	expression tag	UNP P0DTC2
S	300	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	301	SER	-	expression tag	UNP P0DTC2
S	302	PRO	-	expression tag	UNP P0DTC2
S	303	GLY	-	expression tag	UNP P0DTC2
S	304	MET	-	expression tag	UNP P0DTC2
S	305	PRO	-	expression tag	UNP P0DTC2
S	306	ALA	-	expression tag	UNP P0DTC2
S	307	LEU	-	expression tag	UNP P0DTC2
S	308	LEU	-	expression tag	UNP P0DTC2
S	309	SER	-	expression tag	UNP P0DTC2
S	310	LEU	-	expression tag	UNP P0DTC2
S	311	VAL	-	expression tag	UNP P0DTC2
S	312	SER	-	expression tag	UNP P0DTC2
S	313	LEU	-	expression tag	UNP P0DTC2
S	314	LEU	-	expression tag	UNP P0DTC2
S	315	SER	-	expression tag	UNP P0DTC2
S	316	VAL	-	expression tag	UNP P0DTC2
S	317	LEU	-	expression tag	UNP P0DTC2
S	318	LEU	-	expression tag	UNP P0DTC2
S	319	MET	-	expression tag	UNP P0DTC2
S	320	GLY	-	expression tag	UNP P0DTC2
S	321	CYS	-	expression tag	UNP P0DTC2
S	322	VAL	-	expression tag	UNP P0DTC2
S	323	ALA	-	expression tag	UNP P0DTC2
S	324	GLU	-	expression tag	UNP P0DTC2
S	325	THR	-	expression tag	UNP P0DTC2
S	326	GLY	-	expression tag	UNP P0DTC2
S	327	THR	-	expression tag	UNP P0DTC2
S	417	ASN	LYS	conflict	UNP P0DTC2
S	484	LYS	GLU	conflict	UNP P0DTC2
S	501	TYR	ASN	conflict	UNP P0DTC2
S	530	SER	-	expression tag	UNP P0DTC2
S	531	THR	-	expression tag	UNP P0DTC2
S	532	HIS	-	expression tag	UNP P0DTC2
S	533	HIS	-	expression tag	UNP P0DTC2
S	534	HIS	-	expression tag	UNP P0DTC2
S	535	HIS	-	expression tag	UNP P0DTC2
S	536	HIS	-	expression tag	UNP P0DTC2
S	537	HIS	-	expression tag	UNP P0DTC2
S	538	HIS	-	expression tag	UNP P0DTC2
S	539	HIS	-	expression tag	UNP P0DTC2
S	540	GLY	-	expression tag	UNP P0DTC2
S	541	GLY	-	expression tag	UNP P0DTC2

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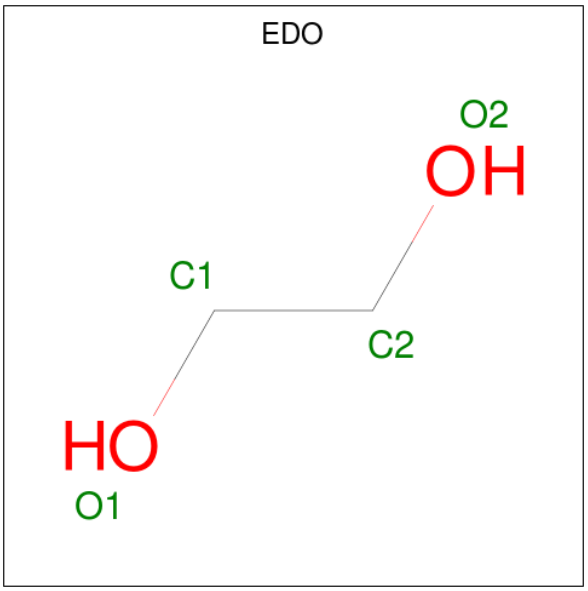
Chain	Residue	Modelled	Actual	Comment	Reference
S	542	SER	-	expression tag	UNP P0DTC2
S	543	SER	-	expression tag	UNP P0DTC2
S	544	GLY	-	expression tag	UNP P0DTC2
S	545	LEU	-	expression tag	UNP P0DTC2
S	546	ASN	-	expression tag	UNP P0DTC2
S	547	ASP	-	expression tag	UNP P0DTC2
S	548	ILE	-	expression tag	UNP P0DTC2
S	549	PHE	-	expression tag	UNP P0DTC2
S	550	GLU	-	expression tag	UNP P0DTC2
S	551	ALA	-	expression tag	UNP P0DTC2
S	552	GLN	-	expression tag	UNP P0DTC2
S	553	LYS	-	expression tag	UNP P0DTC2
S	554	ILE	-	expression tag	UNP P0DTC2
S	555	GLU	-	expression tag	UNP P0DTC2
S	556	TRP	-	expression tag	UNP P0DTC2
S	557	HIS	-	expression tag	UNP P0DTC2
S	558	GLU	-	expression tag	UNP P0DTC2

- Molecule 7 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
7	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0
8	L	1	Total C O 4 2 2	0	0
8	L	1	Total C O 4 2 2	0	0
8	L	1	Total C O 4 2 2	0	0
8	M	1	Total C O 4 2 2	0	0
8	M	1	Total C O 4 2 2	0	0
8	N	1	Total C O 4 2 2	0	0
8	N	1	Total C O 4 2 2	0	0
8	R	1	Total C O 4 2 2	0	0
8	R	1	Total C O 4 2 2	0	0
8	R	1	Total C O 4 2 2	0	0
8	S	1	Total C O 4 2 2	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total Cl 3 3	0	0
9	C	2	Total Cl 2 2	0	0
9	D	2	Total Cl 2 2	0	0

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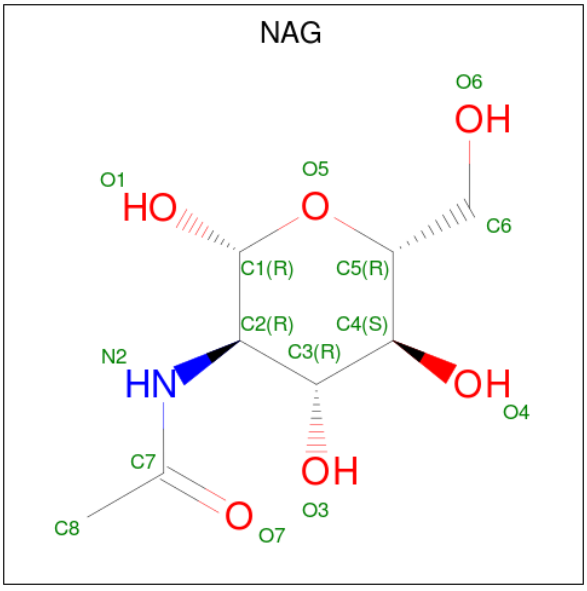
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	5	Total Cl 5 5	0	0
9	F	5	Total Cl 5 5	0	0
9	H	1	Total Cl 1 1	0	0
9	L	2	Total Cl 2 2	0	0
9	R	1	Total Cl 1 1	0	0
9	S	1	Total Cl 1 1	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total Zn 1 1	0	0
10	F	1	Total Zn 1 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0
11	E	1	Total C N O 14 8 1 5	0	0
11	F	1	Total C N O 14 8 1 5	0	0
11	F	1	Total C N O 14 8 1 5	0	0
11	F	1	Total C N O 14 8 1 5	0	0
11	F	1	Total C N O 14 8 1 5	0	0
11	F	1	Total C N O 14 8 1 5	0	0
11	F	1	Total C N O 14 8 1 5	0	0
11	R	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	79	Total O 79 79	0	0
12	B	68	Total O 68 68	0	0
12	C	56	Total O 56 56	0	0
12	D	87	Total O 87 87	0	0
12	E	59	Total O 59 59	0	0
12	F	103	Total O 103 103	0	0
12	H	66	Total O 66 66	0	0

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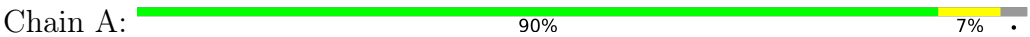
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	118	Total O 118 118	0	0
12	M	69	Total O 69 69	0	0
12	N	98	Total O 98 98	0	0
12	R	104	Total O 104 104	0	0
12	S	110	Total O 110 110	0	0

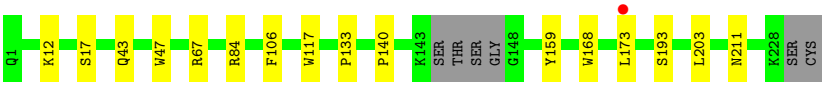
3 Residue-property plots (i)

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: S309 Fab Heavy Chain

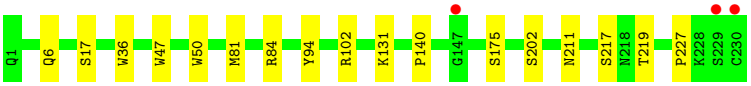
Chain A:





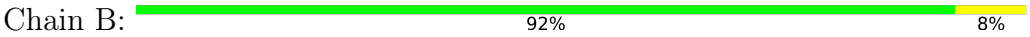
• Molecule 1: S309 Fab Heavy Chain

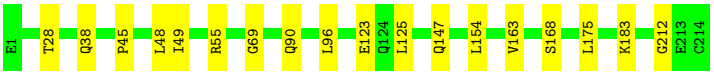
Chain C:



• Molecule 2: S309 Fab Light Chain

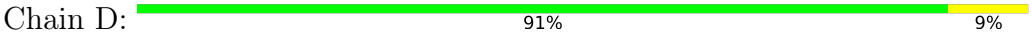
Chain B:

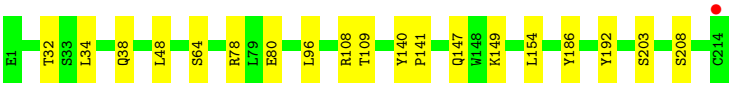




• Molecule 2: S309 Fab Light Chain

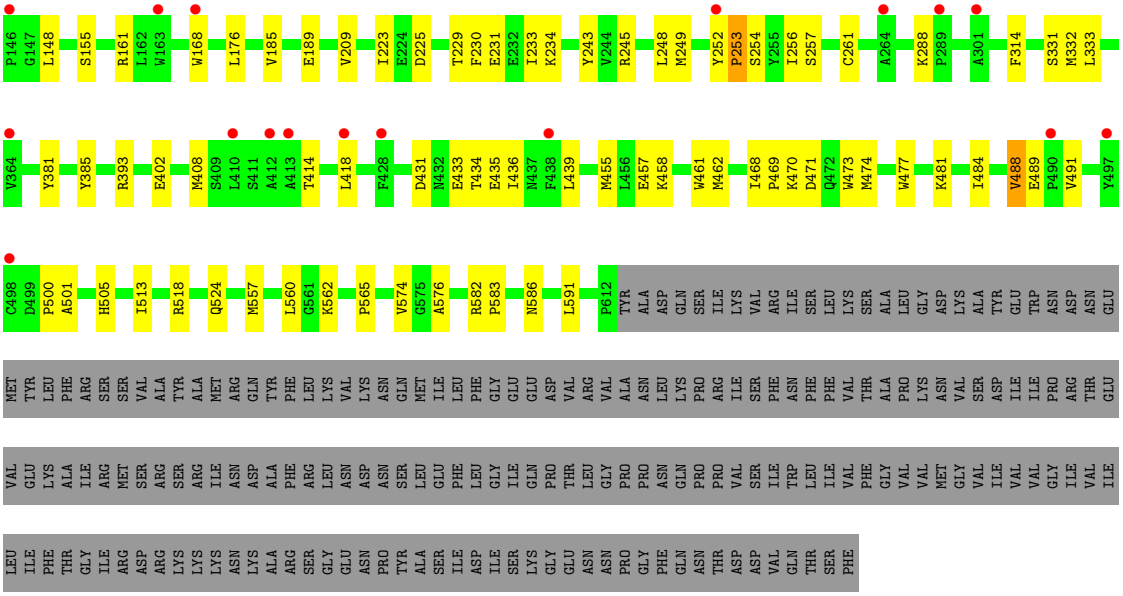
Chain D:





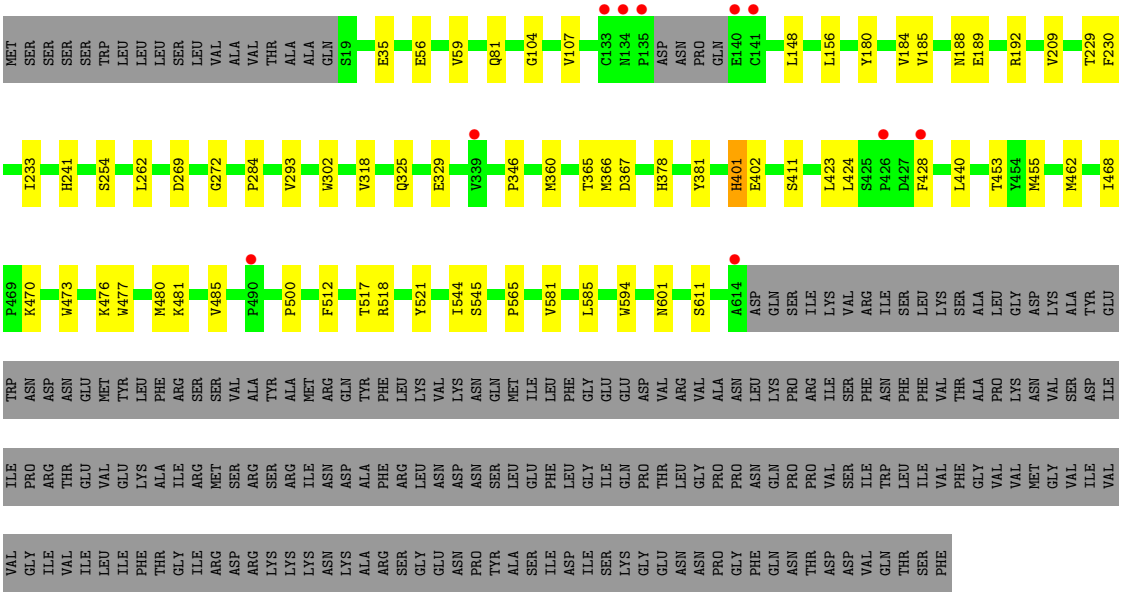
• Molecule 3: Angiotensin-converting enzyme 2

Chain E:



• Molecule 3: Angiotensin-converting enzyme 2

Chain F:



• Molecule 4: S304 Fab Heavy Chain

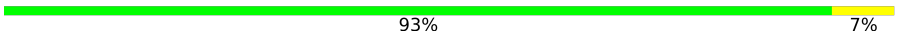
Chain H:

• Molecule 4: S304 Fab Heavy Chain

Chain M:

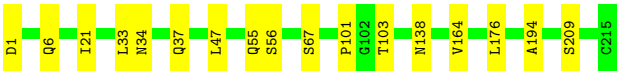
• Molecule 5: S304 Fab Light Chain

Chain L:



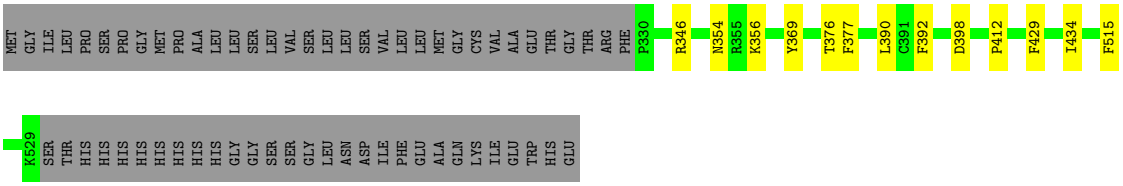
• Molecule 5: S304 Fab Light Chain

Chain N:



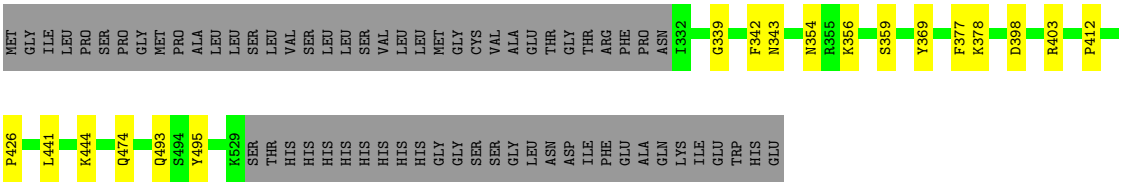
• Molecule 6: Spike protein S1

Chain R:



• Molecule 6: Spike protein S1

Chain S:

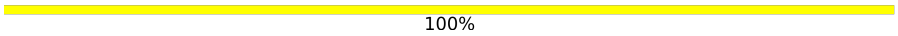


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:




NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.53Å 126.77Å 145.66Å 91.78° 103.66° 96.02°	Depositor
Resolution (Å)	46.27 – 2.70 63.19 – 2.45	Depositor EDS
% Data completeness (in resolution range)	92.2 (46.27-2.70) 90.8 (63.19-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.177 , 0.217 0.180 , 0.219	Depositor DCC
R_{free} test set	9187 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26905	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: NAG, EDO, ZN, CL

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	0.38	0/1703	0.58	0/2327
1	C	0.40	0/1757	0.61	0/2398
2	B	0.39	0/1650	0.61	0/2244
2	D	0.43	0/1641	0.62	0/2233
3	E	0.38	0/4709	0.54	0/6422
3	F	0.35	0/4876	0.53	0/6641
4	H	0.39	0/1644	0.59	0/2247
4	M	0.38	0/1662	0.58	0/2268
5	L	0.40	0/1658	0.59	0/2257
5	N	0.40	0/1651	0.59	0/2252
6	R	0.41	0/1621	0.58	0/2208
6	S	0.40	0/1593	0.57	0/2174
All	All	0.39	0/26165	0.57	0/35671

