wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 10:59 AM EDT

PDB ID	:	3P70
Title	:	Structural basis of thrombin-mediated factor V activation: essential role of the hirudin-like sequence Glu666-Glu672 for processing at the heavy chain-B domain junction
Authors	:	Corral-Rodriguez, M.A.; Bock, P.E.; Hernandez-Carvajal, E.; Gutierrez-Gallego, R.; Fuentes-Prior, P.
Deposited on	:	2010-10-11
Resolution	:	2.55 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

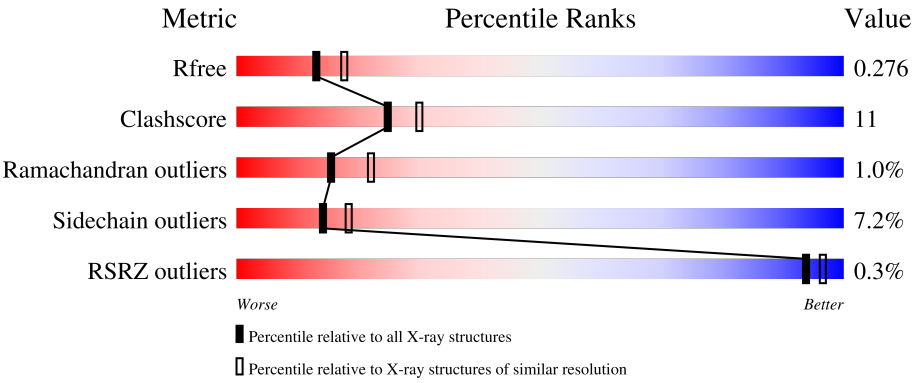
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	36	75% · · 19%
1	C	36	64% 14% · 19%
1	E	36	3% 58% 19% · 19%
1	G	36	64% 14% 22%

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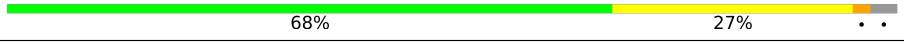
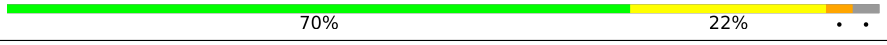
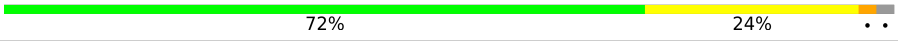
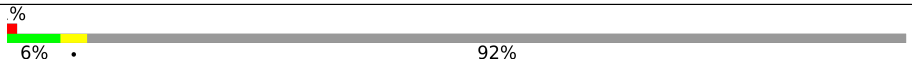
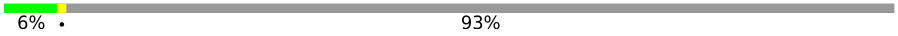
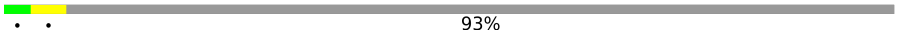
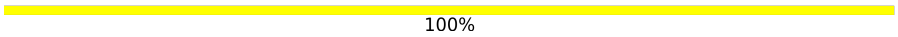
Mol	Chain	Length	Quality of chain
2	B	259	
2	D	259	
2	F	259	
2	H	259	
3	M	71	
3	N	71	
3	O	71	
3	P	71	
4	I	2	
4	J	2	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9477 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 HUMAN ALPHA-THROMBIN, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	29	Total	C	N	O	S	0	0	0
			234	146	38	49	1			
1	C	29	Total	C	N	O	S	0	0	0
			234	146	38	49	1			
1	E	29	Total	C	N	O	S	0	0	0
			234	146	38	49	1			
1	G	28	Total	C	N	O	S	0	0	0
			230	144	37	48	1			

- Molecule 2 is a protein called HUMAN ALPHA-THROMBIN, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	1	0
			2045	1302	364	365	14			
2	D	250	Total	C	N	O	S	0	1	0
			2031	1295	362	360	14			
2	F	252	Total	C	N	O	S	0	0	0
			2047	1309	361	363	14			
2	H	254	Total	C	N	O	S	0	0	0
			2056	1314	363	365	14			

