Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2021 – 12:15 pm GMT

PDB ID	:	7Q0G
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 beta variant spike glycoprotein in complex with Beta-49 and FI-3A Fabs
Authors	:	Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2021-10-14
Resolution	:	1.82 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 following versions of software and data (see references ⓘ) were used in the production of this report:

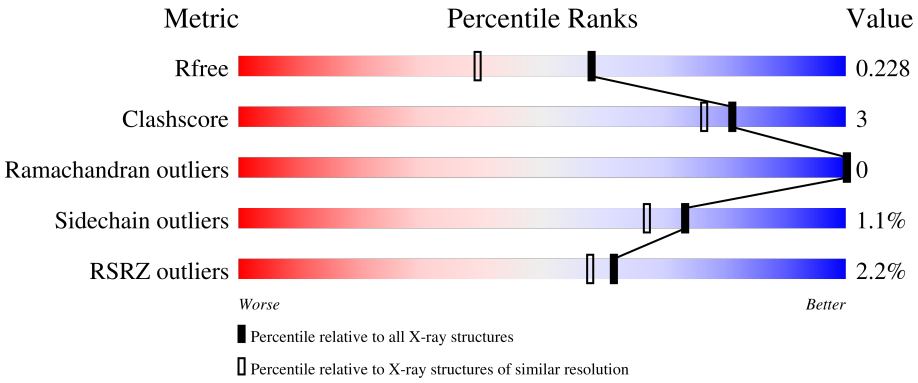
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	E	210	6% 87% 6% 7%
2	H	222	% 90% 9% .
3	L	214	94% 6%
4	B	216	2% 94% 6%
5	A	223	% 91% 7% .

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Mol	Chain	Length	Quality of chain
6	C	5	40% 60%

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
6	MAN	C	4	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 8581 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	196	Total	C	N	O	S	0	0	0
			1549	994	258	289	8			

There are 19 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called FI-3A Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1620	1017	276	319	8			

- Molecule 3 is a protein called FI-3A Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1640	1024	274	337	5			

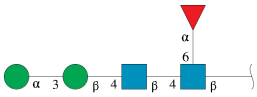
- Molecule 4 is a protein called Beta-49 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	216	Total	C	N	O	S	0	0	0
			1656	1033	283	334	6			

- Molecule 5 is a protein called Beta-49 Fab heavy chain.

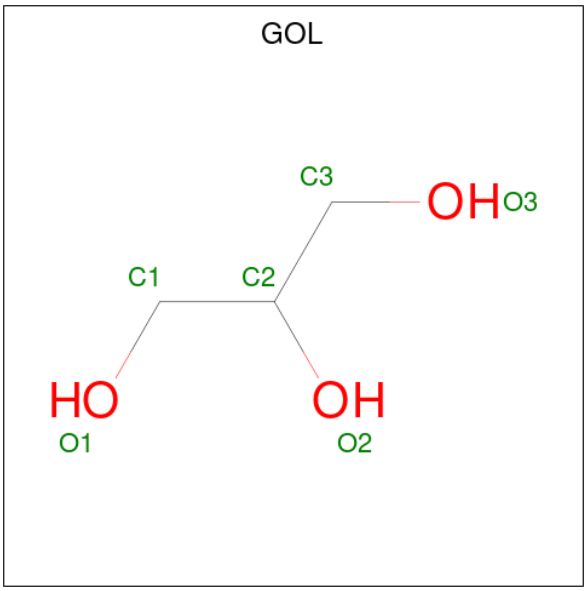
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	219	Total	C	N	O	S	0	0	0
			1603	1015	264	317	7			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
6	C	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

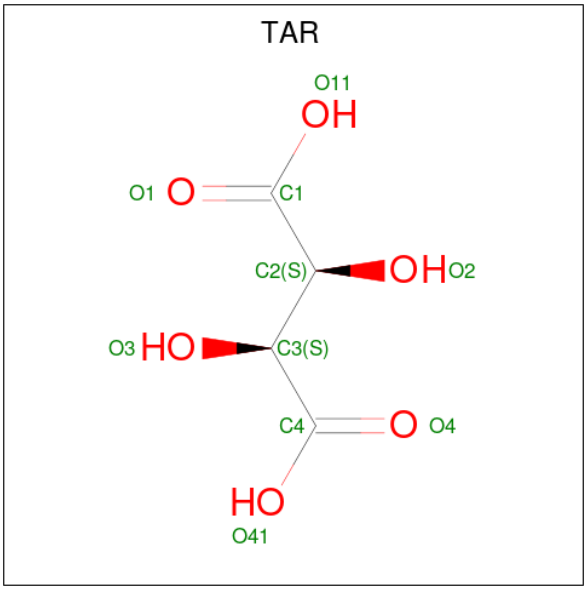
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	4	Total Cl 4 4	0	0
8	H	1	Total Cl 1 1	0	0
8	L	2	Total Cl 2 2	0	0
8	B	3	Total Cl 3 3	0	0
8	A	4	Total Cl 4 4	0	0