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

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	1661	0	1580	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1714	0	1645	9	0
2	B	1617	0	1558	11	0
2	D	1608	0	1545	9	0
3	E	4580	0	4119	59	0
3	F	4741	0	4415	37	0
4	H	1603	0	1510	13	0
4	M	1621	0	1539	13	0
5	L	1622	0	1551	9	0
5	N	1615	0	1529	10	0
6	R	1576	0	1479	9	0
6	S	1548	0	1437	12	0
7	G	28	0	25	0	0
7	I	28	0	25	1	0
8	A	8	0	12	0	0
8	B	24	0	36	2	0
8	C	4	0	6	0	0
8	D	8	0	12	0	0
8	E	16	0	24	0	0
8	F	16	0	24	0	0
8	L	12	0	18	2	0
8	M	8	0	12	2	0
8	N	8	0	12	0	0
8	R	12	0	18	0	0
8	S	4	0	6	0	0
9	A	3	0	0	0	0
9	C	2	0	0	2	0
9	D	2	0	0	0	0
9	E	5	0	0	3	0
9	F	5	0	0	1	0
9	H	1	0	0	0	0
9	L	2	0	0	0	0
9	R	1	0	0	0	0
9	S	1	0	0	1	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
11	E	84	0	78	0	0
11	F	84	0	78	2	0
11	R	14	0	13	0	0
12	A	79	0	0	1	0
12	B	68	0	0	0	1
12	C	56	0	0	3	0
12	D	87	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	E	59	0	0	2	0
12	F	103	0	0	2	0
12	H	66	0	0	2	0
12	L	118	0	0	5	0
12	M	69	0	0	0	0
12	N	98	0	0	0	0
12	R	104	0	0	2	0
12	S	110	0	0	2	0
All	All	26905	0	24306	196	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 (196) 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)
3:E:231:GLU:HA	3:E:234:LYS:HE3	1.49	0.91
8:M:302:EDO:H22	5:N:55:GLN:HE22	1.34	0.89
3:E:113:SER:O	3:E:117:ASN:ND2	2.17	0.78
9:S:602:CL:CL	12:S:798:HOH:O	2.39	0.77
3:F:284:PRO:HD3	3:F:440:LEU:HD22	1.67	0.77
9:E:1115:CL:CL	12:E:1248:HOH:O	2.41	0.75
5:L:144:GLU:N	5:L:144:GLU:OE1	2.19	0.72
2:D:78:ARG:NH1	2:D:80:GLU:OE2	2.22	0.72
9:F:1215:CL:CL	12:F:1338:HOH:O	2.45	0.72
2:B:212:GLY:H	8:B:306:EDO:H11	1.54	0.72
3:E:518:ARG:NH2	9:E:1113:CL:CL	2.59	0.72
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.70	0.71
3:E:402:GLU:HB3	3:E:518:ARG:HD2	1.73	0.71
6:S:474:GLN:NE2	12:S:701:HOH:O	2.25	0.69
3:E:582:ARG:O	3:E:586:ASN:ND2	2.23	0.68
3:E:518:ARG:HD3	9:E:1115:CL:CL	2.31	0.67
3:F:293:VAL:HG22	3:F:366:MET:HG3	1.76	0.67
3:E:185:VAL:O	3:E:189:GLU:HG3	1.95	0.66
4:H:155:GLU:OE1	12:H:401:HOH:O	2.15	0.65
3:E:148:LEU:H	3:E:148:LEU:HD12	1.61	0.64
1:C:102:ARG:NH1	9:C:302:CL:CL	2.68	0.64
3:E:230:PHE:HA	3:E:233:ILE:HG22	1.81	0.63
3:F:402:GLU:HB3	3:F:518:ARG:HD2	1.81	0.62
4:H:66:ARG:NH2	4:H:89:ASP:OD2	2.32	0.62
6:R:346:ARG:NH2	12:R:703:HOH:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:37:GLN:HB2	5:N:47:LEU:HD11	1.81	0.61
9:C:302:CL:CL	12:C:436:HOH:O	2.54	0.59
4:M:56:ASP:HB3	6:S:369:TYR:CG	2.38	0.58
1:C:140:PRO:HG2	1:C:227:PRO:HB3	1.84	0.58
8:L:302:EDO:H11	12:L:488:HOH:O	2.04	0.58
6:S:403:ARG:HG2	6:S:495:TYR:CE1	2.38	0.58
3:E:122:THR:O	3:E:126:ILE:HG23	2.03	0.57
3:F:233:ILE:HD12	3:F:585:LEU:HD21	1.87	0.57
2:B:125:LEU:O	2:B:183:LYS:HD2	2.05	0.57
4:H:56:ASP:OD1	4:H:56:ASP:N	2.31	0.57
3:F:346:PRO:HB3	3:F:360:MET:HG3	1.87	0.57
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.86	0.56
3:F:269:ASP:OD1	3:F:272:GLY:N	2.37	0.56
3:E:288:LYS:HB3	3:E:434:THR:HG22	1.87	0.56
8:M:302:EDO:H22	5:N:55:GLN:NE2	2.13	0.56
3:E:469:PRO:HB2	3:E:471:ASP:OD1	2.06	0.56
3:E:468:ILE:HG22	3:E:473:TRP:HD1	1.71	0.56
3:E:414:THR:O	3:E:418:LEU:HD12	2.06	0.55
3:F:601:ASN:ND2	12:F:1301:HOH:O	2.38	0.55
3:E:37:GLU:OE2	3:E:393:ARG:NH2	2.31	0.55
3:E:455:MET:HG2	3:E:484:ILE:HD12	1.88	0.54
3:E:439:LEU:HB3	3:E:591:LEU:HD13	1.88	0.54
2:B:212:GLY:H	8:B:306:EDO:C1	2.19	0.54
3:F:188:ASN:O	3:F:192:ARG:HG3	2.07	0.54
3:E:144:LEU:HB2	3:E:168:TRP:CH2	2.43	0.54
2:B:123:GLU:OE1	2:B:123:GLU:N	2.26	0.54
4:H:56:ASP:HB3	6:R:369:TYR:CG	2.43	0.54
3:F:302:TRP:CZ2	3:F:423:LEU:HD21	2.44	0.53
3:F:378:HIS:HD1	3:F:401:HIS:HD1	1.56	0.53
2:D:32:THR:HG22	6:S:441:LEU:HD22	1.90	0.53
3:F:56:GLU:O	3:F:59:VAL:HG12	2.08	0.53
4:M:192:PRO:O	4:M:195:SER:OG	2.25	0.52
3:E:223:ILE:HG12	3:E:461:TRP:CZ3	2.45	0.52
2:B:28:THR:HG23	2:B:69:GLY:HA2	1.91	0.52
1:A:140:PRO:HG3	1:A:203:LEU:HD22	1.92	0.52
5:L:18:ARG:NH1	12:L:404:HOH:O	2.41	0.52
5:N:21:ILE:HG12	5:N:103:THR:HG21	1.92	0.52
3:E:233:ILE:O	3:E:233:ILE:HG13	2.10	0.51
4:H:63:VAL:HG13	4:H:67:PHE:HB2	1.92	0.51
3:E:477:TRP:CE3	3:E:500:PRO:HG3	2.46	0.51
3:F:180:TYR:O	3:F:184:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:209:VAL:HG11	3:F:565:PRO:HB3	1.93	0.50
2:B:49:ILE:HD13	2:B:55:ARG:HA	1.94	0.50
1:C:36:TRP:CE2	1:C:81:MET:HB2	2.46	0.50
3:E:56:GLU:O	3:E:59:VAL:HG12	2.12	0.50
3:E:331:SER:HB3	3:E:333:LEU:HD21	1.94	0.50
8:L:302:EDO:H12	12:L:420:HOH:O	2.12	0.50
3:F:318:VAL:HG11	3:F:544:ILE:HD12	1.93	0.49
6:S:354:ASN:O	6:S:398:ASP:HA	2.12	0.49
3:E:248:LEU:O	3:E:252:TYR:N	2.38	0.49
4:M:56:ASP:OD1	4:M:56:ASP:N	2.33	0.49
3:F:517:THR:HG22	3:F:521:TYR:CE2	2.48	0.49
3:E:144:LEU:HB2	3:E:168:TRP:CZ3	2.47	0.49
3:E:225:ASP:O	3:E:229:THR:HG23	2.13	0.49
1:A:47:TRP:CG	2:B:96:LEU:HD22	2.47	0.49
3:E:119:ILE:O	3:E:123:MET:HG3	2.13	0.49
5:N:1:ASP:OD1	6:S:378:LYS:NZ	2.45	0.49
6:S:342:PHE:HB2	7:I:1:NAG:H82	1.95	0.49
3:E:144:LEU:HA	3:E:148:LEU:HD13	1.94	0.49
