wwPDB X-ray Structure Validation Summary Report (i)

Apr 5, 2022 – 01:12 pm BST

PDB ID	:	7AKK
Title	:	Structure of a complement factor-receptor complex
Authors	:	Fernandez, F.J.; Santos-Lopez, J.; Martinez-Barricarte, R.; Querol-Garcia, J.; Navas-Yuste, S.; Savko, M.; Shepard, W.E.; Rodriguez de Cordoba, S.; Vega, M.C.
Deposited on	:	2020-10-01
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

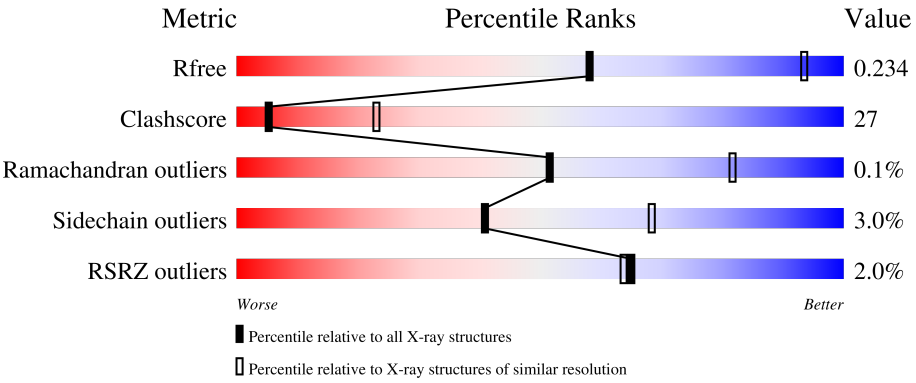
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	B	645	2% 53% 46% ·
1	C	645	2% 49% 49% ·
2	A	898	3% 47% 44% · 6%
2	E	898	2% 27% 28% · 44%
3	D	195	50% 43% · 5%

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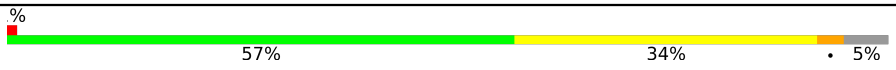
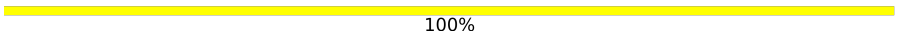
Mol	Chain	Length	Quality of chain
3	H	195	
4	I	3	
5	J	4	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 24012 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	645	Total	C	N	O	S	0	0	0
			5024	3198	851	960	15			
1	C	645	Total	C	N	O	S	0	0	0
			5024	3198	851	960	15			

- Molecule 2 is a protein called Complement C3b alpha' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	842	Total	C	N	O	S	0	0	0
			6736	4276	1128	1295	37			
2	E	504	Total	C	N	O	S	0	0	0
			4084	2585	684	789	26			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	LYS	deletion	UNP P01024
A	?	-	ILE	deletion	UNP P01024
A	?	-	THR	deletion	UNP P01024
A	?	-	HIS	deletion	UNP P01024
A	?	-	ARG	deletion	UNP P01024
A	?	-	ILE	deletion	UNP P01024
A	?	-	HIS	deletion	UNP P01024
A	?	-	TRP	deletion	UNP P01024
A	?	-	GLU	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	ALA	deletion	UNP P01024
A	?	-	SER	deletion	UNP P01024
A	?	-	LEU	deletion	UNP P01024

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P01024
E	?	-	ARG	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	LYS	deletion	UNP P01024
E	?	-	ILE	deletion	UNP P01024
E	?	-	THR	deletion	UNP P01024
E	?	-	HIS	deletion	UNP P01024
E	?	-	ARG	deletion	UNP P01024
E	?	-	ILE	deletion	UNP P01024
E	?	-	HIS	deletion	UNP P01024
E	?	-	TRP	deletion	UNP P01024
E	?	-	GLU	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	ALA	deletion	UNP P01024
E	?	-	SER	deletion	UNP P01024
E	?	-	LEU	deletion	UNP P01024
E	?	-	LEU	deletion	UNP P01024

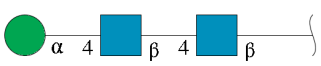
- Molecule 3 is a protein called Integrin alpha-M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	185	Total	C	N	O	S	0	0	0
			1499	951	267	278	3			
3	H	185	Total	C	N	O	S	0	0	0
			1499	951	267	278	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	128	SER	CYS	engineered mutation	UNP P11215
D	316	GLY	ILE	engineered mutation	UNP P11215
H	128	SER	CYS	engineered mutation	UNP P11215
H	316	GLY	ILE	engineered mutation	UNP P11215

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

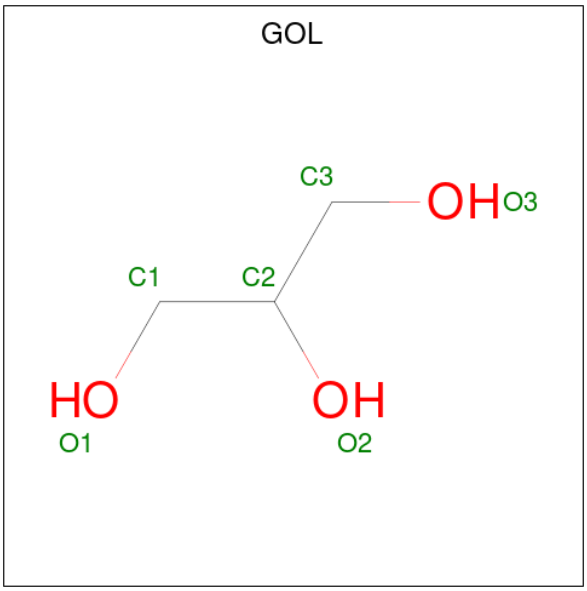


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	J	4	Total C N O 50 28 2 20	0	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

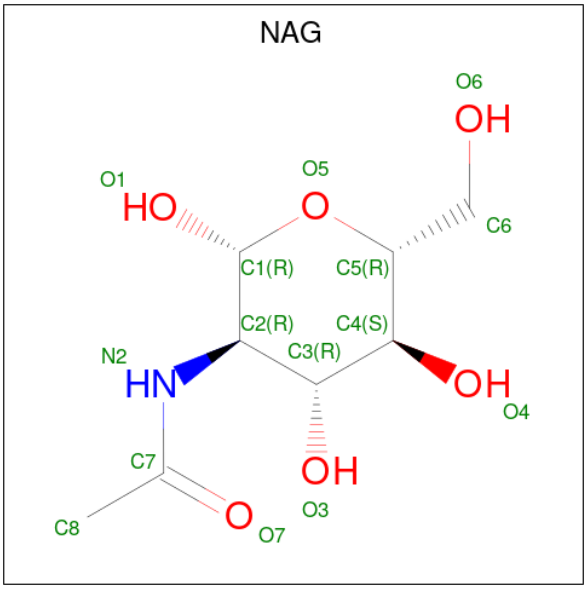
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0
7	C	1	Total K 1 1	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	6	Total O 6 6	0	0
10	A	7	Total O 7 7	0	0