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total K 1 1	0	0
9	H	5	Total K 5 5	0	0
9	L	5	Total K 5 5	0	0
9	B	2	Total K 2 2	0	0
9	A	1	Total K 1 1	0	0

- Molecule 10 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total C O 10 4 6	0	0
10	A	1	Total C O 10 4 6	0	0
10	A	1	Total C O 10 4 6	0	0

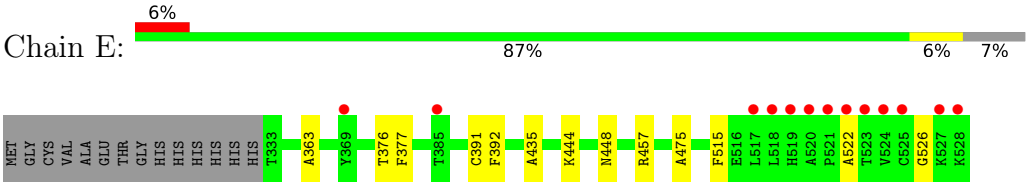
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	47	Total O 47 47	0	0
11	H	90	Total O 90 90	0	0
11	L	67	Total O 67 67	0	0
11	B	43	Total O 43 43	0	0
11	A	70	Total O 70 70	0	0

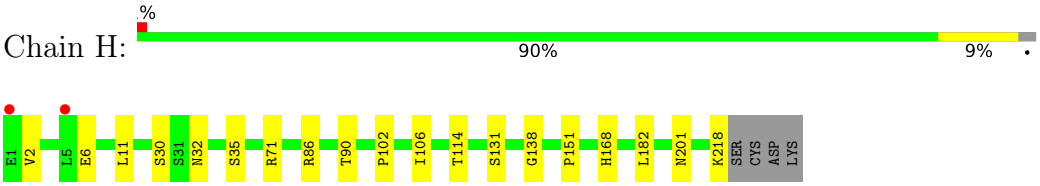
3 Residue-property plots (i)

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.