1:C:131:LYS:NZ	12:C:403:HOH:O	2.38	0.48
3:E:557:MET:HA	3:E:560:LEU:HD12	1.94	0.48
5:L:142:PRO:HB2	5:L:144:GLU:OE1	2.13	0.48
3:E:155:SER:O	3:E:161:ARG:HD2	2.13	0.48
6:S:403:ARG:HG2	6:S:495:TYR:HE1	1.78	0.48
3:F:241:HIS:NE2	3:F:262:LEU:HD23	2.28	0.48
3:F:453:THR:HG23	3:F:512:PHE:CD2	2.48	0.48
3:E:231:GLU:HA	3:E:234:LYS:CE	2.34	0.48
3:F:104:GLY:O	3:F:107:VAL:HG22	2.14	0.48
1:C:50:TRP:CZ2	1:C:102:ARG:HG2	2.48	0.48
1:C:217:SER:OG	1:C:219:THR:OG1	2.25	0.47
4:H:152:TYR:CE1	4:H:157:VAL:HG13	2.49	0.47
3:E:457:GLU:HG2	3:E:513:ILE:HB	1.96	0.47
3:F:477:TRP:CD2	3:F:500:PRO:HG3	2.50	0.47
1:A:12:LYS:HD2	1:A:17:SER:O	2.14	0.47
3:E:230:PHE:O	3:E:233:ILE:HG22	2.15	0.47
3:F:293:VAL:CG2	3:F:366:MET:HG3	2.44	0.47
3:E:431:ASP:O	3:E:435:GLU:HG3	2.15	0.46
3:F:325:GLN:O	3:F:329:GLU:HG3	2.14	0.46
5:N:33:LEU:HG	5:N:34:ASN:N	2.29	0.46
4:H:210:SER:OG	4:H:212:THR:OG1	2.24	0.46
4:H:36:TRP:HD1	4:H:69:ILE:HD12	1.81	0.46
3:F:81:GLN:OE1	11:F:1206:NAG:H5	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:NE2	12:A:401:HOH:O	2.42	0.46
3:E:562:LYS:HG2	3:E:562:LYS:O	2.15	0.46
3:F:476:LYS:O	3:F:480:MET:HG3	2.15	0.46
3:E:314:PHE:HE2	3:E:408:MET:HE3	1.80	0.46
4:M:1:GLN:OE1	4:M:3:GLN:NE2	2.49	0.46
3:E:431:ASP:OD1	3:E:433:GLU:N	2.48	0.46
5:L:14:ALA:O	5:L:17:ASP:HB2	2.16	0.46
3:E:455:MET:HE1	3:E:481:LYS:HE2	1.99	0.45
1:A:133:PRO:HB3	1:A:159:TYR:HB3	1.99	0.45
4:H:18:LEU:HD22	4:H:116:LEU:HD13	1.99	0.45
6:R:354:ASN:O	6:R:398:ASP:HA	2.16	0.45
6:R:376:THR:O	6:R:434:ILE:HA	2.17	0.45
3:F:35:GLU:OE2	6:S:493:GLN:NE2	2.50	0.45
1:A:106:PHE:CG	6:R:356:LYS:HD2	2.52	0.45
4:M:33:ASP:HB2	4:M:105:TYR:OH	2.17	0.45
3:F:230:PHE:O	3:F:233:ILE:HG22	2.17	0.44
4:H:44:GLY:HA2	12:L:460:HOH:O	2.16	0.44
3:E:50:TYR:HE2	3:E:59:VAL:HB	1.83	0.44
4:M:152:TYR:CE1	4:M:157:VAL:HG13	2.52	0.44
3:F:229:THR:HB	3:F:581:VAL:HB	1.97	0.44
6:R:412:PRO:HG3	6:R:429:PHE:HB3	1.97	0.44
12:C:420:HOH:O	6:S:356:LYS:HE3	2.17	0.44
2:D:186:TYR:HA	2:D:192:TYR:OH	2.18	0.44
6:R:346:ARG:NH2	12:R:706:HOH:O	2.49	0.44
6:S:339:GLY:O	6:S:343:ASN:HB2	2.18	0.44
3:E:524:GLN:HG2	3:E:583:PRO:HG2	2.00	0.44
1:A:67:ARG:O	1:A:84:ARG:HG2	2.18	0.44
3:F:284:PRO:HB3	3:F:594:TRP:CH2	2.53	0.43
4:H:124:LYS:NZ	12:H:405:HOH:O	2.51	0.43
2:B:38:GLN:HB2	2:B:48:LEU:HD11	2.00	0.43
5:L:125:GLN:NE2	12:L:406:HOH:O	2.49	0.43
1:A:117:TRP:CZ3	2:B:45:PRO:HG2	2.53	0.43
6:R:392:PHE:CD1	6:R:515:PHE:HB3	2.53	0.43
3:E:505:HIS:H	3:E:505:HIS:HD1	1.65	0.43
3:F:440:LEU:O	3:F:440:LEU:HG	2.16	0.43
3:F:517:THR:HG22	3:F:521:TYR:CZ	2.54	0.43
5:N:164:VAL:HG22	5:N:176:LEU:HD12	2.00	0.43
3:F:185:VAL:O	3:F:189:GLU:HG3	2.19	0.43
3:F:462:MET:HB2	3:F:468:ILE:HD11	2.01	0.42
1:C:17:SER:OG	1:C:84:ARG:HG2	2.19	0.42
3:F:455:MET:HE1	3:F:481:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:176:LEU:HD13	3:E:501:ALA:HB1	2.01	0.42
3:E:253:PRO:HG2	3:E:254:SER:H	1.84	0.42
3:E:470:LYS:HA	3:E:473:TRP:CD1	2.54	0.42
3:E:249:MET:HG3	3:E:256:ILE:HB	2.01	0.42
5:N:194:ALA:HB2	5:N:209:SER:HB3	2.02	0.42
6:R:390:LEU:HD23	6:R:390:LEU:HA	1.81	0.42
3:E:31:LYS:NZ	12:E:1208:HOH:O	2.51	0.42
3:E:574:VAL:HG23	3:E:576:ALA:H	1.84	0.42
6:S:412:PRO:HB3	6:S:426:PRO:O	2.20	0.42
3:E:209:VAL:HG11	3:E:565:PRO:HB3	2.02	0.42
3:E:261:CYS:HB2	3:E:488:VAL:HG13	2.00	0.42
3:F:424:LEU:HD13	3:F:428:PHE:CD2	2.55	0.42
5:N:6:GLN:HG3	5:N:101:PRO:HD2	2.02	0.42
2:D:192:TYR:O	2:D:208:SER:HA	2.19	0.42
3:E:436:ILE:HD13	3:E:436:ILE:HA	1.81	0.42
5:L:120:PRO:HB3	5:L:210:PHE:CE1	2.55	0.42
4:M:63:VAL:HG13	4:M:67:PHE:HB2	2.01	0.42
1:C:6:GLN:NE2	1:C:94:TYR:O	2.39	0.41
4:M:35:HIS:CE1	4:M:50:THR:HG23	2.55	0.41
3:E:474:MET:O	3:E:477:TRP:HB3	2.20	0.41
4:M:190:THR:HG21	5:N:138:ASN:ND2	2.35	0.41
3:E:288:LYS:HG3	3:E:433:GLU:HB2	2.02	0.41
5:L:63:SER:O	5:L:73:LEU:HD12	2.20	0.41
4:H:51:ILE:HD13	4:H:71:ARG:HD2	2.03	0.41
4:M:22:CYS:HB3	4:M:78:LEU:HB3	2.01	0.41
2:D:147:GLN:HG2	2:D:154:LEU:HD11	2.01	0.41
5:L:120:PRO:HB3	5:L:210:PHE:CZ	2.55	0.41
2:D:38:GLN:HB2	2:D:48:LEU:HD21	2.03	0.41
2:D:108:ARG:HG2	2:D:109:THR:N	2.35	0.41
3:E:489:GLU:HG3	3:E:491:VAL:O	2.21	0.41
4:M:11:LEU:HB2	4:M:154:PRO:HG3	2.03	0.41
2:B:147:GLN:HG2	2:B:154:LEU:HD11	2.03	0.41
2:D:140:TYR:CG	2:D:141:PRO:HA	2.55	0.41
3:E:52:THR:HG22	3:E:332:MET:SD	2.61	0.41
3:E:458:LYS:O	3:E:462:MET:HG3	2.21	0.41
3:E:477:TRP:CD2	3:E:500:PRO:HG3	2.56	0.41
1:A:168:TRP:HB3	1:A:173:LEU:HD23	2.02	0.41
3:F:470:LYS:HA	3:F:473:TRP:CD1	2.56	0.41
3:E:245:ARG:HD2	3:E:257:SER:O	2.22	0.40
4:H:36:TRP:NE1	4:H:80:LEU:HB2	2.37	0.40
4:M:8:GLY:O	4:M:18:LEU:HD21	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:TRP:CG	2:D:96:LEU:HD22	2.56	0.40
3:E:148:LEU:HD12	3:E:148:LEU:N	2.33	0.40
3:E:243:TYR:CD1	3:E:243:TYR:C	2.94	0.40
3:F:148:LEU:HD12	3:F:148:LEU:H	1.87	0.40
3:F:365:THR:HG22	3:F:367:ASP:H	1.87	0.40
3:F:545:SER:HB2	11:F:1204:NAG:H82	2.04	0.40
4:M:43:LYS:HB3	4:M:46:GLU:OE2	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)
12:B:448:HOH:O	12:D:478:HOH:O[1_546]	2.05	0.15

