



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:25 AM UTC

PDB ID : 7PS2 / pdb_00007ps2
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 beta variant spike glycoprotein in complex with Beta-29 and Beta-53 Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-09-22
Resolution : 2.99 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

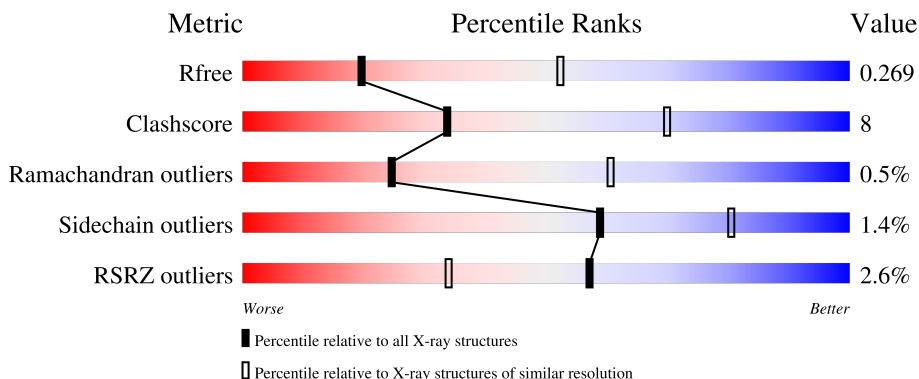
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	B	221	
2	G	210	
3	A	232	
4	H	226	
5	L	215	

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Mol	Chain	Length	Quality of chain
6	E	4	 50% 50%

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
8	SO4	G	608	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8431 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 Beta-29 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	221	1714	1074	287	348	5	0	1	0

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	197	1580	1013	268	291	8	0	1	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	319	MET	-	initiating methionine	UNP P0DTC2
G	320	GLY	-	expression tag	UNP P0DTC2
G	321	CYS	-	expression tag	UNP P0DTC2
G	322	VAL	-	expression tag	UNP P0DTC2
G	323	ALA	-	expression tag	UNP P0DTC2
G	324	GLU	-	expression tag	UNP P0DTC2
G	325	THR	-	expression tag	UNP P0DTC2
G	326	GLY	-	expression tag	UNP P0DTC2
G	327	HIS	-	expression tag	UNP P0DTC2
G	328	HIS	-	expression tag	UNP P0DTC2
G	329	HIS	-	expression tag	UNP P0DTC2
G	330	HIS	-	expression tag	UNP P0DTC2
G	331	HIS	-	expression tag	UNP P0DTC2
G	332	HIS	-	expression tag	UNP P0DTC2
G	417	ASN	LYS	variant	UNP P0DTC2
G	484	LYS	GLU	variant	UNP P0DTC2
G	501	TYR	ASN	variant	UNP P0DTC2
G	527	LYS	-	expression tag	UNP P0DTC2
G	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 is a protein called Beta-29 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	227	Total	C	N	O	S	0	0	0
			1700	1063	294	334	9			

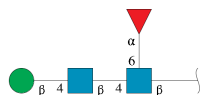
- Molecule 4 is a protein called Beta-53 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	219	Total	C	N	O	S	0	0	0
			1650	1046	276	321	7			

- Molecule 5 is a protein called Beta-53 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	214	Total	C	N	O	S	0	1	0
			1649	1030	280	334	5			

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



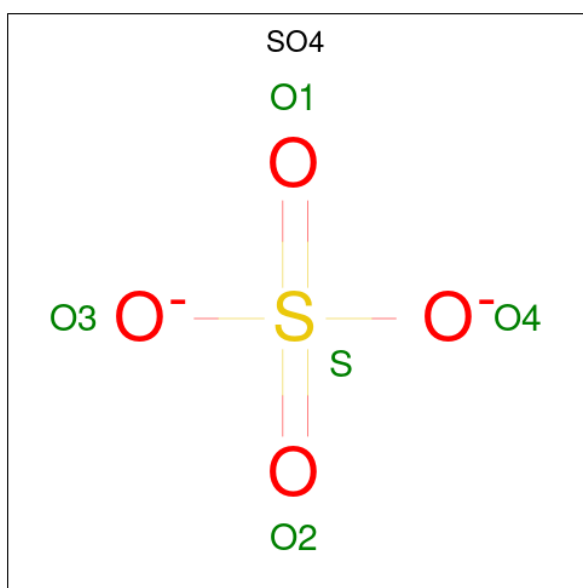
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 6 3 3	0	0
7	G	1	Total C O 6 3 3	0	0