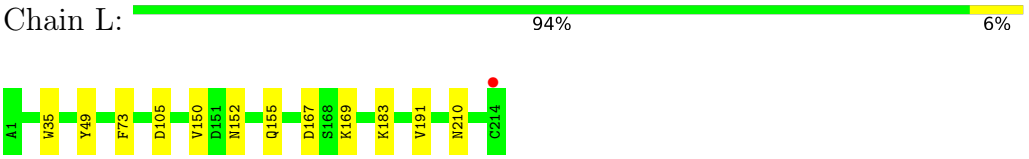
- Molecule 1: Spike protein S1



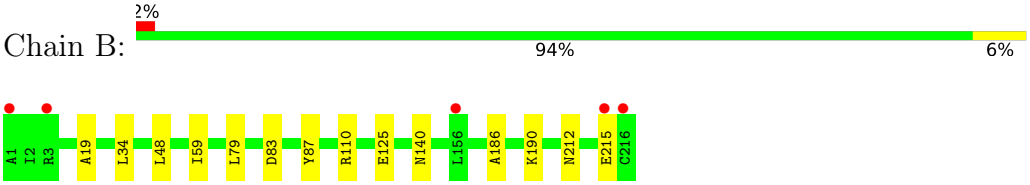
- Molecule 2: FI-3A Fab heavy chain



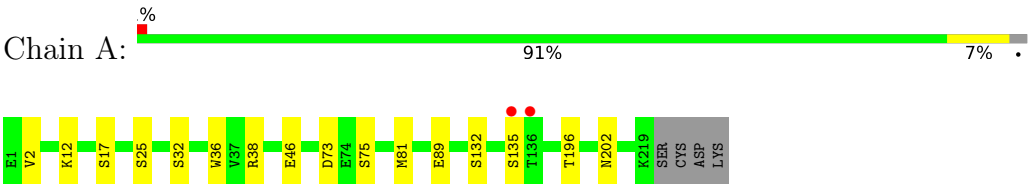
- Molecule 3: FI-3A Fab light chain



- Molecule 4: Beta-49 Fab light chain

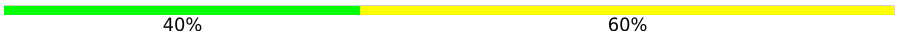


- Molecule 5: Beta-49 Fab heavy chain



• Molecule 6: alpha-D-mannopyranose-(1-3)-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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.29Å 106.54Å 215.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.81 – 1.82 107.81 – 1.82	Depositor EDS
% Data completeness (in resolution range)	51.2 (107.81-1.82) 51.2 (107.81-1.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.192 , 0.224 0.199 , 0.228	Depositor DCC
R_{free} test set	4708 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	8581	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: MAN, NAG, FUC, K, GOL, BMA, CL, TAR

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	E	0.43	0/1593	0.60	0/2169
2	H	0.45	0/1657	0.65	0/2255
3	L	0.46	0/1674	0.65	0/2275
4	B	0.41	0/1693	0.65	0/2298
5	A	0.44	0/1640	0.63	0/2237
All	All	0.44	0/8257	0.64	0/11234

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	E	1549	0	1459	8	0
2	H	1620	0	1598	13	0
3	L	1640	0	1584	6	0
4	B	1656	0	1604	8	0
5	A	1603	0	1583	8	0
6	C	60	0	52	0	0
7	A	6	0	8	0	0
7	B	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	24	0	32	1	0
7	H	24	0	32	4	0
7	L	6	0	7	1	0
8	A	4	0	0	0	0
8	B	3	0	0	0	0
8	E	4	0	0	0	0
8	H	1	0	0	0	0
8	L	2	0	0	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	E	1	0	0	0	0
9	H	5	0	0	0	0
9	L	5	0	0	0	0
10	A	20	0	8	2	0
10	H	10	0	4	0	0
11	A	70	0	0	2	0
11	B	43	0	0	0	0
11	E	47	0	0	0	0
11	H	90	0	0	0	0
11	L	67	0	0	1	0
All	All	8581	0	7995	43	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 3.