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	220/230 (96%)	218 (99%)	2 (1%)	0	100	100
1	C	228/230 (99%)	225 (99%)	3 (1%)	0	100	100
2	B	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
2	D	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
3	E	583/805 (72%)	572 (98%)	10 (2%)	1 (0%)	47	73
3	F	588/805 (73%)	576 (98%)	12 (2%)	0	100	100
4	H	213/223 (96%)	211 (99%)	2 (1%)	0	100	100
4	M	214/223 (96%)	212 (99%)	2 (1%)	0	100	100
5	L	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
5	N	213/215 (99%)	208 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	R	198/263 (75%)	191 (96%)	7 (4%)	0	100	100
6	S	196/263 (74%)	191 (97%)	5 (3%)	0	100	100
All	All	3290/3900 (84%)	3226 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	253	PRO

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	178/192 (93%)	176 (99%)	2 (1%)	73	90
1	C	187/192 (97%)	184 (98%)	3 (2%)	62	85
2	B	181/185 (98%)	179 (99%)	2 (1%)	73	90
2	D	180/185 (97%)	176 (98%)	4 (2%)	52	79
3	E	454/711 (64%)	448 (99%)	6 (1%)	69	87
3	F	495/711 (70%)	488 (99%)	7 (1%)	67	86
4	H	173/185 (94%)	173 (100%)	0	100	100
4	M	177/185 (96%)	174 (98%)	3 (2%)	60	84
5	L	182/188 (97%)	179 (98%)	3 (2%)	62	85
5	N	180/188 (96%)	178 (99%)	2 (1%)	73	90
6	R	169/226 (75%)	168 (99%)	1 (1%)	86	95
6	S	165/226 (73%)	162 (98%)	3 (2%)	59	83
All	All	2721/3374 (81%)	2685 (99%)	36 (1%)	69	87

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	SER

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Mol	Chain	Res	Type
1	A	211	ASN
2	B	90	GLN
2	B	168	SER
1	C	175	SER
1	C	202	SER
1	C	211	ASN
2	D	34	LEU
2	D	64	SER
2	D	149	LYS
2	D	203	SER
3	E	30	ASP
3	E	94	LYS
3	E	103	ASN
3	E	381	TYR
3	E	385	TYR
3	E	488	VAL
3	F	156	LEU
3	F	254	SER
3	F	381	TYR
3	F	401	HIS
3	F	411	SER
3	F	485	VAL
3	F	611	SER
5	L	9	SER
5	L	56	SER
5	L	191	LYS
4	M	186	SER
4	M	193	SER
4	M	204	ASN
5	N	56	SER
5	N	67	SER
6	R	377	PHE
6	S	359	SER
6	S	377	PHE
6	S	444	LYS

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	3	GLN
1	C	57	ASN
2	D	160	GLN

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Mol	Chain	Res	Type
3	E	325	GLN
3	E	552	GLN
3	F	325	GLN
5	L	3	GLN
4	M	3	GLN
5	N	211	ASN
6	S	474	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)

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	$\#\|Z\| > 2$
7	NAG	G	1	6,7	14,14,15	0.48	0	17,19,21	0.62	0
7	NAG	G	2	7	14,14,15	1.13	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	I	1	6,7	14,14,15	0.36	0	17,19,21	0.58	0
7	NAG	I	2	7	14,14,15	0.34	0	17,19,21	1.30	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
7	NAG	G	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	NAG	I	1	6,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	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)
7	G	2	NAG	O5-C1	-3.62	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	2	NAG	C1-O5-C5	4.64	118.48	112.19
7	G	2	NAG	C1-O5-C5	3.35	116.73	112.19

There are no chirality outliers.

There are no torsion outliers.

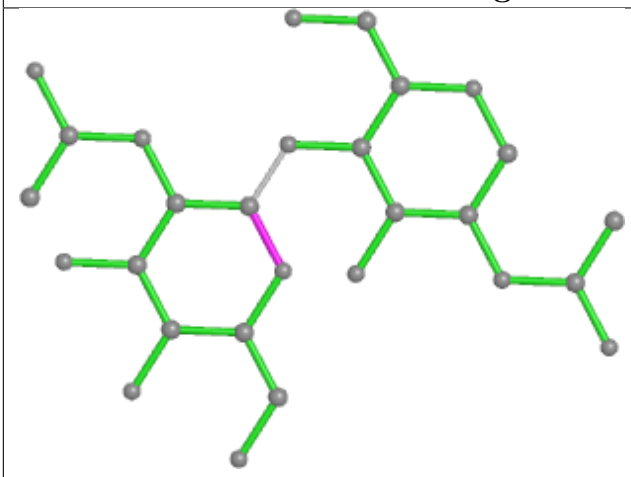
There are no ring outliers.

1 monomer is involved in 1 short contact:

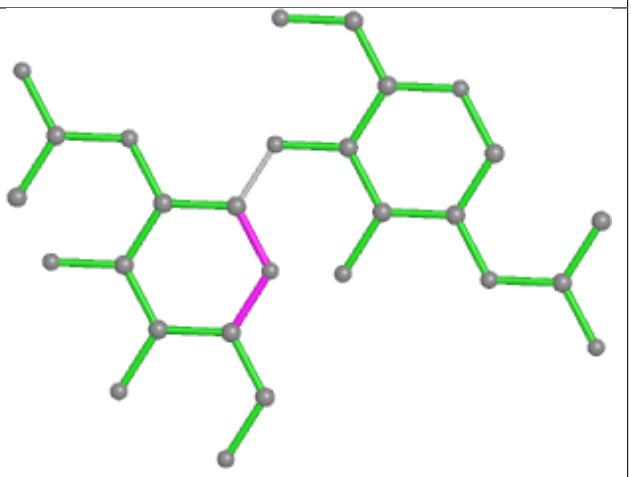
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	1	NAG	1	0