- Molecule 8 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



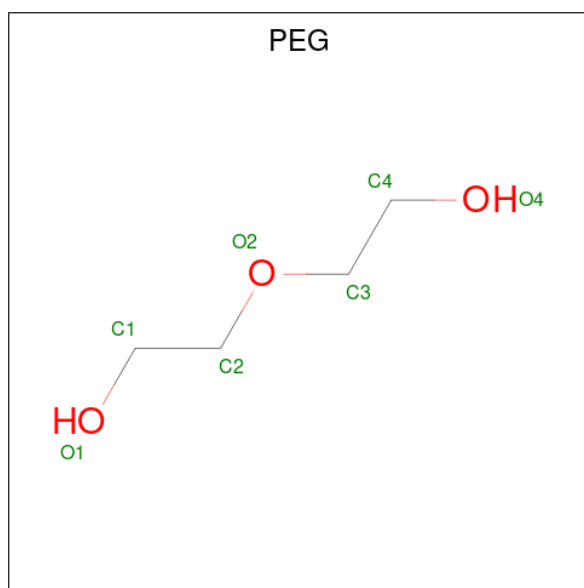
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

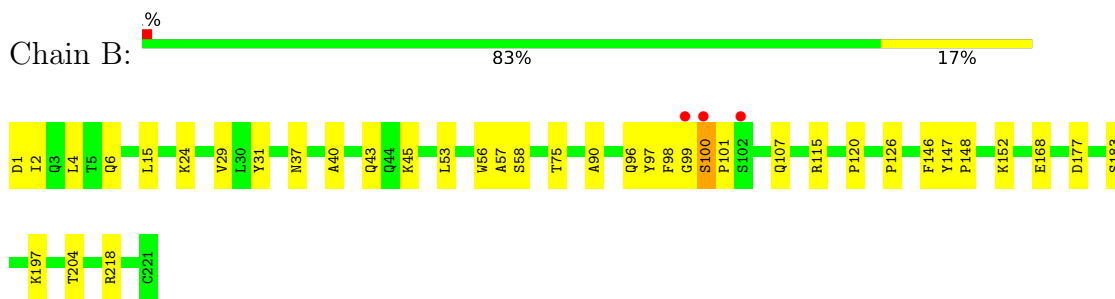


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			7	4	3		

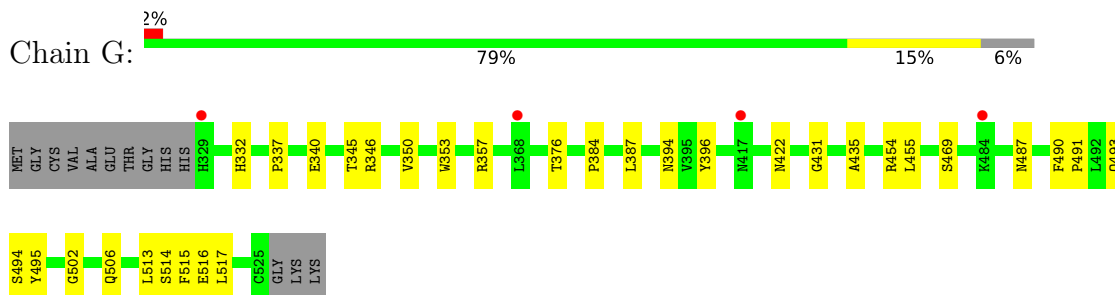
3 Residue-property plots [i](#)

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.