All (43) 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)
2:H:86:ARG:HH22	7:H:402:GOL:H2	1.49	0.78
4:B:110:ARG:NH2	7:B:401:GOL:O1	2.24	0.70
5:A:89:GLU:OE2	11:A:401:HOH:O	2.10	0.69
1:E:391:CYS:HB3	1:E:522:ALA:HB1	1.78	0.66
4:B:19:ALA:HB2	4:B:79:LEU:HD21	1.80	0.63
5:A:38:ARG:NH1	5:A:46:GLU:OE1	2.33	0.61
4:B:140:ASN:HD22	7:B:401:GOL:H31	1.65	0.60
10:A:302:TAR:O4	10:A:302:TAR:O2	2.19	0.59
4:B:212:ASN:HB2	4:B:215:GLU:HG3	1.88	0.55
2:H:168:HIS:CE1	7:L:301:GOL:H11	2.42	0.54
1:E:444:LYS:HG3	1:E:448:ASN:HB2	1.90	0.54
2:H:138:GLY:O	7:H:403:GOL:O2	2.24	0.54
1:E:457:ARG:HH22	7:E:703:GOL:H2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:212:ASN:HB2	4:B:215:GLU:CG	2.39	0.53
3:L:191:VAL:HG22	3:L:210:ASN:OD1	2.09	0.53
2:H:30:SER:HA	2:H:71:ARG:HD2	1.92	0.51
5:A:38:ARG:NE	11:A:407:HOH:O	2.45	0.49
3:L:150:VAL:CG2	3:L:155:GLN:HG3	2.42	0.49
2:H:11:LEU:HB2	2:H:151:PRO:HG3	1.95	0.49
2:H:2:VAL:HG12	2:H:106:ILE:HD13	1.95	0.48
2:H:35:SER:OG	7:H:401:GOL:O1	2.31	0.48
1:E:376:THR:HB	1:E:435:ALA:HB3	1.94	0.48
2:H:86:ARG:NH2	7:H:402:GOL:H2	2.25	0.48
5:A:132:SER:CB	5:A:135:SER:HB3	2.44	0.48
5:A:12:LYS:HE2	5:A:17:SER:O	2.15	0.47
2:H:90:THR:HG23	2:H:114:THR:HA	1.97	0.46
2:H:102:PRO:HG3	3:L:49:TYR:CZ	2.51	0.46
5:A:2:VAL:HA	5:A:25:SER:O	2.16	0.46
2:H:131:SER:OG	2:H:218:LYS:HE3	2.16	0.45
5:A:73:ASP:OD1	5:A:75:SER:OG	2.34	0.45
1:E:392:PHE:CD1	1:E:515:PHE:HB3	2.52	0.45
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.52	0.45
1:E:475:ALA:HB1	2:H:32:ASN:HD21	1.82	0.45
1:E:391:CYS:CB	1:E:522:ALA:HB1	2.44	0.44
1:E:363:ALA:O	1:E:526:GLY:HA2	2.18	0.43
4:B:83:ASP:O	4:B:87:TYR:OH	2.24	0.43
2:H:182:LEU:C	2:H:182:LEU:HD12	2.40	0.42
4:B:48:LEU:HD23	4:B:59:ILE:HD12	2.00	0.42
4:B:186:ALA:O	4:B:190:LYS:HG3	2.20	0.41
5:A:36:TRP:CE2	5:A:81:MET:HB2	2.56	0.41
10:A:302:TAR:O11	10:A:302:TAR:O3	2.35	0.41
3:L:167:ASP:OD2	3:L:169:LYS:HB3	2.20	0.41
3:L:183:LYS:NZ	11:L:414:HOH:O	2.55	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	E	194/210 (92%)	189 (97%)	5 (3%)	0	100	100
2	H	216/222 (97%)	213 (99%)	3 (1%)	0	100	100
3	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
4	B	214/216 (99%)	208 (97%)	6 (3%)	0	100	100
5	A	217/223 (97%)	214 (99%)	3 (1%)	0	100	100
All	All	1053/1085 (97%)	1031 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	E	167/180 (93%)	166 (99%)	1 (1%)	86	83
2	H	183/187 (98%)	181 (99%)	2 (1%)	73	67
3	L	187/188 (100%)	185 (99%)	2 (1%)	73	67
4	B	186/186 (100%)	184 (99%)	2 (1%)	73	67
5	A	180/187 (96%)	177 (98%)	3 (2%)	60	50
All	All	903/928 (97%)	893 (99%)	10 (1%)	73	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	377	PHE
2	H	6	GLU
2	H	201	ASN
3	L	105	ASP
3	L	152	ASN
4	B	34	LEU
4	B	125	GLU

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Mol	Chain	Res	Type
5	A	32	SER
5	A	196	THR
5	A	202	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	189	HIS

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	$\#\|Z\| > 2$
6	NAG	C	1	1,6	14,14,15	0.39	0	17,19,21	0.51	0
6	NAG	C	2	6	14,14,15	0.45	0	17,19,21	0.56	0
6	BMA	C	3	6	11,11,12	1.06	1 (9%)	15,15,17	0.74	0
6	MAN	C	4	6	11,11,12	1.24	1 (9%)	15,15,17	1.13	1 (6%)
6	FUC	C	5	6	10,10,11	1.12	1 (10%)	14,14,16	0.83	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	C	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	BMA	C	3	6	-	2/2/19/22	0/1/1/1
6	MAN	C	4	6	-	0/2/19/22	0/1/1/1
6	FUC	C	5	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3	BMA	C4-C5	2.58	1.58	1.53
6	C	5	FUC	C2-C3	2.16	1.55	1.52
6	C	4	MAN	O5-C5	2.03	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	4	MAN	C1-C2-C3	-2.30	106.84	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