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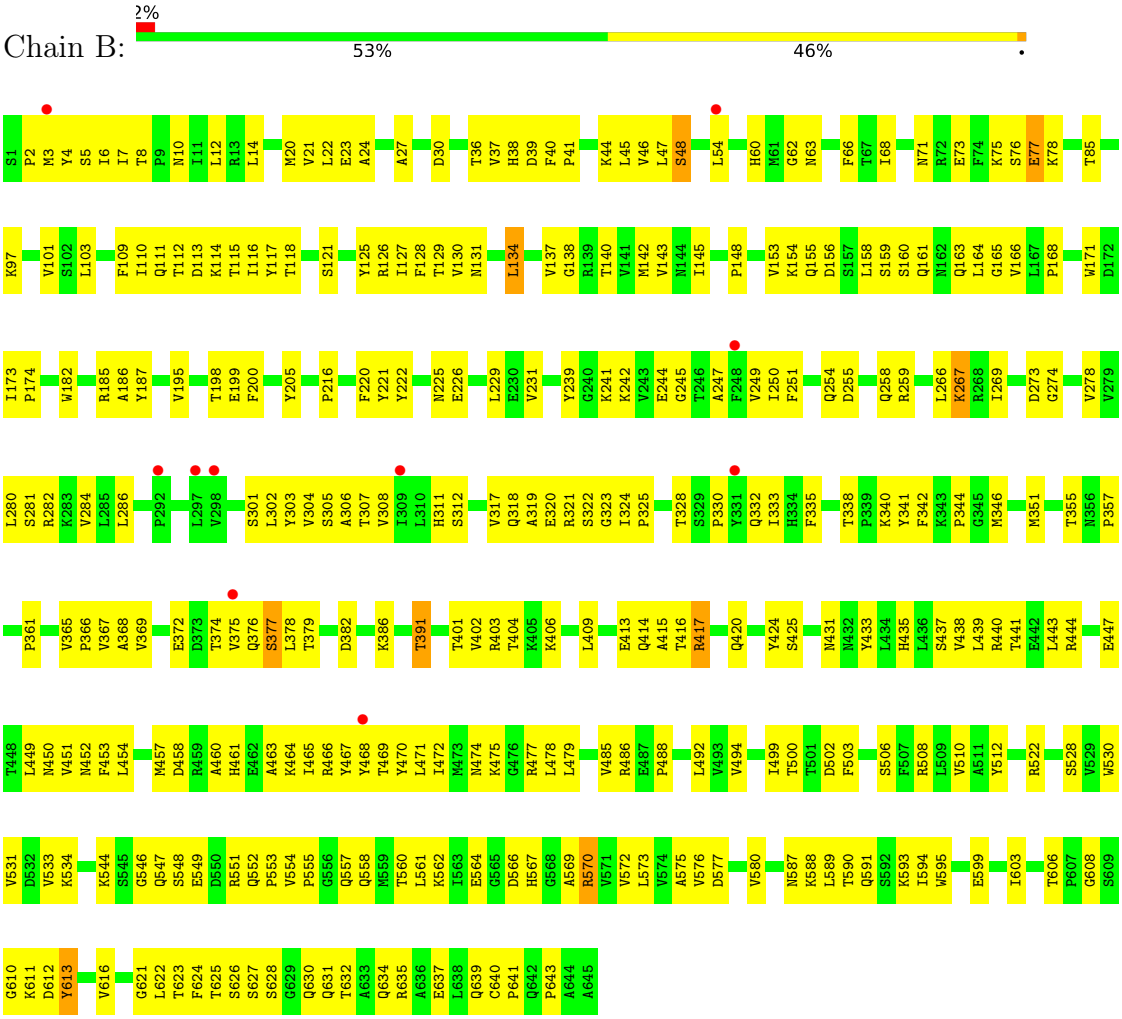
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total O 2 2	0	0
10	C	4	Total O 4 4	0	0
10	E	2	Total O 2 2	0	0

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.