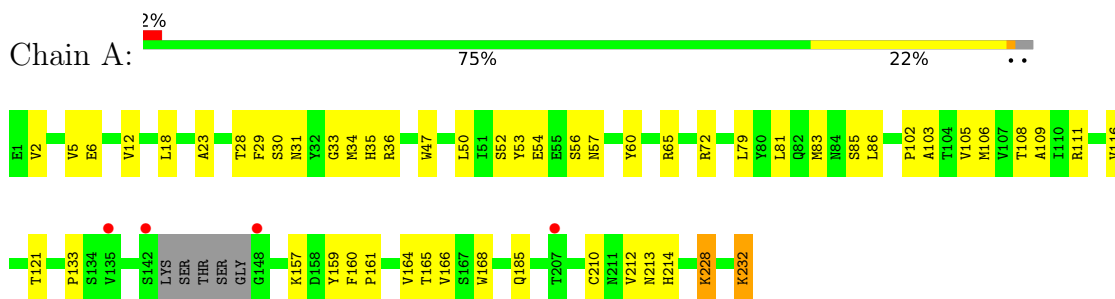
- Molecule 1: Beta-29 Fab light chain



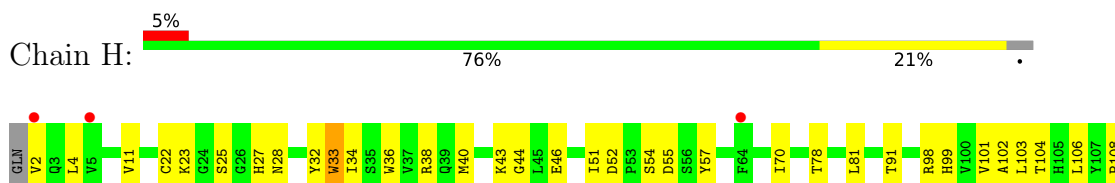
- Molecule 2: Spike protein S1

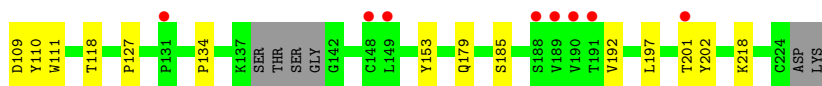


- Molecule 3: Beta-29 Fab heavy chain

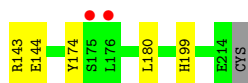
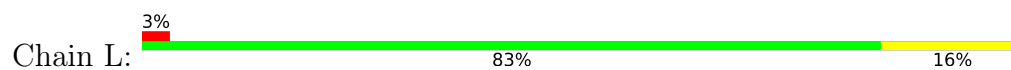


- Molecule 4: Beta-53 heavy chain





- Molecule 5: Beta-53 Fab light chain



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	213.40Å 213.40Å 226.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.33 – 2.99 48.33 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.33-2.99) 99.8 (48.33-2.99)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.233 , 0.266 0.235 , 0.269	Depositor DCC
R_{free} test set	2017 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	103.1	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 116.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8431	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: BMA, NAG, FUC, PEG, GOL, SO4

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	B	0.13	0/1754	0.32	0/2383
2	G	0.14	0/1631	0.30	0/2221
3	A	0.14	0/1736	0.32	0/2360
4	H	0.13	0/1696	0.35	0/2317
5	L	0.11	0/1688	0.29	0/2295
All	All	0.13	0/8505	0.32	0/11576

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	L	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	92	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1714	0	1662	24	0
2	G	1580	0	1486	26	0
3	A	1700	0	1673	40	0
4	H	1650	0	1605	32	0
5	L	1649	0	1598	18	0
6	E	49	0	43	1	0
7	B	6	0	8	0	0
7	G	6	0	8	0	0
8	A	20	0	0	1	0
8	B	5	0	0	0	0
8	G	30	0	0	2	0
8	H	10	0	0	0	0
8	L	5	0	0	0	0
9	G	7	0	10	0	0
All	All	8431	0	8093	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 8.