- Molecule 3 is a protein called HUMAN FACTOR V, A2-B DOMAIN LINKER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	0	0	0
			51	35	6	10			
3	N	5	Total	C	N	O	0	0	0
			42	30	5	7			
3	O	5	Total	C	N	O	0	0	0
			42	30	5	7			
3	P	5	Total	C	N	O	0	0	0
			44	30	5	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	639	ALA	-	expression tag	UNP P12259
M	640	HIS	-	expression tag	UNP P12259
M	641	HIS	-	expression tag	UNP P12259
M	642	HIS	-	expression tag	UNP P12259
M	643	HIS	-	expression tag	UNP P12259
M	644	HIS	-	expression tag	UNP P12259
M	645	HIS	-	expression tag	UNP P12259
M	646	VAL	-	expression tag	UNP P12259
M	647	GLY	-	expression tag	UNP P12259
M	648	THR	-	expression tag	UNP P12259
M	649	TRP	-	expression tag	UNP P12259
M	650	GLU	-	expression tag	UNP P12259
M	651	ASN	-	expression tag	UNP P12259
M	652	LEU	-	expression tag	UNP P12259
M	653	TYR	-	expression tag	UNP P12259
M	654	PHE	-	expression tag	UNP P12259
M	655	GLN	-	expression tag	UNP P12259
M	656	SER	-	expression tag	UNP P12259
N	639	ALA	-	expression tag	UNP P12259
N	640	HIS	-	expression tag	UNP P12259
N	641	HIS	-	expression tag	UNP P12259
N	642	HIS	-	expression tag	UNP P12259
N	643	HIS	-	expression tag	UNP P12259
N	644	HIS	-	expression tag	UNP P12259
N	645	HIS	-	expression tag	UNP P12259
N	646	VAL	-	expression tag	UNP P12259
N	647	GLY	-	expression tag	UNP P12259
N	648	THR	-	expression tag	UNP P12259
N	649	TRP	-	expression tag	UNP P12259
N	650	GLU	-	expression tag	UNP P12259
N	651	ASN	-	expression tag	UNP P12259
N	652	LEU	-	expression tag	UNP P12259
N	653	TYR	-	expression tag	UNP P12259
N	654	PHE	-	expression tag	UNP P12259
N	655	GLN	-	expression tag	UNP P12259
N	656	SER	-	expression tag	UNP P12259
O	639	ALA	-	expression tag	UNP P12259
O	640	HIS	-	expression tag	UNP P12259
O	641	HIS	-	expression tag	UNP P12259
O	642	HIS	-	expression tag	UNP P12259
O	643	HIS	-	expression tag	UNP P12259
O	644	HIS	-	expression tag	UNP P12259

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Chain	Residue	Modelled	Actual	Comment	Reference
O	645	HIS	-	expression tag	UNP P12259
O	646	VAL	-	expression tag	UNP P12259
O	647	GLY	-	expression tag	UNP P12259
O	648	THR	-	expression tag	UNP P12259
O	649	TRP	-	expression tag	UNP P12259
O	650	GLU	-	expression tag	UNP P12259
O	651	ASN	-	expression tag	UNP P12259
O	652	LEU	-	expression tag	UNP P12259
O	653	TYR	-	expression tag	UNP P12259
O	654	PHE	-	expression tag	UNP P12259
O	655	GLN	-	expression tag	UNP P12259
O	656	SER	-	expression tag	UNP P12259
P	639	ALA	-	expression tag	UNP P12259
P	640	HIS	-	expression tag	UNP P12259
P	641	HIS	-	expression tag	UNP P12259
P	642	HIS	-	expression tag	UNP P12259
P	643	HIS	-	expression tag	UNP P12259
P	644	HIS	-	expression tag	UNP P12259
P	645	HIS	-	expression tag	UNP P12259
P	646	VAL	-	expression tag	UNP P12259
P	647	GLY	-	expression tag	UNP P12259
P	648	THR	-	expression tag	UNP P12259
P	649	TRP	-	expression tag	UNP P12259
P	650	GLU	-	expression tag	UNP P12259
P	651	ASN	-	expression tag	UNP P12259
P	652	LEU	-	expression tag	UNP P12259
P	653	TYR	-	expression tag	UNP P12259
P	654	PHE	-	expression tag	UNP P12259
P	655	GLN	-	expression tag	UNP P12259
P	656	SER	-	expression tag	UNP P12259