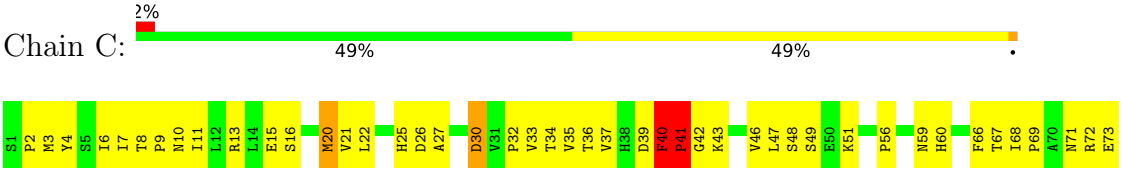
• Molecule 1: Complement C3 beta chain

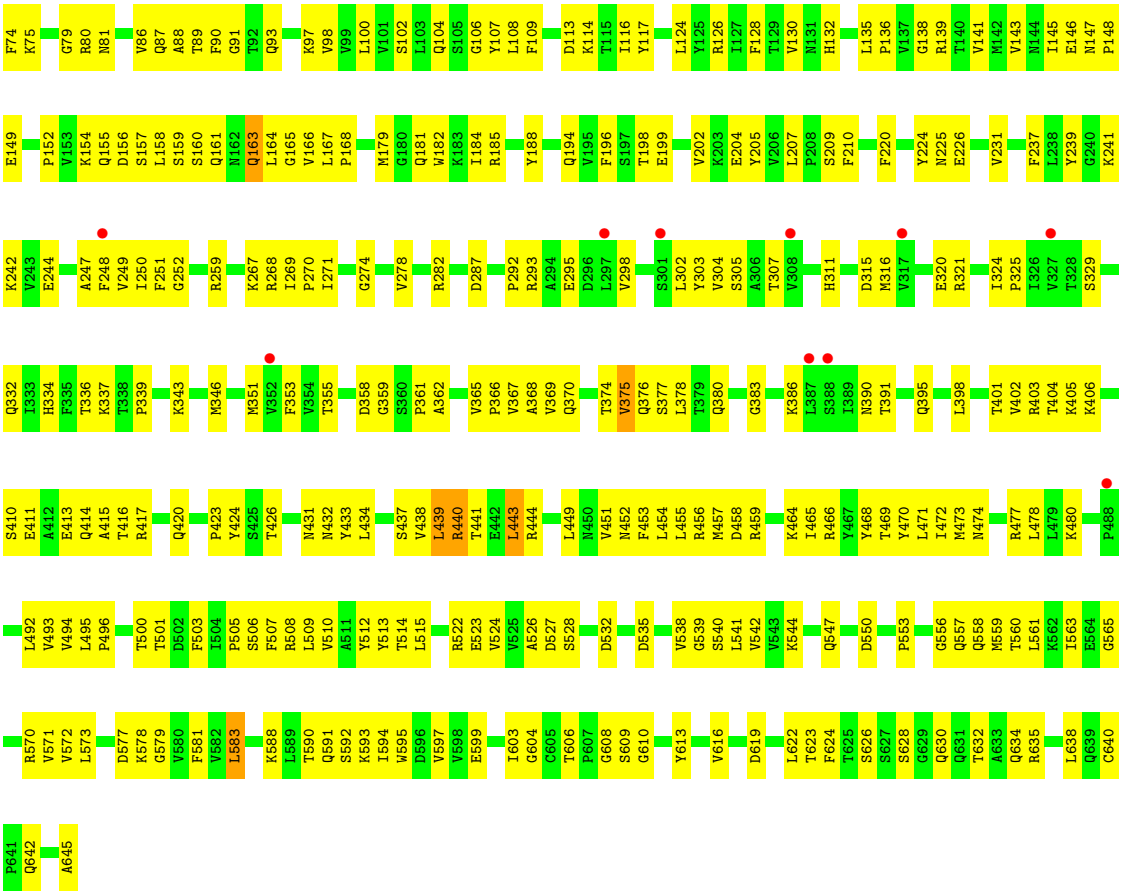
Chain B:



• Molecule 1: Complement C3 beta chain

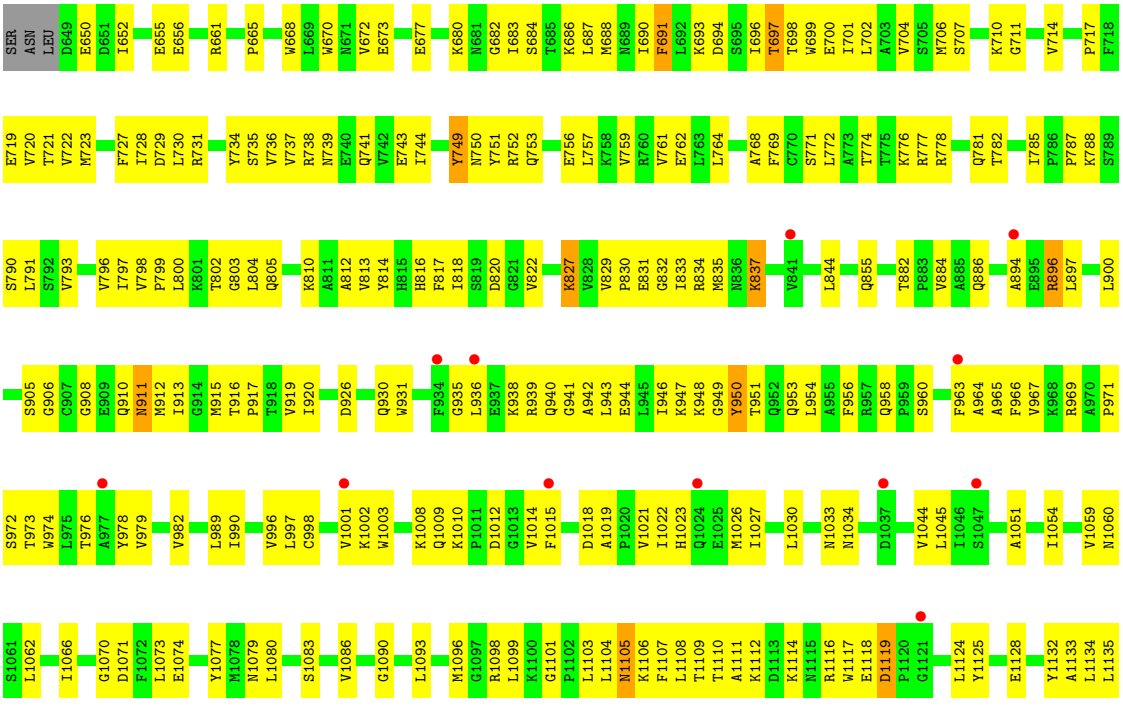
Chain C:

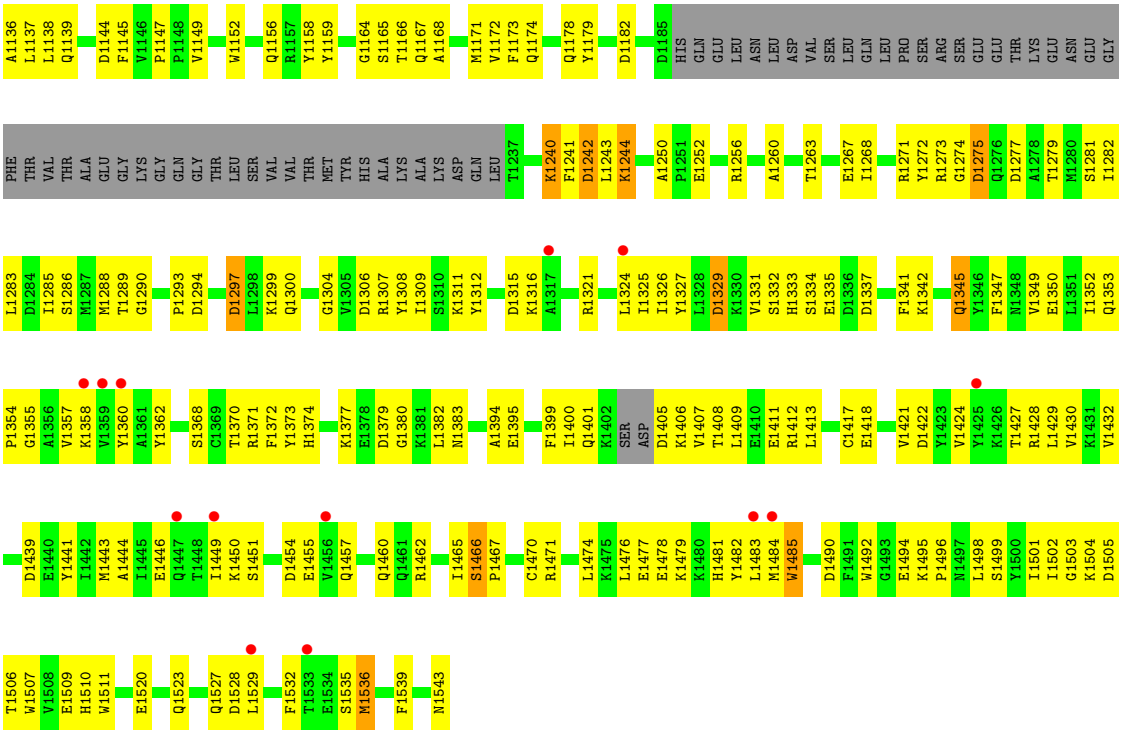




• Molecule 2: Complement C3b alpha' chain

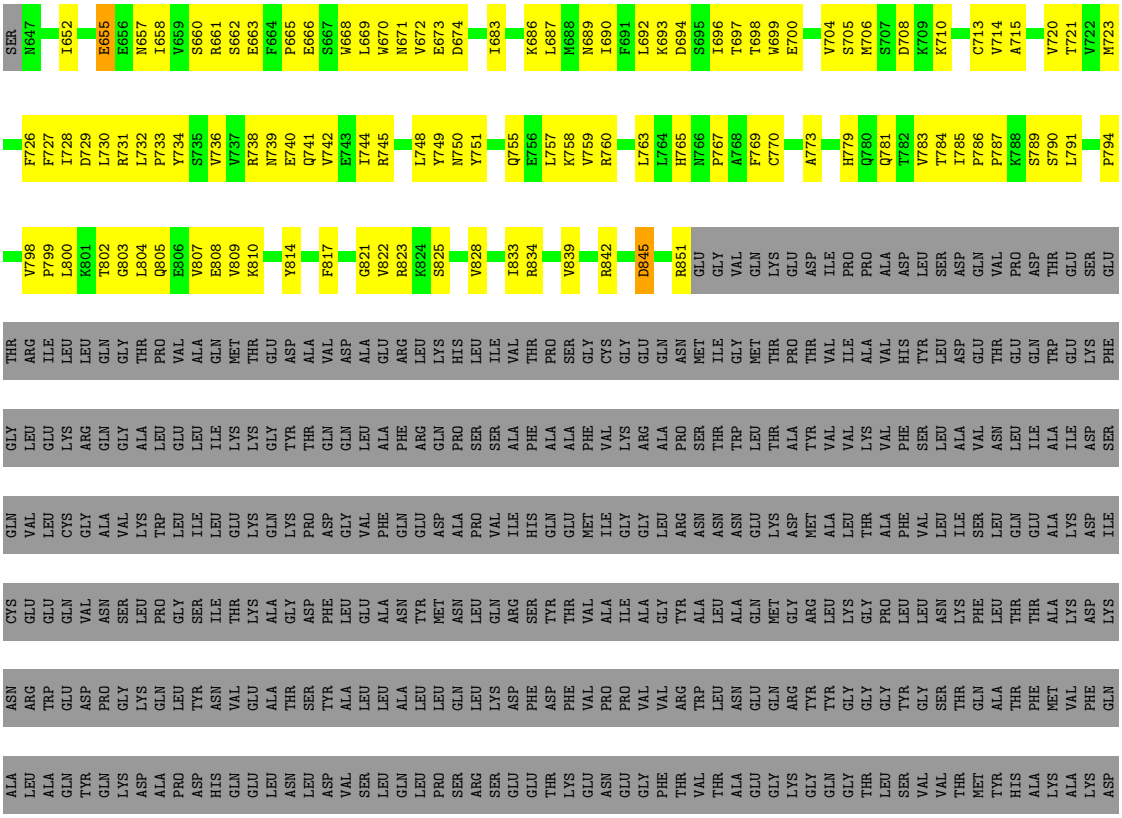
Chain A:

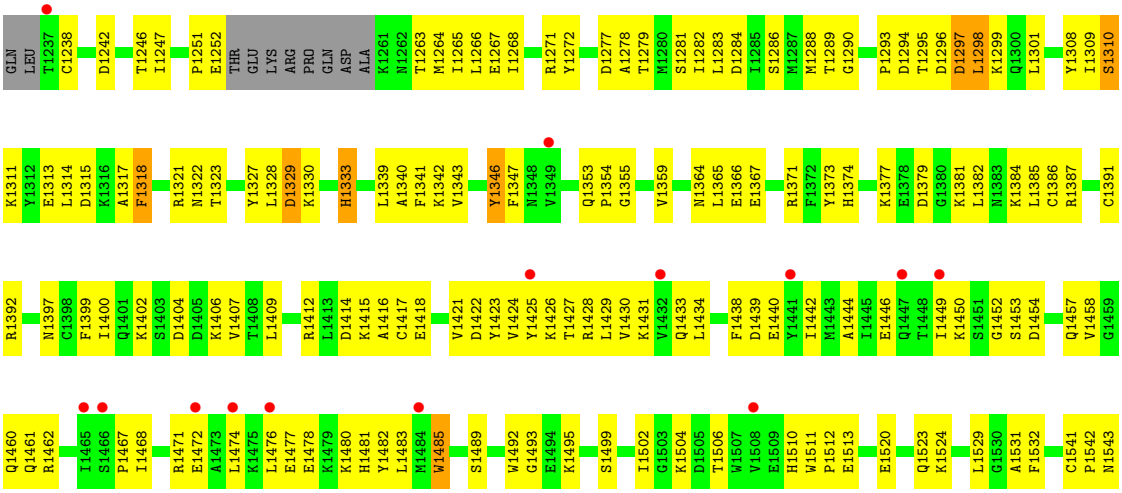




• Molecule 2: Complement C3b alpha' chain

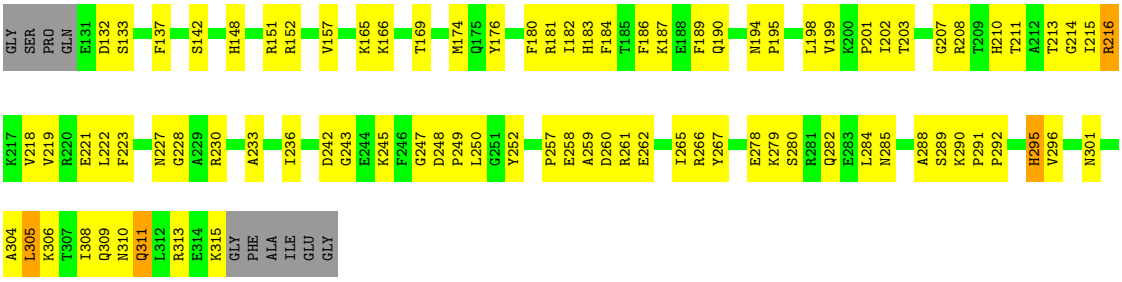
Chain E:





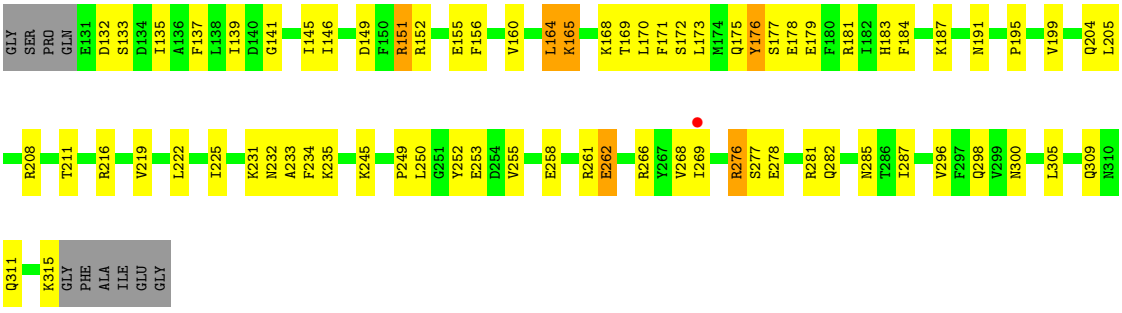
• Molecule 3: Integrin alpha-M

Chain D:



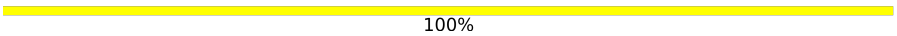
• Molecule 3: Integrin alpha-M

Chain H:



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

Chain I:



• Molecule 5: beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.29Å 150.73Å 111.30Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	53.77 – 3.40 53.77 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (53.77-3.40) 99.3 (53.77-3.40)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.192 , 0.229 0.192 , 0.234	Depositor DCC
R_{free} test set	2520 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	105.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.109 for l,k,-h 0.117 for h,-k,-l 0.326 for l,-k,h	Xtriage
Reported twinning fraction	0.500 for l,-k,h	Depositor
Outliers	0 of 50383 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24012	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: GOL, MG, MAN, K, NAG, BMA

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	0.63	0/5126	0.82	4/6966 (0.1%)
1	C	0.61	1/5126 (0.0%)	0.83	2/6966 (0.0%)
2	A	0.56	1/6871 (0.0%)	0.73	5/9303 (0.1%)
2	E	0.61	0/4164	0.77	1/5629 (0.0%)
3	D	0.55	0/1527	0.70	0/2054
3	H	0.67	2/1527 (0.1%)	0.80	1/2054 (0.0%)
All	All	0.60	4/24341 (0.0%)	0.78	13/32972 (0.0%)

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
1	B	0	1
1	C	0	1
2	A	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	640	CYS	CB-SG	6.77	1.93	1.82
3	H	262	GLU	CG-CD	5.90	1.60	1.51
2	A	749	TYR	CD1-CE1	-5.24	1.31	1.39
3	H	262	GLU	CB-CG	5.21	1.62	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1119	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	B	391	THR	C-N-CA	-7.50	102.95	121.70
1	C	41	PRO	CA-N-CD	-6.88	101.87	111.50
2	E	713	CYS	CA-CB-SG	6.30	125.35	114.00
2	A	1119	ASP	CB-CG-OD1	6.14	123.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	817	PHE	Peptide
1	B	640	CYS	Peptide
1	C	40	PHE	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	5024	0	5084	275	0
1	C	5024	0	5084	332	1
2	A	6736	0	6668	365	2
2	E	4084	0	4022	250	0
3	D	1499	0	1509	66	1
3	H	1499	0	1511	68	2
4	I	39	0	33	2	0
5	J	50	0	43	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	E	6	0	8	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	D	1	0	0	0	0
8	H	1	0	0	0	0
9	E	14	0	13	0	0
10	A	7	0	0	0	0
10	B	6	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	2	0	0	0	0
All	All	24012	0	23991	1272	3

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 27.

The worst 5 of 1272 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLN:HG3	1:C:401:THR:HB	1.14	1.12
1:C:369:VAL:H	1:C:375:VAL:CG2	1.65	1.09
1:C:369:VAL:H	1:C:375:VAL:HG21	0.94	1.07
1:C:369:VAL:HG22	1:C:375:VAL:HG11	1.34	1.07
1:B:155:GLN:HE21	2:E:804:LEU:HD13	1.13	1.06

All (3) 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)
2:A:756:GLU:OE2	3:H:300:ASN:ND2[2_747]	1.93	0.27
2:A:1428:ARG:NH2	3:H:191:ASN:O[1_455]	2.07	0.13
3:D:249:PRO:O	1:C:71:ASN:ND2[2_657]	2.08	0.12

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	643/645 (100%)	609 (95%)	34 (5%)	0	100	100
1	C	643/645 (100%)	617 (96%)	25 (4%)	1 (0%)	47	78
2	A	836/898 (93%)	743 (89%)	92 (11%)	1 (0%)	51	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	498/898 (56%)	441 (89%)	57 (11%)	0	100	100
3	D	183/195 (94%)	169 (92%)	14 (8%)	0	100	100
3	H	183/195 (94%)	173 (94%)	9 (5%)	1 (0%)	29	61
All	All	2986/3476 (86%)	2752 (92%)	231 (8%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	PRO
2	A	656	GLU
3	H	177	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	567/567 (100%)	551 (97%)	16 (3%)	43	70
1	C	567/567 (100%)	555 (98%)	12 (2%)	53	76
2	A	745/794 (94%)	720 (97%)	25 (3%)	37	65
2	E	463/794 (58%)	448 (97%)	15 (3%)	39	67
3	D	166/172 (96%)	159 (96%)	7 (4%)	30	59
3	H	166/172 (96%)	162 (98%)	4 (2%)	49	74
All	All	2674/3066 (87%)	2595 (97%)	79 (3%)	41	68

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	440	ARG
2	E	1346	TYR
1	C	583	LEU
2	E	1297	ASP
3	H	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	642	GLN
3	H	191	ASN
2	E	689	ASN
2	E	1383	ASN
2	A	1276	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)