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)
3:A:36:ARG:HG2	3:A:81:LEU:HD22	1.63	0.80
3:A:52:SER:HB3	3:A:57:ASN:HB2	1.65	0.77
5:L:106:ASP:OD2	5:L:174:TYR:OH	2.02	0.77
5:L:12:SER:HB3	5:L:108:LYS:HA	1.73	0.70
1:B:100:SER:HB2	1:B:101:PRO:HD3	1.75	0.69
5:L:13:VAL:HG13	5:L:17:GLU:HB2	1.75	0.68
2:G:455:LEU:HD21	3:A:102:PRO:HG3	1.74	0.68
1:B:197:LYS:HA	1:B:218:ARG:HB3	1.76	0.68
1:B:2:ILE:H	1:B:101:PRO:HG3	1.60	0.66
3:A:52:SER:O	3:A:72:ARG:NH1	2.28	0.66
2:G:357:ARG:NH1	8:G:608:SO4:O1	2.28	0.66
4:H:51:ILE:HD11	4:H:70:ILE:HG13	1.80	0.64
2:G:376:THR:HB	2:G:435:ALA:HB3	1.79	0.64
5:L:143:ARG:O	5:L:143:ARG:NH1	2.30	0.62
2:G:337:PRO:HB2	2:G:340:GLU:HG3	1.81	0.61
3:A:50:LEU:HD11	3:A:103:ALA:HB1	1.81	0.61
1:B:29:VAL:HG13	1:B:98:PHE:HB2	1.83	0.61
1:B:43:GLN:HB2	1:B:53:LEU:HD11	1.83	0.61
3:A:108:THR:HA	3:A:111:ARG:HG2	1.84	0.60
2:G:345:THR:HA	4:H:101:VAL:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:29:PHE:C	3:A:31:ASN:H	2.10	0.59
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.83	0.59
2:G:396:TYR:HB2	2:G:514:SER:HB2	1.85	0.58
5:L:133:VAL:HB	5:L:180:LEU:HB3	1.84	0.58
3:A:2:VAL:HG11	3:A:116:VAL:HG21	1.86	0.57
3:A:6:GLU:HB2	3:A:121:THR:HG23	1.85	0.57
4:H:25:SER:O	4:H:98:ARG:NH2	2.38	0.57
5:L:54:ARG:HH21	5:L:63:SER:HB3	1.67	0.57
2:G:494:SER:O	3:A:31:ASN:ND2	2.38	0.57
4:H:108:PRO:HG2	5:L:46:LEU:HD22	1.85	0.57
3:A:133:PRO:HB3	3:A:159:TYR:HB3	1.87	0.56
5:L:29:VAL:HG11	5:L:90:GLN:HB2	1.88	0.56
4:H:99:HIS:CE1	4:H:108:PRO:HB3	2.41	0.56
4:H:98:ARG:NH1	4:H:109:ASP:OD2	2.38	0.55
2:G:495:TYR:O	3:A:28:THR:OG1	2.18	0.55
3:A:105:VAL:HA	3:A:111:ARG:HH11	1.73	0.54
4:H:43:LYS:HG2	4:H:44:GLY:H	1.73	0.53
1:B:100:SER:HB2	1:B:101:PRO:CD	2.38	0.53
2:G:346:ARG:NH2	4:H:57:TYR:HB3	2.23	0.53
4:H:22:CYS:SG	4:H:34:ILE:HD11	2.48	0.53
1:B:4:LEU:HD11	1:B:96:GLN:H	1.74	0.53
5:L:33:LEU:HD11	5:L:88:CYS:HB2	1.90	0.52
3:A:12:VAL:HG11	3:A:18:LEU:HB2	1.91	0.52
3:A:35:HIS:CE1	3:A:50:LEU:HD13	2.45	0.52
4:H:98:ARG:HB3	4:H:109:ASP:OD1	2.10	0.52
3:A:33:GLY:HA3	3:A:103:ALA:HB3	1.92	0.51
3:A:54:GLU:OE1	3:A:54:GLU:N	2.37	0.51
5:L:61:ARG:HB2	5:L:76:SER:O	2.11	0.51
3:A:12:VAL:HG21	3:A:86:LEU:HD13	1.92	0.50
3:A:47:TRP:HZ2	3:A:50:LEU:HB2	1.77	0.50
2:G:357:ARG:NH1	8:G:608:SO4:O3	2.45	0.50
5:L:2:ILE:HG23	5:L:27:GLN:HG2	1.92	0.50
2:G:431:GLY:HA2	2:G:515:PHE:CD2	2.46	0.50
3:A:166:VAL:HG22	3:A:212:VAL:HG22	1.94	0.49
2:G:455:LEU:HD22	2:G:493:GLN:OE1	2.12	0.49
4:H:2:VAL:HG12	4:H:110:TYR:HB2	1.95	0.49
2:G:346:ARG:HH22	4:H:55:ASP:HB3	1.77	0.48
4:H:33:TRP:CE3	4:H:33:TRP:HA	2.47	0.48
4:H:40:MET:HB2	4:H:43:LYS:HB2	1.95	0.48
2:G:490:PHE:CD1	2:G:491:PRO:HD2	2.47	0.48
2:G:346:ARG:HH21	4:H:52:ASP:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:52:SER:HG	3:A:56:SER:H	1.62	0.47