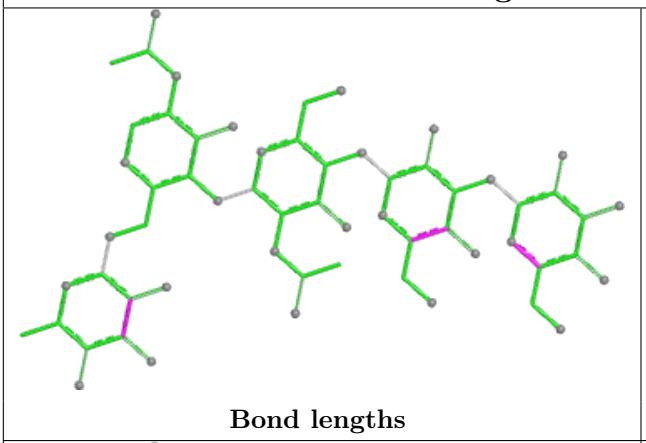
Mol	Chain	Res	Type	Atoms
6	C	3	BMA	O5-C5-C6-O6
6	C	3	BMA	C4-C5-C6-O6

There are no ring outliers.

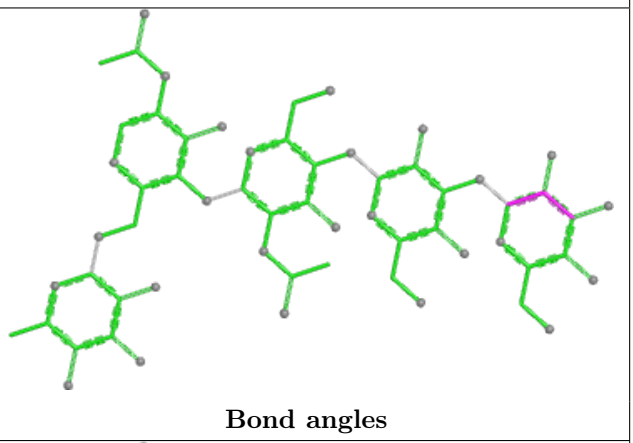
No monomer is involved in short contacts.