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

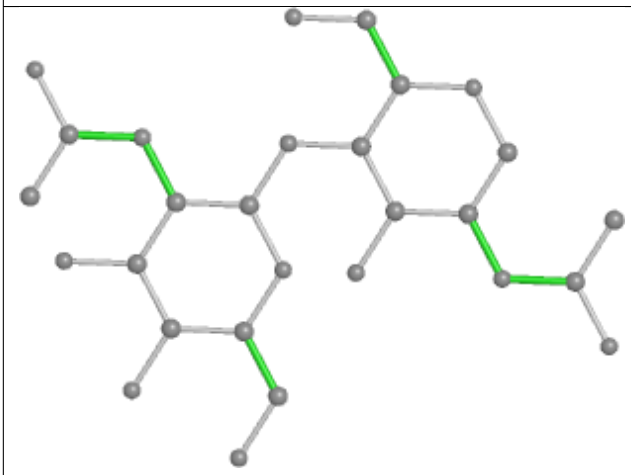
Oligosaccharide Chain G



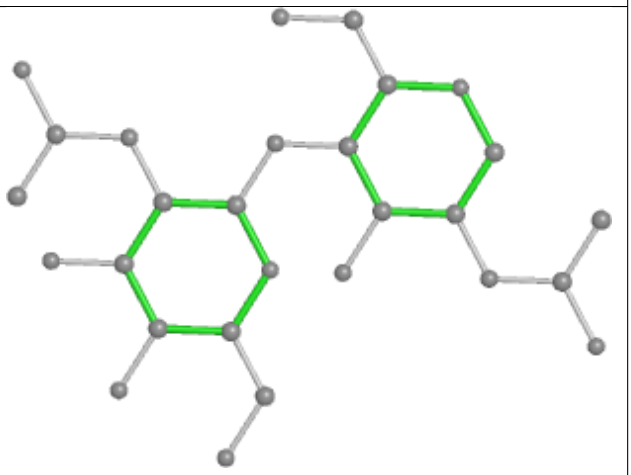
Bond lengths



Bond angles

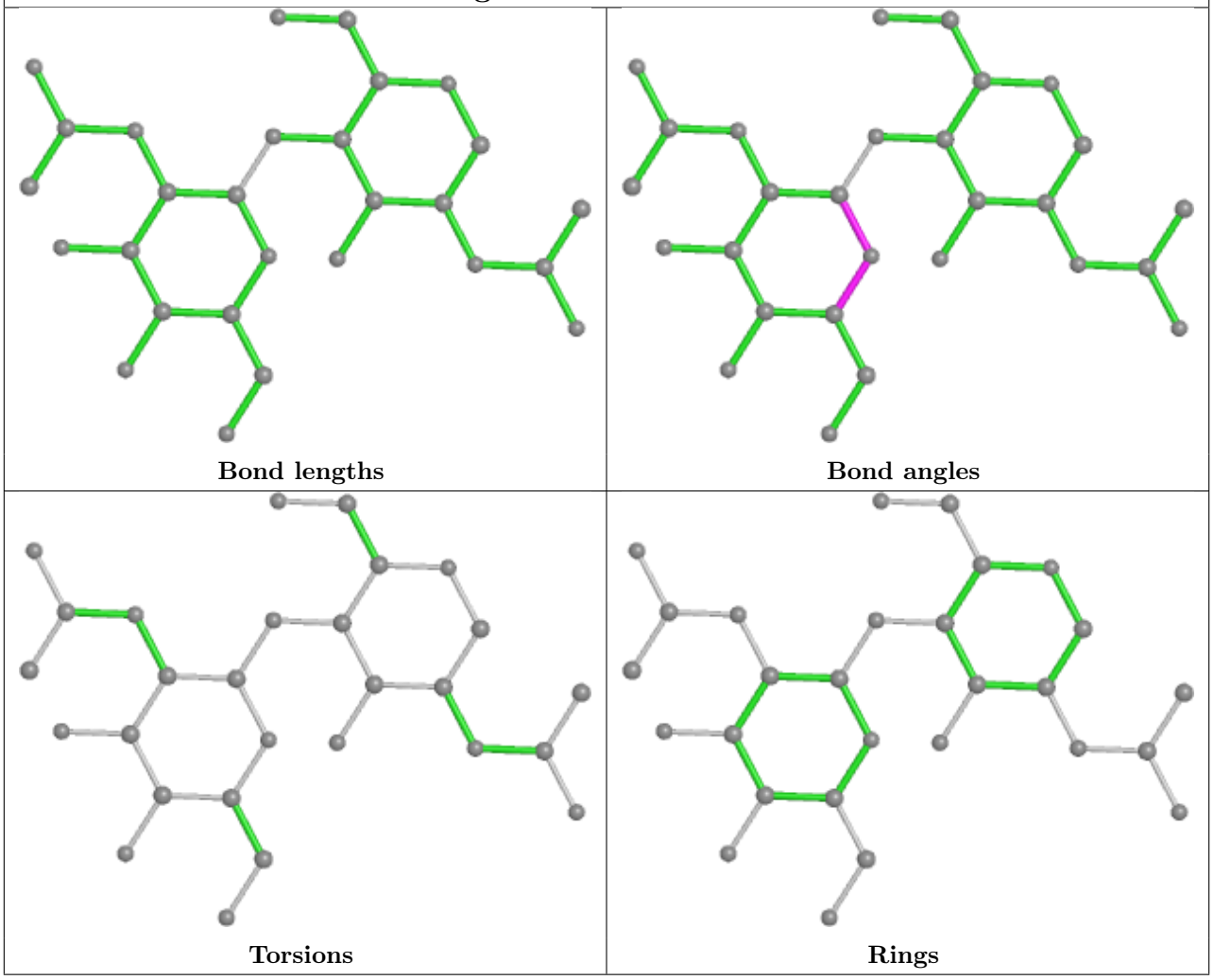


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 24 are monoatomic - leaving 43 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	$\#\|Z\| > 2$
8	EDO	C	301	-	3,3,3	0.56	0	2,2,2	0.18	0
8	EDO	R	603	-	3,3,3	0.45	0	2,2,2	0.41	0
8	EDO	L	301	-	3,3,3	0.55	0	2,2,2	0.06	0
8	EDO	F	1209	-	3,3,3	1.63	0	2,2,2	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	EDO	B	301	-	3,3,3	0.42	0	2,2,2	0.41	0
8	EDO	N	302	-	3,3,3	0.70	0	2,2,2	0.48	0
11	NAG	E	1106	3	14,14,15	0.43	0	17,19,21	0.38	0
8	EDO	B	306	-	3,3,3	0.99	0	2,2,2	2.27	1 (50%)
8	EDO	M	301	-	3,3,3	0.49	0	2,2,2	0.52	0
11	NAG	E	1102	3	14,14,15	0.14	0	17,19,21	0.50	0
11	NAG	F	1203	3	14,14,15	0.31	0	17,19,21	0.52	0
8	EDO	L	302	-	3,3,3	1.84	1 (33%)	2,2,2	0.77	0
8	EDO	B	302	-	3,3,3	0.56	0	2,2,2	0.13	0
8	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.31	0
11	NAG	F	1207	3	14,14,15	0.46	0	17,19,21	0.59	1 (5%)
8	EDO	F	1210	-	3,3,3	1.74	1 (33%)	2,2,2	1.93	1 (50%)
8	EDO	N	301	-	3,3,3	0.54	0	2,2,2	0.10	0
8	EDO	E	1109	-	3,3,3	1.80	1 (33%)	2,2,2	1.18	0
11	NAG	E	1107	3	14,14,15	0.52	0	17,19,21	0.60	0
8	EDO	D	302	-	3,3,3	0.53	0	2,2,2	0.21	0
8	EDO	A	301	-	3,3,3	0.53	0	2,2,2	0.19	0
8	EDO	M	302	-	3,3,3	1.42	0	2,2,2	0.83	0
11	NAG	R	601	6	14,14,15	0.48	0	17,19,21	0.38	0
11	NAG	E	1103	3	14,14,15	0.33	0	17,19,21	0.68	0
8	EDO	A	302	-	3,3,3	0.48	0	2,2,2	0.20	0
11	NAG	F	1206	3	14,14,15	0.54	0	17,19,21	0.44	0
11	NAG	F	1205	3	14,14,15	0.37	0	17,19,21	0.71	1 (5%)
8	EDO	F	1211	-	3,3,3	1.33	0	2,2,2	2.20	1 (50%)
11	NAG	E	1105	3	14,14,15	0.71	0	17,19,21	0.84	1 (5%)
8	EDO	E	1110	-	3,3,3	1.51	0	2,2,2	1.32	0
8	EDO	F	1208	-	3,3,3	0.57	0	2,2,2	0.40	0
8	EDO	L	303	-	3,3,3	1.78	1 (33%)	2,2,2	0.43	0
11	NAG	E	1104	3	14,14,15	0.31	0	17,19,21	0.66	1 (5%)
8	EDO	S	601	-	3,3,3	0.46	0	2,2,2	0.44	0
8	EDO	B	303	-	3,3,3	0.49	0	2,2,2	0.32	0
11	NAG	F	1202	3	14,14,15	0.21	0	17,19,21	0.71	1 (5%)
8	EDO	D	301	-	3,3,3	0.47	0	2,2,2	0.26	0
8	EDO	R	604	-	3,3,3	0.43	0	2,2,2	0.42	0
8	EDO	R	602	-	3,3,3	0.50	0	2,2,2	0.28	0
11	NAG	F	1204	3	14,14,15	0.35	0	17,19,21	0.48	0
8	EDO	E	1108	-	3,3,3	0.42	0	2,2,2	0.54	0
8	EDO	B	305	-	3,3,3	0.50	0	2,2,2	0.28	0
8	EDO	E	1111	-	3,3,3	1.67	1 (33%)	2,2,2	1.54	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
8	EDO	C	301	-	-	0/1/1/1	-
8	EDO	R	603	-	-	0/1/1/1	-
8	EDO	L	301	-	-	0/1/1/1	-
8	EDO	F	1209	-	-	1/1/1/1	-
8	EDO	B	301	-	-	0/1/1/1	-
8	EDO	N	302	-	-	0/1/1/1	-
11	NAG	E	1106	3	-	1/6/23/26	0/1/1/1
8	EDO	B	306	-	-	1/1/1/1	-
8	EDO	M	301	-	-	0/1/1/1	-
11	NAG	E	1102	3	-	0/6/23/26	0/1/1/1
11	NAG	F	1203	3	-	0/6/23/26	0/1/1/1
8	EDO	L	302	-	-	0/1/1/1	-
8	EDO	B	302	-	-	0/1/1/1	-
8	EDO	B	304	-	-	0/1/1/1	-
11	NAG	F	1207	3	-	0/6/23/26	0/1/1/1
8	EDO	F	1210	-	-	0/1/1/1	-
8	EDO	N	301	-	-	0/1/1/1	-
8	EDO	E	1109	-	-	0/1/1/1	-
11	NAG	E	1107	3	-	0/6/23/26	0/1/1/1
8	EDO	D	302	-	-	1/1/1/1	-
8	EDO	A	301	-	-	0/1/1/1	-
8	EDO	M	302	-	-	0/1/1/1	-
11	NAG	R	601	6	-	0/6/23/26	0/1/1/1
11	NAG	E	1103	3	-	0/6/23/26	0/1/1/1
8	EDO	A	302	-	-	0/1/1/1	-
11	NAG	F	1206	3	-	0/6/23/26	0/1/1/1
11	NAG	F	1205	3	-	1/6/23/26	0/1/1/1
8	EDO	F	1211	-	-	0/1/1/1	-
11	NAG	E	1105	3	-	0/6/23/26	0/1/1/1
8	EDO	E	1110	-	-	0/1/1/1	-
8	EDO	F	1208	-	-	0/1/1/1	-
8	EDO	L	303	-	-	1/1/1/1	-
11	NAG	E	1104	3	-	0/6/23/26	0/1/1/1
8	EDO	S	601	-	-	0/1/1/1	-
8	EDO	B	303	-	-	0/1/1/1	-
11	NAG	F	1202	3	-	0/6/23/26	0/1/1/1
8	EDO	D	301	-	-	0/1/1/1	-
8	EDO	R	604	-	-	1/1/1/1	-
8	EDO	R	602	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	F	1204	3	-	2/6/23/26	0/1/1/1
8	EDO	E	1108	-	-	0/1/1/1	-
8	EDO	B	305	-	-	0/1/1/1	-
8	EDO	E	1111	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	1109	EDO	O1-C1	2.17	1.53	1.42
8	L	303	EDO	O1-C1	2.12	1.53	1.42
8	F	1210	EDO	O1-C1	2.09	1.52	1.42
8	L	302	EDO	C2-C1	2.05	1.62	1.48
8	E	1111	EDO	O1-C1	2.01	1.52	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	1105	NAG	C1-O5-C5	2.83	116.03	112.19
8	B	306	EDO	O1-C1-C2	-2.73	92.25	111.91
11	F	1205	NAG	C1-O5-C5	2.43	115.48	112.19
8	F	1211	EDO	O1-C1-C2	-2.42	94.47	111.91
11	F	1202	NAG	C1-O5-C5	2.28	115.29	112.19
11	E	1104	NAG	C1-O5-C5	2.17	115.14	112.19
8	F	1210	EDO	O2-C2-C1	-2.11	96.72	111.91
11	F	1207	NAG	C1-O5-C5	2.02	114.94	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	303	EDO	O1-C1-C2-O2
11	F	1205	NAG	O5-C5-C6-O6
11	F	1204	NAG	C4-C5-C6-O6
11	F	1204	NAG	O5-C5-C6-O6
11	E	1106	NAG	C4-C5-C6-O6
8	F	1209	EDO	O1-C1-C2-O2
8	B	306	EDO	O1-C1-C2-O2
8	E	1111	EDO	O1-C1-C2-O2
8	D	302	EDO	O1-C1-C2-O2
8	R	604	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	306	EDO	2	0
8	L	302	EDO	2	0
8	M	302	EDO	2	0
11	F	1206	NAG	1	0
11	F	1204	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, 95^{th} 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	224/230 (97%)	-0.06	1 (0%) 92 93	43, 65, 83, 105	0
1	C	230/230 (100%)	-0.10	3 (1%) 77 78	44, 59, 81, 114	0
2	B	214/214 (100%)	-0.24	0 100 100	43, 55, 77, 97	0
2	D	214/214 (100%)	-0.17	1 (0%) 91 92	43, 53, 70, 107	0
3	E	587/805 (72%)	0.06	20 (3%) 45 45	50, 85, 126, 150	0
3	F	592/805 (73%)	-0.01	10 (1%) 70 72	50, 74, 98, 136	0
4	H	217/223 (97%)	-0.22	1 (0%) 91 92	42, 57, 78, 133	0
4	M	218/223 (97%)	-0.12	0 100 100	41, 58, 78, 107	0
5	L	215/215 (100%)	-0.18	0 100 100	39, 48, 70, 99	0
5	N	215/215 (100%)	-0.03	0 100 100	40, 51, 82, 105	0
6	R	200/263 (76%)	-0.06	0 100 100	40, 50, 75, 104	0
6	S	198/263 (75%)	-0.06	0 100 100	41, 50, 76, 95	0
All	All	3324/3900 (85%)	-0.07	36 (1%) 80 82	39, 61, 103, 150	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	135	PRO	4.5
3	E	133	CYS	4.3
2	D	214	CYS	3.8
3	F	133	CYS	3.5
3	E	497	TYR	3.4
1	C	147	GLY	3.4
3	E	301	ALA	3.3
3	E	103	ASN	3.2
3	E	428	PHE	3.2
3	F	339	VAL	2.9
3	F	614	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
4	H	223	CYS	2.8
3	E	498	CYS	2.8
3	E	413	ALA	2.7
1	C	230	CYS	2.7
3	E	289	PRO	2.6
3	E	141	CYS	2.6
3	E	168	TRP	2.6
3	F	141	CYS	2.6
3	F	490	PRO	2.5
1	C	229	SER	2.5
3	E	364	VAL	2.5
3	F	134	ASN	2.5
3	F	140	GLU	2.4
3	E	438	PHE	2.4
3	E	412	ALA	2.4
3	E	146	PRO	2.3
1	A	173	LEU	2.3
3	E	264	ALA	2.2
3	F	426	PRO	2.2
3	E	418	LEU	2.1
3	E	252	TYR	2.1
3	F	428	PHE	2.1
3	E	410	LEU	2.1
3	E	490	PRO	2.0
3	E	163	TRP	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^{th} 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
7	NAG	I	2	14/15	0.79	0.20	65,85,92,97	0
7	NAG	G	2	14/15	0.88	0.20	72,80,90,100	0
7	NAG	I	1	14/15	0.94	0.14	53,59,67,71	0