7 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	$\#\|Z\| > 2$
4	NAG	I	1	1,4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	I	2	4	14,14,15	0.75	0	17,19,21	1.12	2 (11%)
4	MAN	I	3	4	11,11,12	2.27	4 (36%)	15,15,17	1.58	4 (26%)
5	NAG	J	1	5,1	14,14,15	0.94	1 (7%)	17,19,21	0.57	0
5	NAG	J	2	5	14,14,15	0.87	1 (7%)	17,19,21	0.80	0
5	MAN	J	3	5	11,11,12	2.16	4 (36%)	15,15,17	1.87	2 (13%)
5	BMA	J	4	5	11,11,12	1.85	4 (36%)	15,15,17	1.13	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	MAN	I	3	4	-	1/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	MAN	J	3	5	-	1/2/19/22	0/1/1/1
5	BMA	J	4	5	-	0/2/19/22	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	MAN	O5-C1	5.53	1.52	1.43
5	J	3	MAN	C2-C3	4.80	1.59	1.52
5	J	4	BMA	C4-C3	3.18	1.60	1.52
5	J	1	NAG	O5-C1	2.98	1.48	1.43
5	J	4	BMA	O5-C1	2.89	1.48	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	3	MAN	C1-O5-C5	5.18	119.21	112.19
4	I	3	MAN	C1-C2-C3	3.22	113.63	109.67
5	J	3	MAN	C1-C2-C3	3.16	113.55	109.67
4	I	3	MAN	C1-O5-C5	2.72	115.87	112.19
4	I	3	MAN	O5-C1-C2	-2.55	106.84	110.77

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6

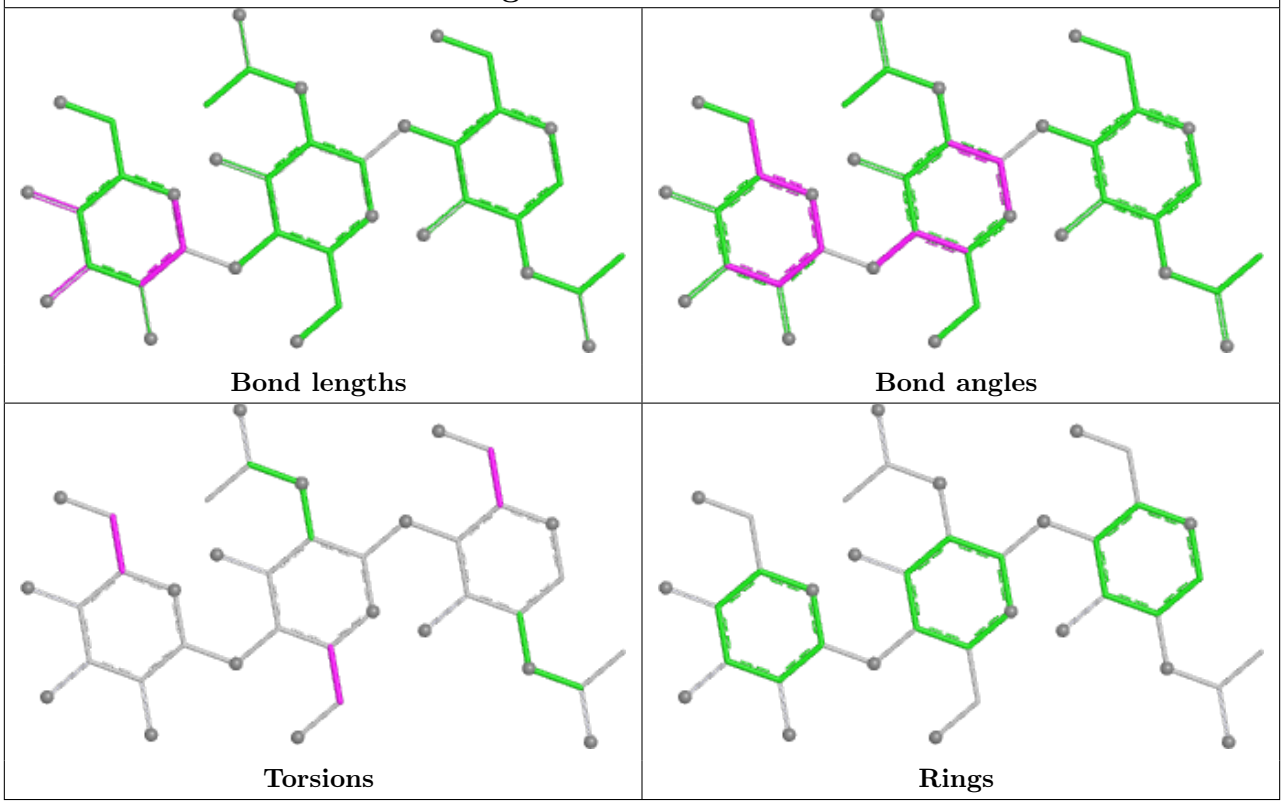
There are no ring outliers.

3 monomers are involved in 3 short contacts:

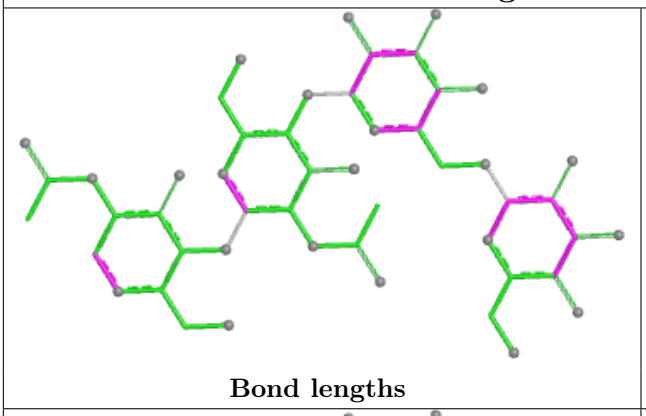
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	4	BMA	1	0
5	J	2	NAG	1	0
4	I	1	NAG	2	0