4:H:102:ALA:O	4:H:104:THR:N	2.47	0.47
5:L:10:THR:OG1	5:L:144:GLU:OE2	2.28	0.47
1:B:1:ASP:HA	1:B:101:PRO:HG3	1.96	0.47
4:H:28:ASN:ND2	6:E:1:NAG:O5	2.39	0.47
3:A:157:LYS:NZ	3:A:185:GLN:OE1	2.46	0.47
4:H:127:PRO:HB3	4:H:153:TYR:HB3	1.97	0.47
1:B:40:ALA:HB2	1:B:97:TYR:HE2	1.79	0.47
3:A:83:MET:HE2	3:A:86:LEU:HD21	1.96	0.46
1:B:152:LYS:HB3	1:B:204:THR:OG1	2.16	0.46
1:B:45:LYS:HG2	1:B:90:ALA:HB2	1.97	0.46
2:G:353:TRP:H	2:G:353:TRP:CD1	2.33	0.46
2:G:394:ASN:HB3	2:G:516:GLU:HB2	1.97	0.46
3:A:232:LYS:HD2	3:A:232:LYS:HA	1.42	0.46
1:B:120:PRO:HB3	1:B:146:PHE:HB3	1.98	0.46
4:H:23:LYS:HG2	4:H:78:THR:HG23	1.97	0.45
1:B:31:TYR:HE2	3:A:109:ALA:HB2	1.80	0.45
2:G:350:VAL:HG22	2:G:422:ASN:HB3	1.99	0.45
3:A:29:PHE:O	3:A:31:ASN:N	2.49	0.45
4:H:4:LEU:HA	4:H:23:LYS:O	2.16	0.45
3:A:34:MET:HB3	3:A:79:LEU:HD22	1.98	0.45
3:A:85:SER:O	3:A:85:SER:OG	2.33	0.45
5:L:10:THR:HG22	5:L:104:LYS:HB3	1.98	0.45
1:B:115:ARG:NH1	1:B:177:ASP:O	2.50	0.45
4:H:201:THR:HB	4:H:218:LYS:HE3	1.99	0.44
1:B:2:ILE:N	1:B:101:PRO:HG3	2.28	0.44
4:H:38:ARG:CZ	4:H:40:MET:HE3	2.47	0.44
2:G:431:GLY:HA2	2:G:515:PHE:HD2	1.82	0.44
2:G:384:PRO:HA	2:G:387:LEU:HG	2.00	0.44
5:L:19:ALA:HB3	5:L:75:ILE:HB	1.99	0.44
1:B:147:TYR:CG	1:B:148:PRO:HA	2.52	0.44
3:A:165:THR:OG1	3:A:213:ASN:HB3	2.18	0.44
3:A:105:VAL:HA	3:A:111:ARG:NH1	2.33	0.43
1:B:37:ASN:HB2	1:B:57:ALA:HB2	2.00	0.43
2:G:487:ASN:HD21	3:A:106:MET:HG3	1.83	0.43
4:H:91:THR:HG23	4:H:118:THR:HA	1.99	0.43
4:H:179:GLN:NE2	4:H:185:SER:OG	2.51	0.43
4:H:4:LEU:HG	4:H:110:TYR:HD2	1.83	0.43
2:G:346:ARG:NH1	4:H:55:ASP:OD2	2.45	0.43
2:G:502:GLY:O	2:G:506:GLN:HG3	2.19	0.42
4:H:4:LEU:HG	4:H:110:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:141:TYR:O	5:L:199:HIS:HE1	2.01	0.42
4:H:33:TRP:HA	4:H:33:TRP:HE3	1.82	0.42
4:H:52:ASP:OD1	4:H:54:SER:OG	2.31	0.42
4:H:192:VAL:HG11	4:H:202:TYR:CE1	2.55	0.42
1:B:24:LYS:HA	1:B:75:THR:O	2.19	0.42
3:A:60:TYR:OH	8:A:301:SO4:O2	2.30	0.42
1:B:126:PRO:HG2	3:A:228:LYS:NZ	2.35	0.42
1:B:99:GLY:HA2	3:A:111:ARG:NH1	2.35	0.41
3:A:53:TYR:CD1	3:A:102:PRO:HB2	2.55	0.41
4:H:36:TRP:CE2	4:H:81:LEU:HB2	2.54	0.41
2:G:387:LEU:HD23	2:G:387:LEU:HA	1.89	0.41
2:G:454:ARG:NH2	2:G:469:SER:O	2.43	0.41
3:A:29:PHE:C	3:A:31:ASN:N	2.75	0.41
3:A:160:PHE:HA	3:A:161:PRO:HA	1.88	0.41
3:A:164:VAL:HG12	3:A:214:HIS:HB2	2.02	0.41
5:L:35:TRP:CE2	5:L:73:LEU:HB2	2.56	0.41
1:B:56:TRP:C	1:B:58:SER:H	2.29	0.41
4:H:134:PRO:HG3	4:H:197:LEU:HD22	2.02	0.41
1:B:4:LEU:HD11	1:B:96:GLN:N	2.36	0.41
3:A:168:TRP:CH2	3:A:210:CYS:HB3	2.56	0.40
1:B:168:GLU:HA	1:B:183:SER:O	2.21	0.40
2:G:396:TYR:O	2:G:513:LEU:HA	2.21	0.40
1:B:6:GLN:O	1:B:107:GLN:NE2	2.54	0.40
3:A:5:VAL:HG23	3:A:23:ALA:HB3	2.04	0.40
5:L:33:LEU:HG	5:L:34:ALA:N	2.37	0.40