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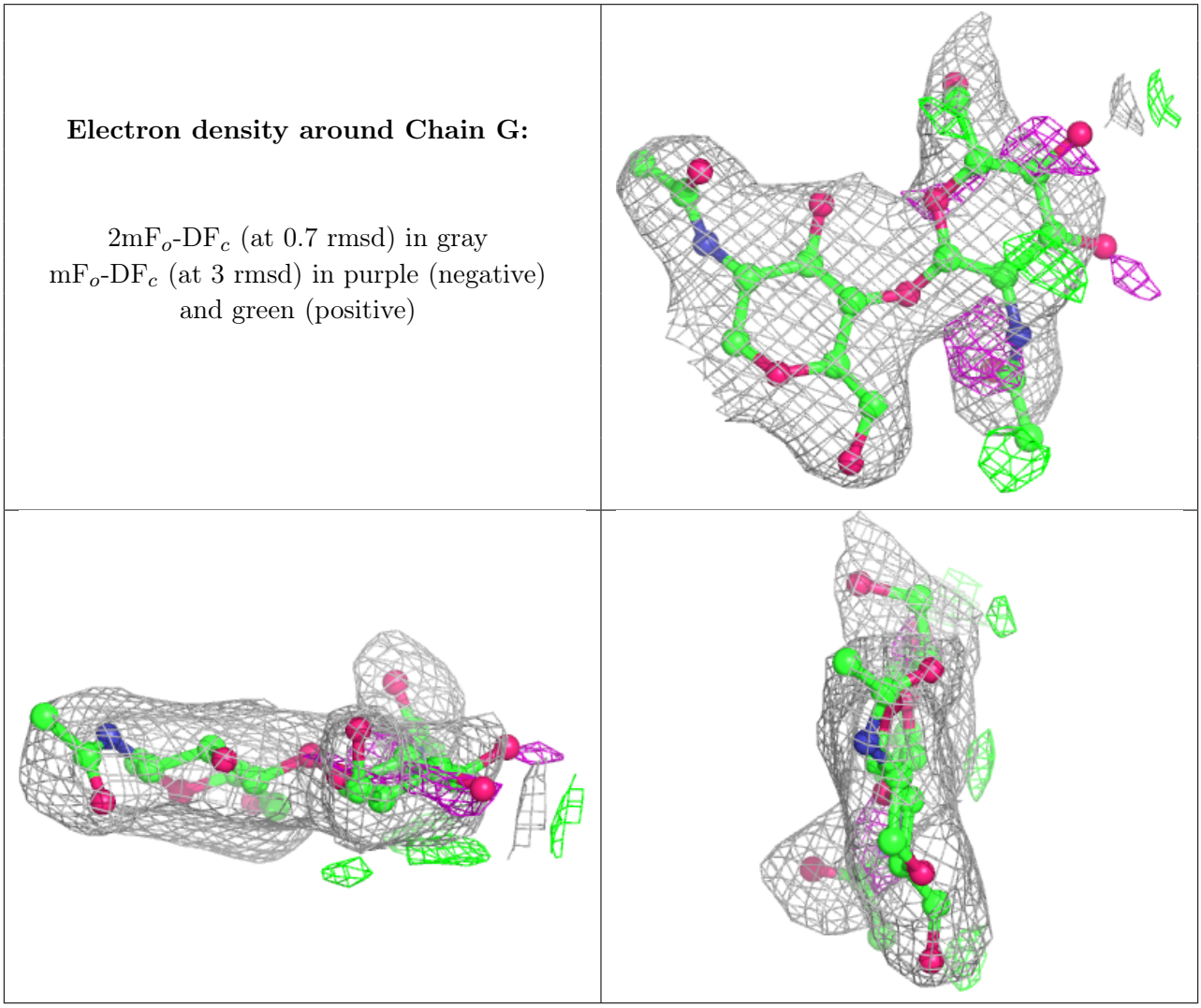
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	G	1	14/15	0.97	0.17	53,56,63,71	0