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

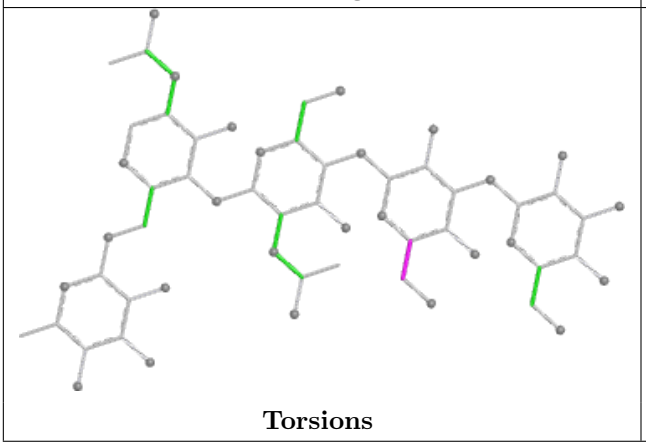
Oligosaccharide Chain C



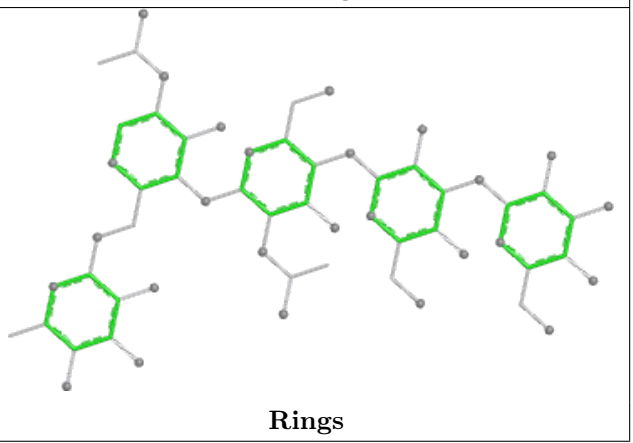
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 28 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
7	GOL	E	703	-	5,5,5	0.99	0	5,5,5	0.95	0
7	GOL	H	401	-	5,5,5	1.23	0	5,5,5	0.73	0
7	GOL	A	303	-	5,5,5	0.85	0	5,5,5	1.02	0
10	TAR	A	301	-	3,9,9	0.34	0	6,12,12	1.17	0
7	GOL	E	704	-	5,5,5	1.30	1 (20%)	5,5,5	1.09	0
7	GOL	E	702	-	5,5,5	1.06	0	5,5,5	1.04	0
7	GOL	H	403	-	5,5,5	1.20	0	5,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	B	402	-	5,5,5	1.50	2 (40%)	5,5,5	1.03	0
7	GOL	E	701	-	5,5,5	1.00	0	5,5,5	0.90	0
7	GOL	H	402	-	5,5,5	1.09	0	5,5,5	0.91	0
7	GOL	B	403	-	5,5,5	0.99	0	5,5,5	0.92	0
7	GOL	L	301	9	5,5,5	1.36	0	5,5,5	0.67	0
7	GOL	B	401	-	5,5,5	0.87	0	5,5,5	1.29	1 (20%)
7	GOL	H	405	-	5,5,5	1.00	0	5,5,5	0.92	0
10	TAR	H	404	-	3,9,9	0.17	0	6,12,12	1.14	1 (16%)
10	TAR	A	302	-	3,9,9	0.32	0	6,12,12	0.62	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
7	GOL	E	703	-	-	2/4/4/4	-
7	GOL	H	401	-	-	1/4/4/4	-
7	GOL	A	303	-	-	1/4/4/4	-
10	TAR	A	301	-	-	3/4/12/12	-
7	GOL	E	704	-	-	2/4/4/4	-
7	GOL	E	702	-	-	1/4/4/4	-
7	GOL	H	403	-	-	4/4/4/4	-
7	GOL	B	402	-	-	1/4/4/4	-
7	GOL	E	701	-	-	2/4/4/4	-
7	GOL	H	402	-	-	2/4/4/4	-
7	GOL	B	403	-	-	4/4/4/4	-
7	GOL	L	301	9	-	2/4/4/4	-
7	GOL	B	401	-	-	1/4/4/4	-
7	GOL	H	405	-	-	3/4/4/4	-
10	TAR	H	404	-	-	4/4/12/12	-
10	TAR	A	302	-	-	4/4/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	402	GOL	C3-C2	2.57	1.62	1.51
7	E	704	GOL	C3-C2	2.24	1.60	1.51
7	B	402	GOL	C1-C2	2.06	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	401	GOL	C3-C2-C1	-2.27	102.86	111.70
10	H	404	TAR	C4-C3-C2	-2.18	108.41	113.11

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	703	GOL	C1-C2-C3-O3
7	E	703	GOL	O2-C2-C3-O3
7	E	704	GOL	C1-C2-C3-O3
7	H	403	GOL	C1-C2-C3-O3
7	L	301	GOL	O1-C1-C2-O2
7	L	301	GOL	O1-C1-C2-C3
7	B	403	GOL	O1-C1-C2-C3
10	H	404	TAR	C1-C2-C3-C4
10	A	301	TAR	C1-C2-C3-C4
10	A	302	TAR	C1-C2-C3-O3
10	A	302	TAR	O2-C2-C3-O3
10	A	302	TAR	O2-C2-C3-C4
7	B	403	GOL	O2-C2-C3-O3
7	H	401	GOL	C1-C2-C3-O3
7	H	402	GOL	O1-C1-C2-C3
7	H	403	GOL	O1-C1-C2-C3
7	H	405	GOL	O1-C1-C2-C3
7	B	403	GOL	C1-C2-C3-O3
7	H	403	GOL	O2-C2-C3-O3
10	H	404	TAR	O2-C2-C3-O3
10	A	302	TAR	C1-C2-C3-C4
7	E	704	GOL	O2-C2-C3-O3
7	H	405	GOL	O2-C2-C3-O3
7	B	402	GOL	O2-C2-C3-O3
7	E	701	GOL	O2-C2-C3-O3
7	B	403	GOL	O1-C1-C2-O2
7	A	303	GOL	O1-C1-C2-C3
7	H	405	GOL	O1-C1-C2-O2
10	H	404	TAR	O2-C2-C3-C4
7	E	702	GOL	C1-C2-C3-O3
10	H	404	TAR	C1-C2-C3-O3
10	A	301	TAR	C1-C2-C3-O3
10	A	301	TAR	O2-C2-C3-C4
7	H	403	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	H	402	GOL	O1-C1-C2-O2
7	E	701	GOL	C1-C2-C3-O3
7	B	401	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	703	GOL	1	0
7	H	401	GOL	1	0
7	H	403	GOL	1	0
7	H	402	GOL	2	0
7	L	301	GOL	1	0
7	B	401	GOL	2	0
10	A	302	TAR	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	E	196/210 (93%)	0.59	13 (6%)	18	14	31, 46, 97, 142	0
2	H	218/222 (98%)	0.36	2 (0%)	84	82	27, 37, 59, 90	0
3	L	214/214 (100%)	0.28	1 (0%)	91	89	29, 43, 60, 99	0
4	B	216/216 (100%)	0.33	5 (2%)	60	56	32, 48, 77, 120	0
5	A	219/223 (98%)	0.26	2 (0%)	84	82	31, 42, 68, 103	0
All	All	1063/1085 (97%)	0.36	23 (2%)	62	58	27, 43, 74, 142	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	522	ALA	6.8
4	B	216	CYS	6.2
1	E	519	HIS	6.0
1	E	528	LYS	6.0
1	E	520	ALA	5.6
5	A	136	THR	5.5
1	E	523	THR	4.5
1	E	518	LEU	4.4
5	A	135	SER	4.3
1	E	521	PRO	3.7
3	L	214	CYS	3.5
1	E	517	LEU	3.1
2	H	1	GLU	2.9
1	E	527	LYS	2.7
1	E	369	TYR	2.4
4	B	156	LEU	2.4
1	E	524	VAL	2.4
4	B	1	ALA	2.3
2	H	5	LEU	2.2
1	E	385	THR	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	3	ARG	2.1
1	E	525	CYS	2.1
4	B	215	GLU	2.1