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	B	220/221 (100%)	209 (95%)	10 (4%)	1 (0%)	24 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	196/210 (93%)	183 (93%)	13 (7%)	0	100	100
3	A	223/232 (96%)	204 (92%)	17 (8%)	2 (1%)	14	48
4	H	215/226 (95%)	192 (89%)	22 (10%)	1 (0%)	24	60
5	L	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	24	60
All	All	1067/1104 (97%)	987 (92%)	75 (7%)	5 (0%)	24	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	30	SER
4	H	103	LEU
1	B	100	SER
3	A	228	LYS
5	L	30	SER

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	B	196/195 (100%)	195 (100%)	1 (0%)	81	89
2	G	172/180 (96%)	170 (99%)	2 (1%)	63	82
3	A	191/195 (98%)	189 (99%)	2 (1%)	68	84
4	H	188/195 (96%)	181 (96%)	7 (4%)	30	64
5	L	186/186 (100%)	185 (100%)	1 (0%)	81	89
All	All	933/951 (98%)	920 (99%)	13 (1%)	59	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	LEU
2	G	332	HIS
2	G	517	LEU

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Mol	Chain	Res	Type
3	A	65	ARG
3	A	232	LYS
4	H	11	VAL
4	H	27	HIS
4	H	32	TYR
4	H	33	TRP
4	H	46	GLU
4	H	106	LEU
4	H	111	TRP
5	L	99	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	144	ASN
1	B	145	ASN
1	B	167	GLN
2	G	450	ASN
2	G	487	ASN
3	A	178	HIS
5	L	138	ASN
5	L	200	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$
6	NAG	E	1	6,2	14,14,15	0.39	0	17,19,21	0.42	0
6	NAG	E	2	6	14,14,15	0.44	0	17,19,21	0.40	0
6	BMA	E	3	6	11,11,12	0.80	0	15,15,17	0.83	0
6	FUC	E	4	6	10,10,11	0.73	0	14,14,16	0.98	1 (7%)

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	E	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	BMA	E	3	6	-	0/2/19/22	0/1/1/1
6	FUC	E	4	6	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	4	FUC	C1-O5-C5	2.03	117.76	112.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

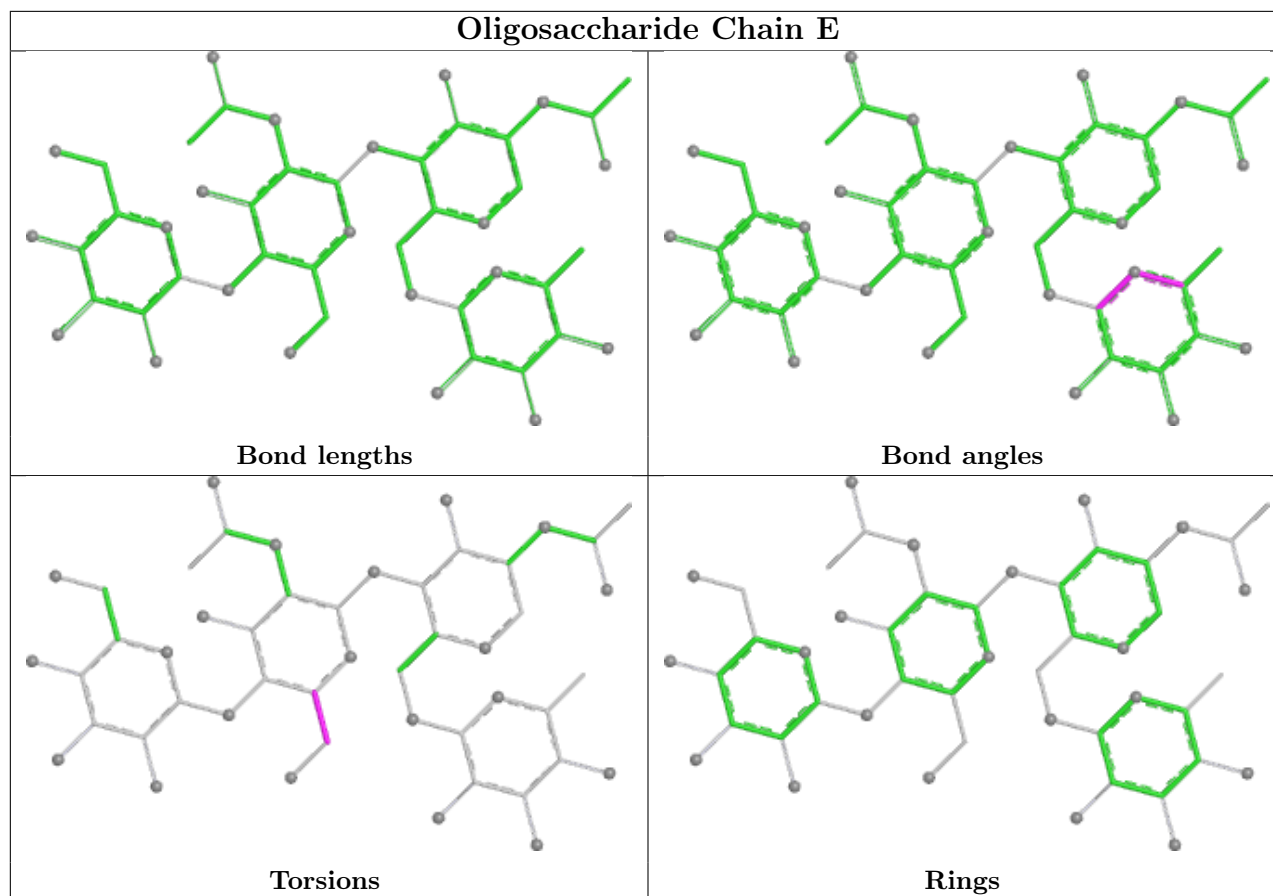
Mol	Chain	Res	Type	Atoms
6	E	2	NAG	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	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.