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

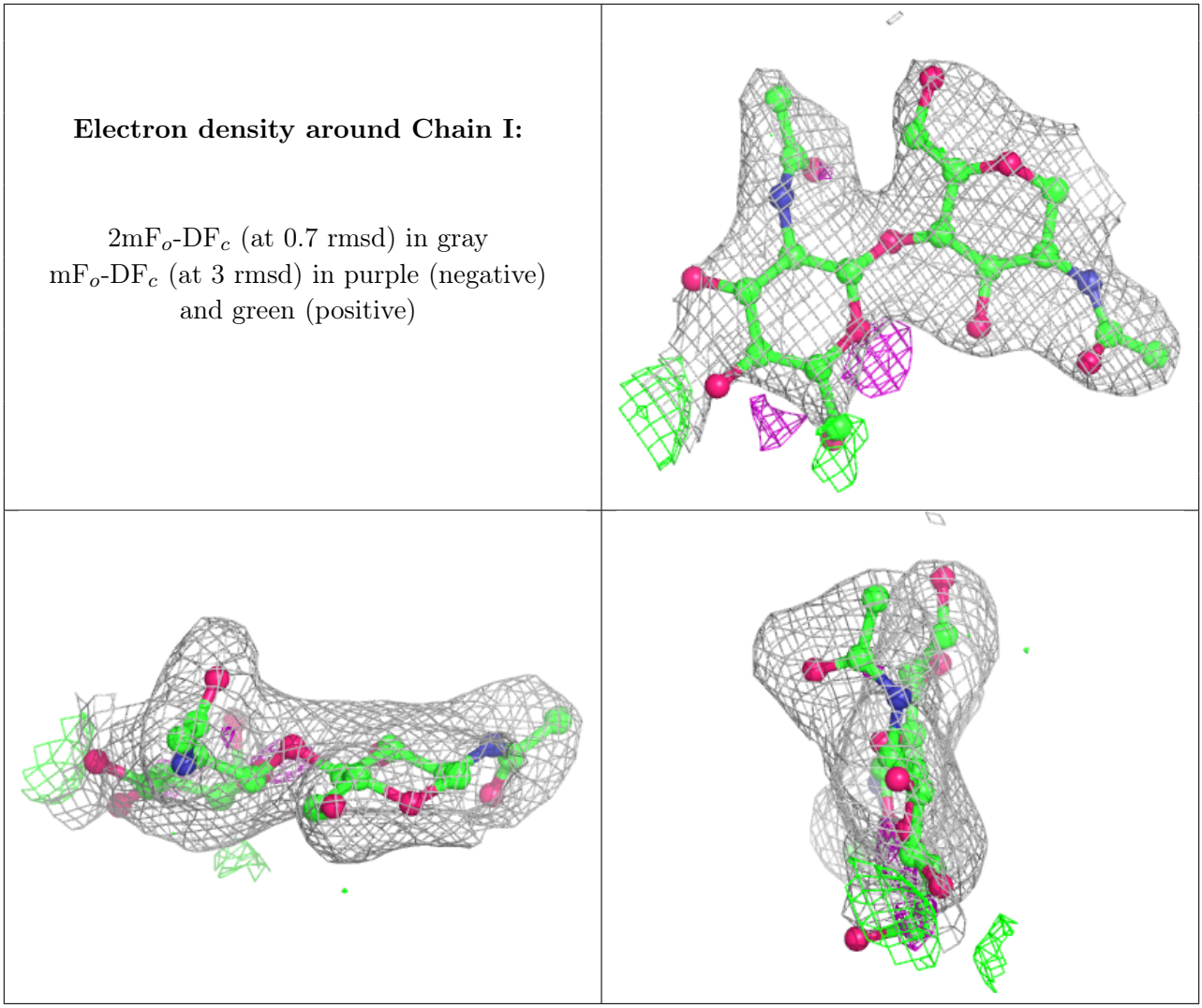
Electron density around Chain G:

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



Electron density around Chain I:

$2mF_o$-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, 95^{th} 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	CL	E	1113	1/1	0.69	0.13	88,88,88,88	0
11	NAG	E	1107	14/15	0.69	0.27	111,123,127,129	0
9	CL	F	1216	1/1	0.70	0.17	94,94,94,94	0
11	NAG	E	1106	14/15	0.71	0.40	101,110,114,114	0
9	CL	C	303	1/1	0.73	0.22	77,77,77,77	0
11	NAG	E	1105	14/15	0.73	0.46	91,104,108,109	0
8	EDO	L	302	4/4	0.75	0.18	63,69,71,72	0
8	EDO	L	303	4/4	0.76	0.23	59,64,69,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	F	1207	14/15	0.76	0.31	100,115,120,121	0
11	NAG	F	1206	14/15	0.78	0.32	91,98,102,103	0
9	CL	R	605	1/1	0.78	0.11	88,88,88,88	0
8	EDO	E	1108	4/4	0.80	0.19	79,81,81,87	0
9	CL	C	302	1/1	0.82	0.11	76,76,76,76	0
8	EDO	B	302	4/4	0.82	0.17	58,65,70,73	0
9	CL	A	304	1/1	0.83	0.10	90,90,90,90	0
8	EDO	N	302	4/4	0.85	0.27	57,63,63,64	0
8	EDO	B	305	4/4	0.85	0.31	56,62,63,66	0
11	NAG	R	601	14/15	0.85	0.28	91,99,103,104	0
11	NAG	F	1204	14/15	0.86	0.37	91,99,102,105	0
8	EDO	F	1211	4/4	0.86	0.25	69,70,85,86	0
9	CL	H	301	1/1	0.87	0.20	85,85,85,85	0
8	EDO	M	302	4/4	0.88	0.22	54,58,76,80	0
8	EDO	S	601	4/4	0.88	0.18	60,61,62,70	0
11	NAG	F	1205	14/15	0.89	0.16	93,100,103,110	0
8	EDO	E	1109	4/4	0.89	0.27	70,76,80,80	0
9	CL	A	305	1/1	0.90	0.11	65,65,65,65	0
8	EDO	E	1111	4/4	0.90	0.22	96,97,101,107	0
9	CL	L	305	1/1	0.90	0.07	82,82,82,82	0
8	EDO	A	301	4/4	0.91	0.15	62,64,66,67	0
8	EDO	C	301	4/4	0.91	0.12	53,61,62,62	0
8	EDO	D	302	4/4	0.91	0.19	58,60,62,63	0
11	NAG	E	1103	14/15	0.91	0.20	66,71,76,83	0
8	EDO	R	604	4/4	0.92	0.29	47,49,52,59	0
8	EDO	F	1210	4/4	0.92	0.37	88,90,92,101	0
8	EDO	E	1110	4/4	0.92	0.21	82,87,100,104	0
11	NAG	E	1104	14/15	0.92	0.11	77,89,94,95	0
9	CL	A	303	1/1	0.93	0.10	86,86,86,86	0
9	CL	E	1114	1/1	0.93	0.10	80,80,80,80	0
9	CL	F	1214	1/1	0.93	0.09	80,80,80,80	0
8	EDO	B	304	4/4	0.93	0.21	58,58,64,67	0
8	EDO	B	303	4/4	0.93	0.23	53,62,64,66	0
8	EDO	F	1208	4/4	0.93	0.09	69,71,73,76	0
8	EDO	F	1209	4/4	0.93	0.14	74,79,85,91	0
11	NAG	E	1102	14/15	0.93	0.15	70,81,85,86	0
9	CL	E	1112	1/1	0.93	0.08	96,96,96,96	0
9	CL	S	602	1/1	0.94	0.15	66,66,66,66	0
8	EDO	D	301	4/4	0.94	0.25	52,53,56,58	0
8	EDO	M	301	4/4	0.94	0.30	50,53,55,57	0
8	EDO	R	602	4/4	0.94	0.20	55,56,57,59	0
9	CL	F	1215	1/1	0.95	0.08	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CL	L	304	1/1	0.95	0.10	79,79,79,79	0
11	NAG	F	1203	14/15	0.95	0.13	68,70,75,78	0
8	EDO	R	603	4/4	0.95	0.28	49,49,53,53	0
11	NAG	F	1202	14/15	0.96	0.13	63,68,75,80	0
8	EDO	N	301	4/4	0.96	0.23	46,47,48,49	0
8	EDO	B	301	4/4	0.96	0.15	55,58,58,59	0
9	CL	E	1115	1/1	0.96	0.09	82,82,82,82	0
9	CL	F	1213	1/1	0.96	0.14	67,67,67,67	0
9	CL	D	303	1/1	0.96	0.14	64,64,64,64	0
8	EDO	A	302	4/4	0.96	0.23	59,60,62,65	0
8	EDO	B	306	4/4	0.97	0.17	68,70,75,92	0
10	ZN	F	1201	1/1	0.97	0.16	86,86,86,86	0
8	EDO	L	301	4/4	0.97	0.23	43,45,46,47	0
10	ZN	E	1101	1/1	0.98	0.12	88,88,88,88	0
9	CL	F	1212	1/1	0.98	0.09	78,78,78,78	0
9	CL	E	1116	1/1	0.98	0.06	88,88,88,88	0
9	CL	D	304	1/1	0.99	0.17	66,66,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.