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)

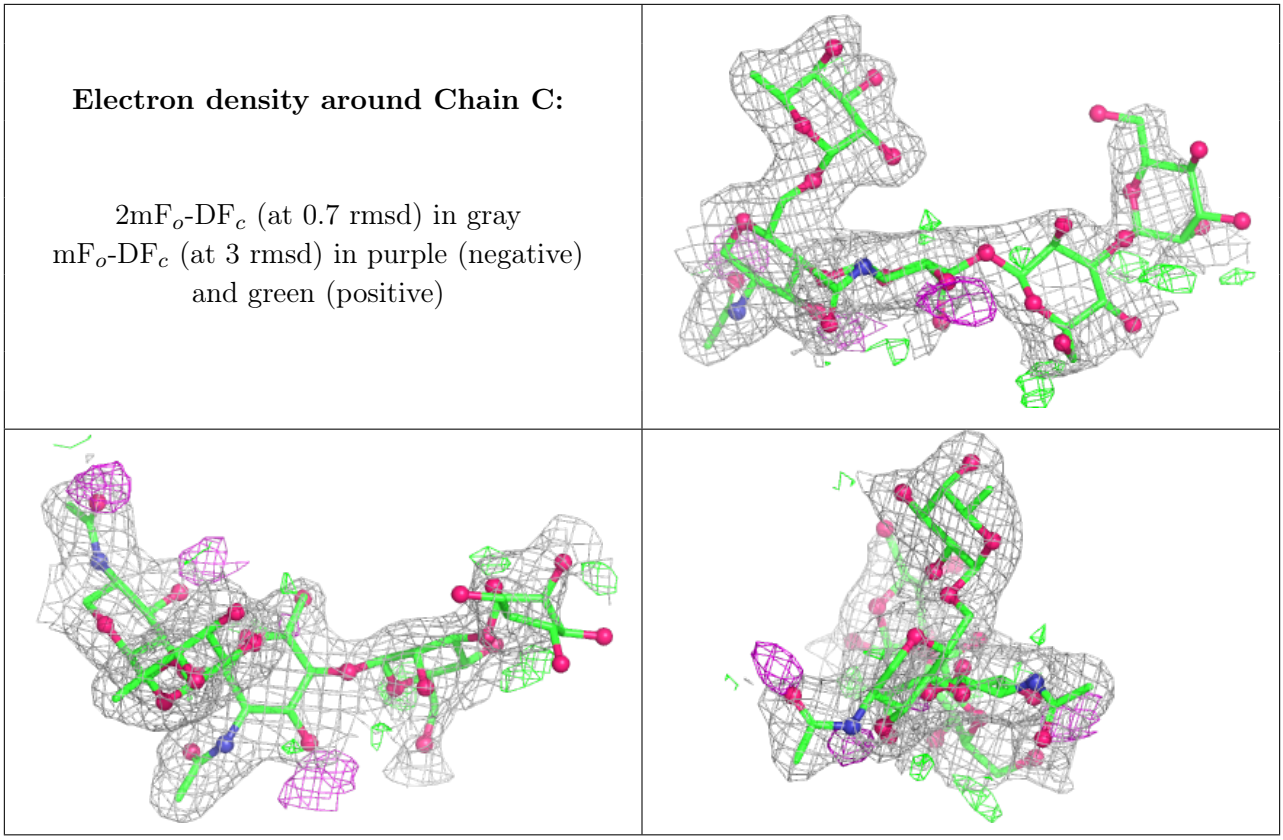
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	MAN	C	4	11/12	0.72	0.46	100,117,131,132	0
6	BMA	C	3	11/12	0.79	0.22	82,96,112,113	0
6	NAG	C	2	14/15	0.93	0.12	40,53,73,82	0
6	FUC	C	5	10/11	0.94	0.11	39,50,59,63	0
6	NAG	C	1	14/15	0.97	0.12	32,40,46,47	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