5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SO4	G	603	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	G	606	-	4,4,4	0.51	0	6,6,6	0.40	0
8	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.11	0
7	GOL	B	301	-	5,5,5	0.71	0	5,5,5	1.19	1 (20%)
9	PEG	G	602	-	6,6,6	0.23	0	5,5,5	0.04	0
8	SO4	A	304	-	4,4,4	0.54	0	6,6,6	0.52	0
8	SO4	H	301	-	4,4,4	0.26	0	6,6,6	0.11	0
8	SO4	G	608	-	4,4,4	0.52	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	A	301	-	4,4,4	0.22	0	6,6,6	0.12	0
8	SO4	B	302	-	4,4,4	0.48	0	6,6,6	0.38	0
8	SO4	G	604	-	4,4,4	0.23	0	6,6,6	0.14	0
8	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.15	0
7	GOL	G	601	-	5,5,5	0.70	0	5,5,5	1.27	1 (20%)
8	SO4	H	302	-	4,4,4	0.25	0	6,6,6	0.11	0
8	SO4	G	607	-	4,4,4	0.41	0	6,6,6	0.41	0
8	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.15	0
8	SO4	G	605	-	4,4,4	0.24	0	6,6,6	0.13	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	301	-	-	4/4/4/4	-
7	GOL	G	601	-	-	0/4/4/4	-
9	PEG	G	602	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	301	GOL	C3-C2-C1	-2.16	103.87	111.80
7	G	601	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	301	GOL	C1-C2-C3-O3
9	G	602	PEG	O2-C3-C4-O4
7	B	301	GOL	O1-C1-C2-C3
7	B	301	GOL	O2-C2-C3-O3
7	B	301	GOL	O1-C1-C2-O2
9	G	602	PEG	O1-C1-C2-O2
9	G	602	PEG	C4-C3-O2-C2
9	G	602	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	608	SO4	2	0
8	A	301	SO4	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	B	221/221 (100%)	-0.04	3 (1%) 73 51	81, 134, 198, 248	1 (0%)
2	G	197/210 (93%)	0.02	4 (2%) 65 41	62, 90, 129, 179	1 (0%)
3	A	227/232 (97%)	0.11	4 (1%) 67 44	83, 133, 195, 235	0
4	H	219/226 (96%)	0.45	11 (5%) 34 18	88, 144, 302, 366	0
5	L	214/215 (99%)	0.34	6 (2%) 55 32	99, 207, 286, 347	1 (0%)
All	All	1078/1104 (97%)	0.18	28 (2%) 57 34	62, 132, 270, 366	3 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	188	SER	4.2
3	A	135	VAL	4.2
5	L	137	LEU	4.2
5	L	136	LEU	4.1
4	H	189	VAL	4.1
4	H	149	LEU	4.0
3	A	142	SER	3.0
5	L	115	SER	3.0
5	L	176	LEU	3.0
4	H	191	THR	3.0
4	H	190	VAL	2.9
4	H	201	THR	2.7
1	B	100	SER	2.7
4	H	5	VAL	2.5
4	H	148	CYS	2.5
1	B	102	SER	2.4
5	L	175	SER	2.4
4	H	2	VAL	2.4
4	H	131	PRO	2.3
4	H	64	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	484	LYS	2.2
3	A	207	THR	2.1
1	B	99	GLY	2.1
2	G	368	LEU	2.1
3	A	148	GLY	2.1
2	G	329	HIS	2.1
5	L	89	GLN	2.0
2	G	417[A]	ASN	2.0