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

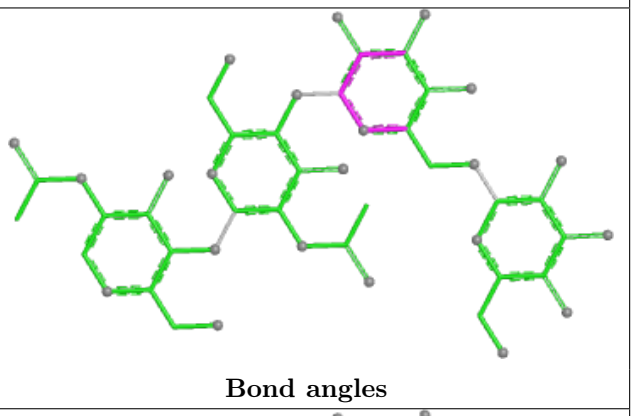
Oligosaccharide Chain I



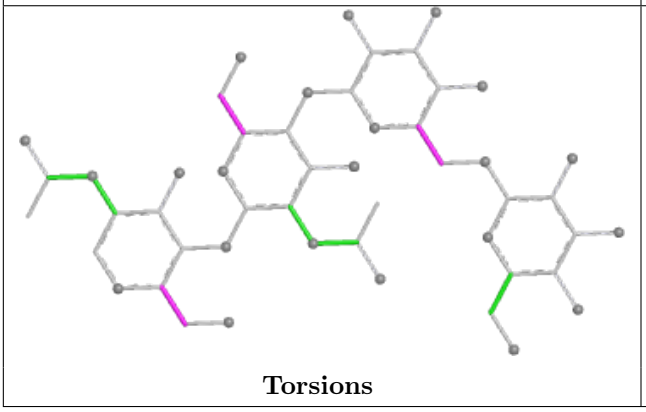
Oligosaccharide Chain J



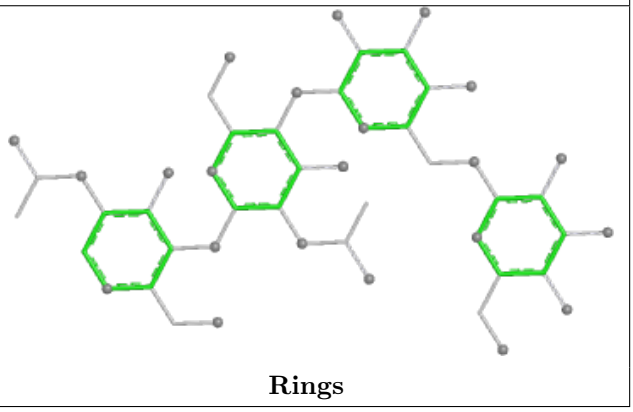
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	C	1601	-	5,5,5	0.90	0	5,5,5	0.99	0
9	NAG	E	1601	2	14,14,15	0.38	0	17,19,21	0.79	1 (5%)
6	GOL	E	1602	-	5,5,5	1.11	0	5,5,5	1.00	0
6	GOL	B	1601	-	5,5,5	1.66	2 (40%)	5,5,5	0.58	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	GOL	C	1601	-	-	0/4/4/4	-
9	NAG	E	1601	2	-	0/6/23/26	0/1/1/1
6	GOL	E	1602	-	-	2/4/4/4	-
6	GOL	B	1601	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1601	GOL	C3-C2	2.93	1.63	1.51
6	B	1601	GOL	C1-C2	2.08	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	1601	NAG	C1-O5-C5	2.19	115.16	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1601	GOL	C1-C2-C3-O3
6	E	1602	GOL	O1-C1-C2-C3
6	E	1602	GOL	O1-C1-C2-O2
6	B	1601	GOL	O2-C2-C3-O3
6	B	1601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1602	GOL	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	B	645/645 (100%)	-0.09	10 (1%)	72	70	47, 108, 152, 185	0
1	C	645/645 (100%)	-0.09	10 (1%)	72	70	57, 104, 150, 179	0
2	A	842/898 (93%)	-0.15	25 (2%)	50	49	55, 127, 164, 192	0
2	E	504/898 (56%)	-0.16	14 (2%)	53	51	58, 111, 170, 204	0
3	D	185/195 (94%)	-0.18	0	100	100	78, 108, 133, 155	0
3	H	185/195 (94%)	-0.26	1 (0%)	91	90	68, 93, 123, 145	0
All	All	3006/3476 (86%)	-0.14	60 (1%)	65	64	47, 111, 159, 204	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	388	SER	6.9
2	A	1317	ALA	5.3
2	E	1447	GLN	5.2
2	A	1447	GLN	5.1
2	A	1037	ASP	4.9

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

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

6.3 Carbohydrates

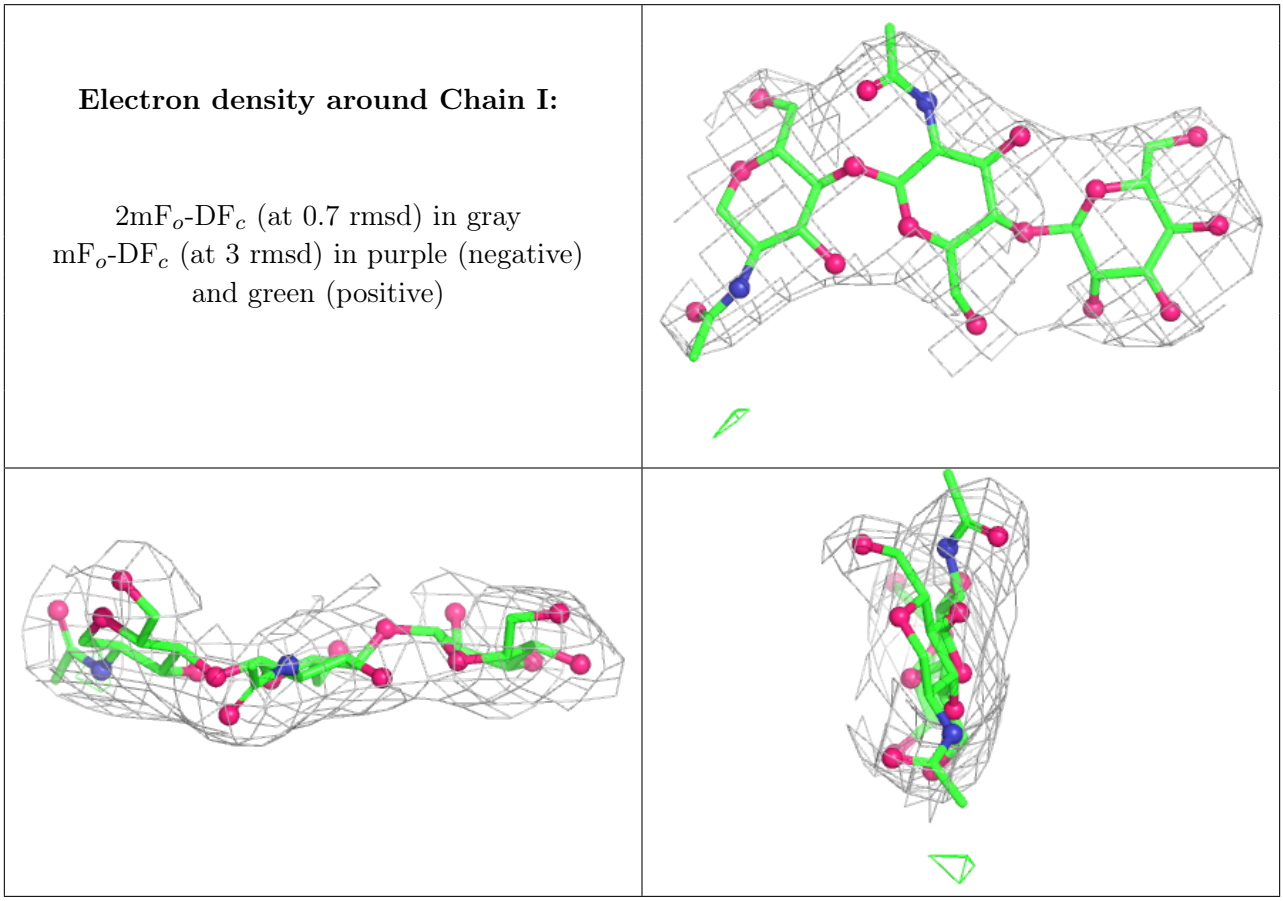
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	BMA	J	4	11/12	0.91	0.23	119,126,140,143	0
5	MAN	J	3	11/12	0.92	0.16	135,144,147,150	0
4	MAN	I	3	11/12	0.94	0.11	120,126,137,141	0
4	NAG	I	1	14/15	0.95	0.14	123,128,134,135	0
4	NAG	I	2	14/15	0.96	0.08	138,141,144,145	0
5	NAG	J	1	14/15	0.96	0.20	98,107,131,132	0
5	NAG	J	2	14/15	0.97	0.17	106,118,132,140	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.