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	K	L	305	1/1	0.72	0.11	81,81,81,81	0
7	GOL	B	401	6/6	0.73	0.30	52,64,74,74	0
9	K	H	409	1/1	0.77	0.16	79,79,79,79	0
7	GOL	H	405	6/6	0.78	0.20	48,49,59,64	0
7	GOL	B	402	6/6	0.78	0.20	43,55,58,63	0
8	CL	B	404	1/1	0.79	0.24	65,65,65,65	0
8	CL	A	305	1/1	0.80	0.10	58,58,58,58	0
8	CL	A	306	1/1	0.80	0.18	71,71,71,71	0
10	TAR	A	302	10/10	0.80	0.22	46,65,77,85	0
9	K	L	306	1/1	0.81	0.15	70,70,70,70	0
10	TAR	A	301	10/10	0.82	0.28	36,68,77,92	0
9	K	A	308	1/1	0.82	0.06	87,87,87,87	0
7	GOL	E	701	6/6	0.83	0.21	63,66,75,76	0
9	K	L	307	1/1	0.84	0.10	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	H	402	6/6	0.86	0.25	39,54,64,84	0
7	GOL	E	704	6/6	0.86	0.25	42,60,67,70	0
8	CL	E	707	1/1	0.86	0.19	73,73,73,73	0
9	K	L	304	1/1	0.86	0.06	73,73,73,73	0
7	GOL	L	301	6/6	0.86	0.20	35,48,56,63	0
9	K	H	410	1/1	0.87	0.19	79,79,79,79	0
8	CL	E	706	1/1	0.89	0.07	61,61,61,61	0
7	GOL	H	403	6/6	0.89	0.30	45,49,57,71	0
10	TAR	H	404	10/10	0.90	0.21	37,64,71,72	0
9	K	L	308	1/1	0.90	0.08	74,74,74,74	0
8	CL	B	405	1/1	0.90	0.14	60,60,60,60	0
7	GOL	E	703	6/6	0.91	0.28	46,66,72,85	0
7	GOL	B	403	6/6	0.91	0.24	44,56,63,66	0
8	CL	L	303	1/1	0.91	0.11	70,70,70,70	0
7	GOL	E	702	6/6	0.92	0.13	45,57,68,81	0
7	GOL	A	303	6/6	0.92	0.23	52,58,68,70	0
9	K	H	407	1/1	0.92	0.09	61,61,61,61	0
9	K	H	408	1/1	0.92	0.11	69,69,69,69	0
8	CL	H	406	1/1	0.92	0.29	66,66,66,66	0
8	CL	E	708	1/1	0.93	0.12	66,66,66,66	0
9	K	B	408	1/1	0.94	0.05	56,56,56,56	0
7	GOL	H	401	6/6	0.95	0.21	34,48,52,52	0
9	K	E	709	1/1	0.95	0.07	78,78,78,78	0
8	CL	A	307	1/1	0.97	0.16	63,63,63,63	0
8	CL	L	302	1/1	0.97	0.06	73,73,73,73	0
9	K	B	407	1/1	0.98	0.12	56,56,56,56	0
9	K	H	411	1/1	0.98	0.12	60,60,60,60	0
8	CL	B	406	1/1	0.98	0.07	64,64,64,64	0
8	CL	A	304	1/1	0.99	0.07	34,34,34,34	0
8	CL	E	705	1/1	1.00	0.07	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.