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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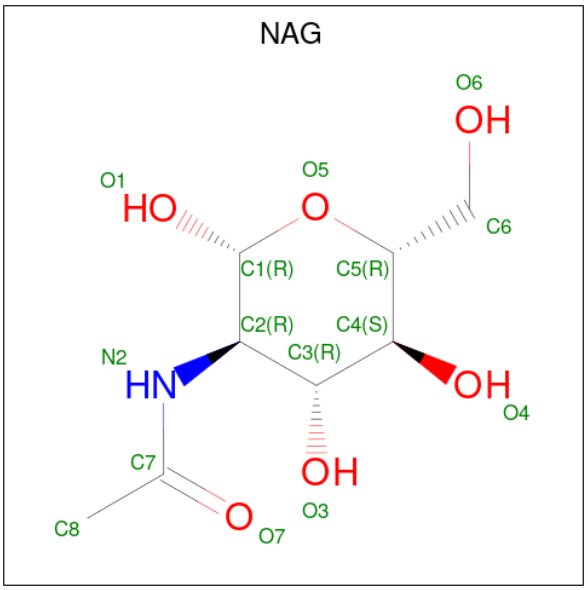
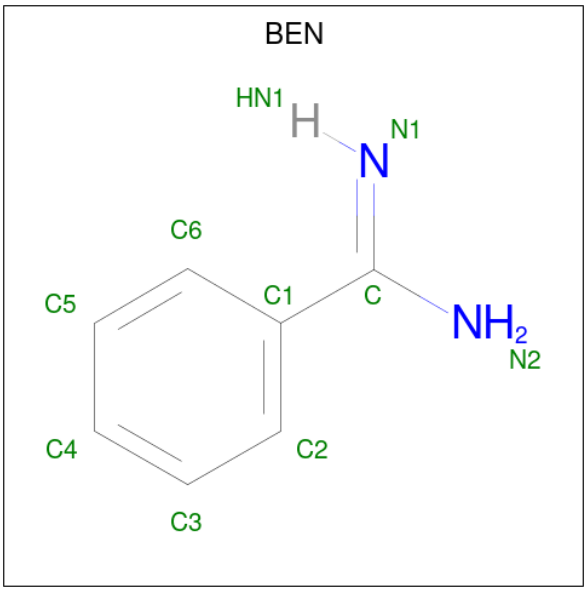
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	J	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is BENZAMIDINE (three-letter code: BEN) (formula: $C_7H_8N_2$).

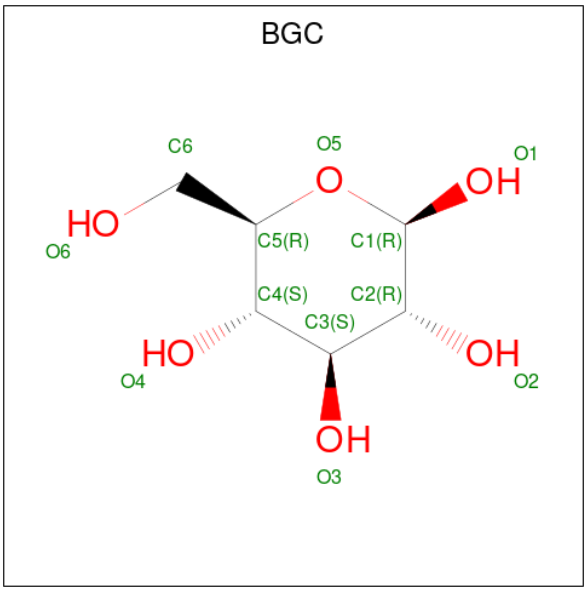


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N 9 7 2	0	0
6	D	1	Total C N 9 7 2	0	0
6	F	1	Total C N 9 7 2	0	0
6	H	1	Total C N 9 7 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Na 2 2	0	0
7	C	1	Total Na 1 1	0	0
7	D	1	Total Na 1 1	0	0
7	F	1	Total Na 1 1	0	0
7	G	1	Total Na 1 1	0	0
7	H	1	Total Na 1 1	0	0

- Molecule 8 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 12 6 6	0	0
8	F	1	Total C O 12 6 6	0	0
8	H	1	Total C O 12 6 6	0	0

- Molecule 9 is water.