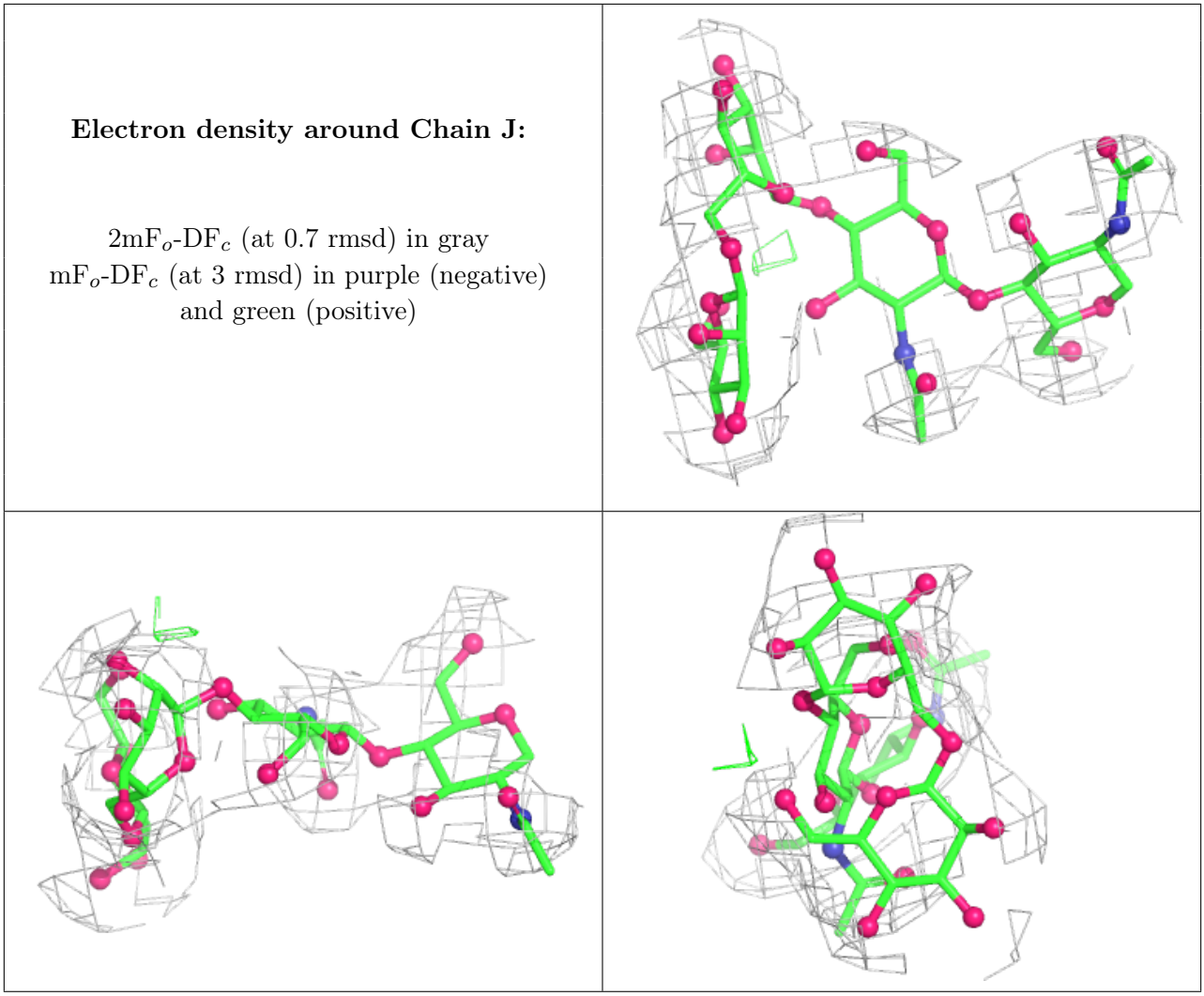
Electron density around Chain I:

$2mF_o$-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 J:

$2mF_o$-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	NAG	E	1601	14/15	0.74	0.24	157,161,166,168	0
6	GOL	C	1601	6/6	0.90	0.19	81,91,93,93	0
6	GOL	E	1602	6/6	0.95	0.20	69,73,75,76	0
6	GOL	B	1601	6/6	0.96	0.23	67,70,71,73	0
7	K	C	1602	1/1	0.98	0.14	71,71,71,71	0
8	MG	D	2101	1/1	0.99	0.11	117,117,117,117	0
8	MG	H	2001	1/1	0.99	0.15	82,82,82,82	0
7	K	A	1601	1/1	0.99	0.22	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.