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

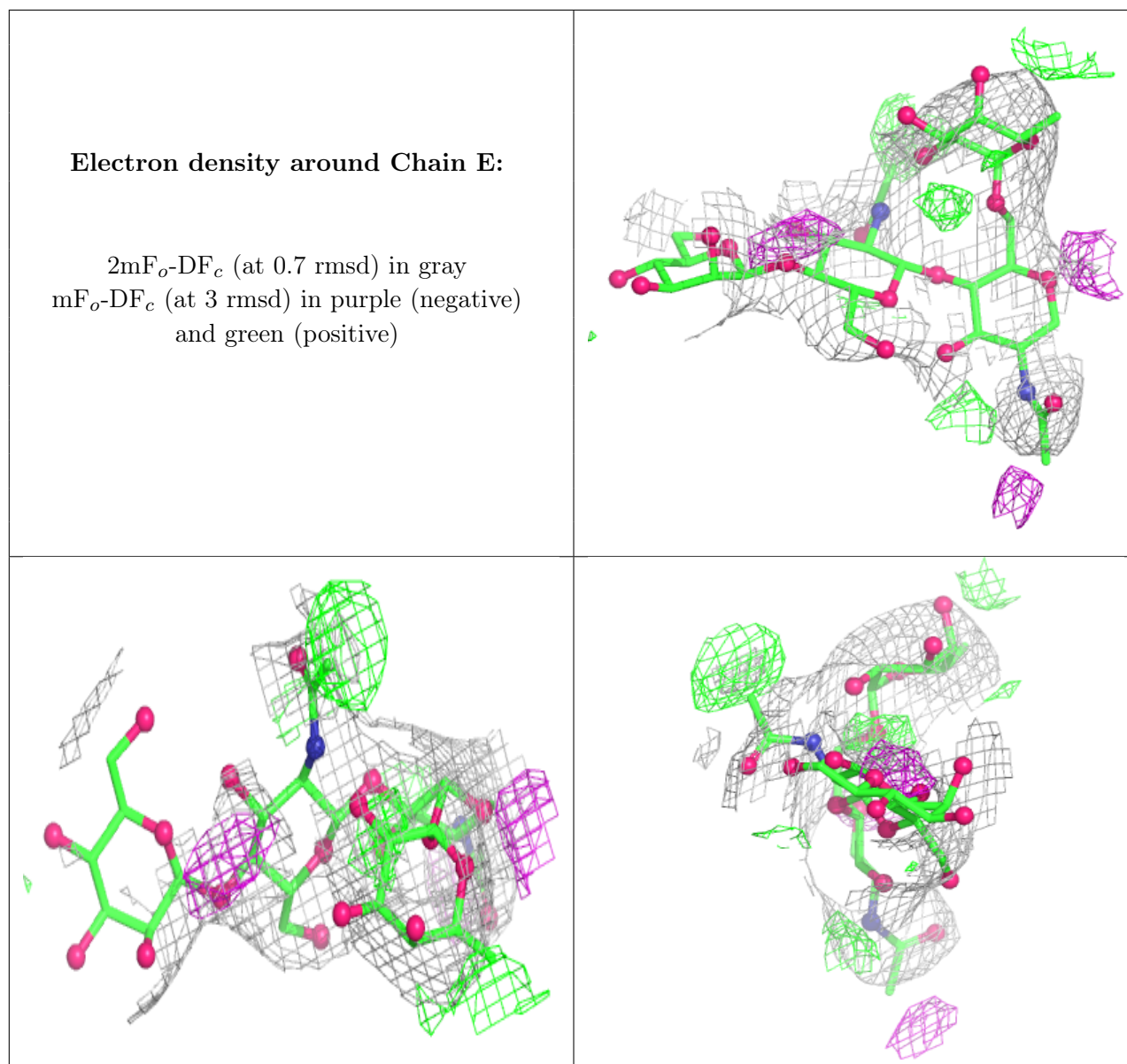
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	E	1	14/15	-	-	84,125,139,157	0
6	NAG	E	2	14/15	-	-	149,172,183,186	0
6	BMA	E	3	11/12	-	-	129,156,170,170	0
6	FUC	E	4	10/11	-	-	123,157,176,189	0

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	SO4	A	303	5/5	0.48	0.10	145,158,184,233	0
8	SO4	A	304	5/5	0.62	0.09	158,164,174,259	0
8	SO4	A	301	5/5	0.63	0.16	108,139,161,484	0
8	SO4	G	608	5/5	0.66	0.09	144,151,205,283	0
8	SO4	G	607	5/5	0.67	0.09	119,137,164,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SO4	G	604	5/5	0.72	0.10	123,133,175,221	0
8	SO4	A	302	5/5	0.72	0.08	151,168,184,231	0
8	SO4	H	302	5/5	0.72	0.09	152,163,206,272	0
8	SO4	B	302	5/5	0.78	0.07	141,152,173,241	0
8	SO4	G	605	5/5	0.79	0.08	101,133,153,197	0
8	SO4	G	603	5/5	0.81	0.08	120,121,172,211	0
8	SO4	L	301	5/5	0.81	0.08	124,147,157,171	0
7	GOL	B	301	6/6	0.82	0.14	102,106,109,125	0
8	SO4	G	606	5/5	0.85	0.12	110,119,178,225	0
8	SO4	H	301	5/5	0.85	0.13	100,118,137,141	0
7	GOL	G	601	6/6	0.86	0.13	89,106,119,124	0
9	PEG	G	602	7/7	0.86	0.14	93,94,112,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.