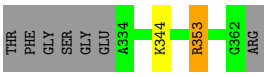
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O 1 1	0	0
9	B	11	Total O 11 11	0	0
9	C	2	Total O 2 2	0	0
9	F	6	Total O 6 6	0	0
9	H	3	Total O 3 3	0	0
9	N	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

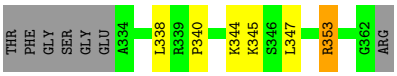
• Molecule 1: HUMAN ALPHA-THROMBIN, LIGHT CHAIN

Chain A:



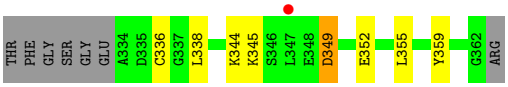
• Molecule 1: HUMAN ALPHA-THROMBIN, LIGHT CHAIN

Chain C:



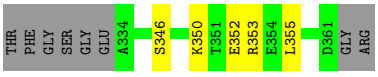
• Molecule 1: HUMAN ALPHA-THROMBIN, LIGHT CHAIN

Chain E:



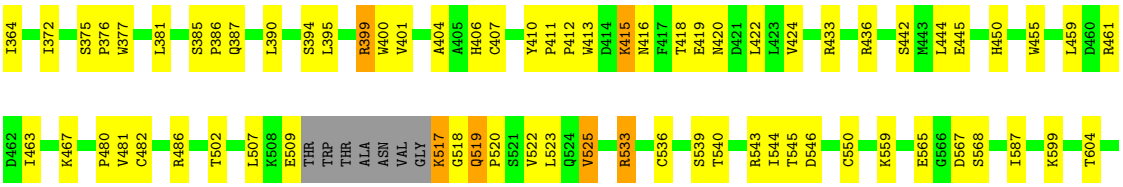
• Molecule 1: HUMAN ALPHA-THROMBIN, LIGHT CHAIN

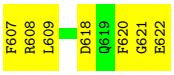
Chain G:



• Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN

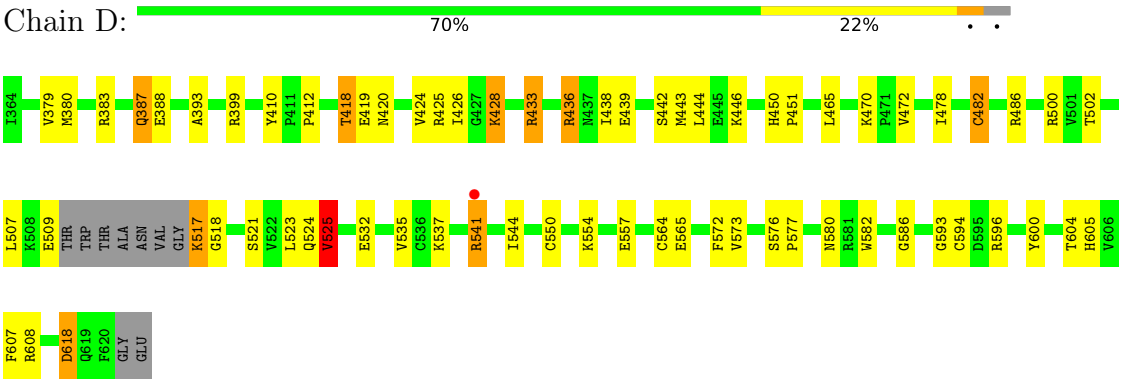
Chain B:





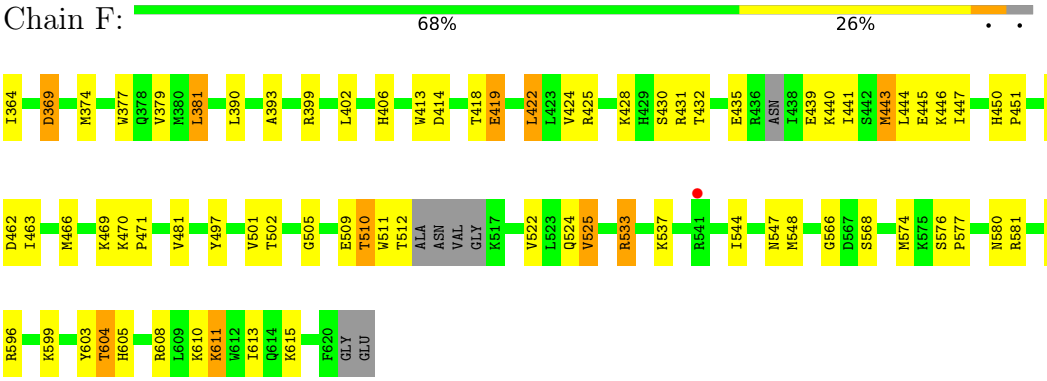
• Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN

Chain D:



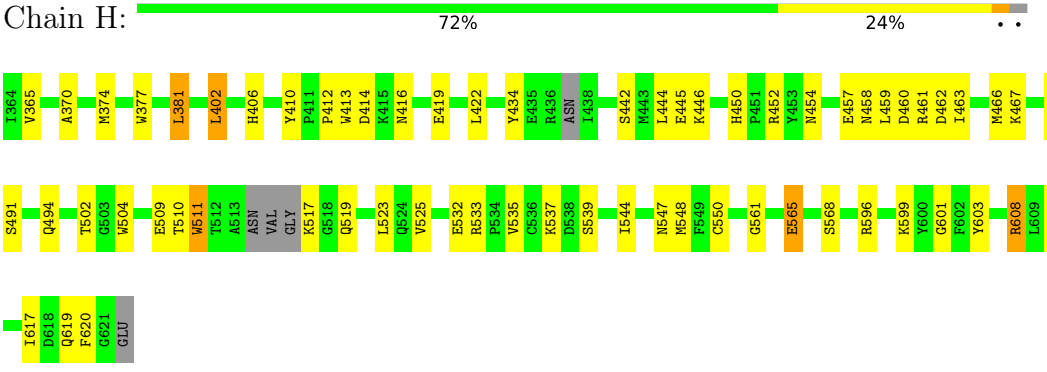
• Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN

Chain F:



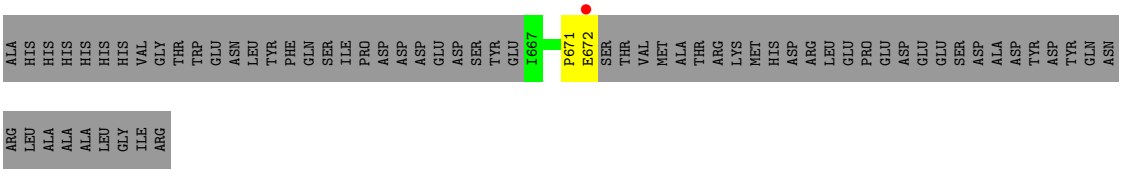
• Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN

Chain H:



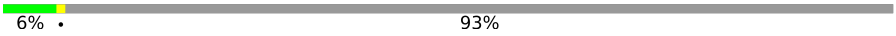
• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER

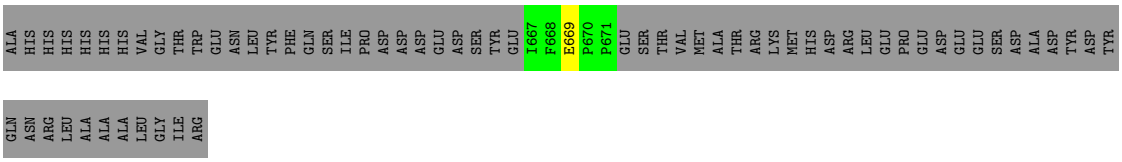
Chain M:



• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER

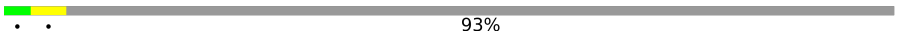
Chain N:

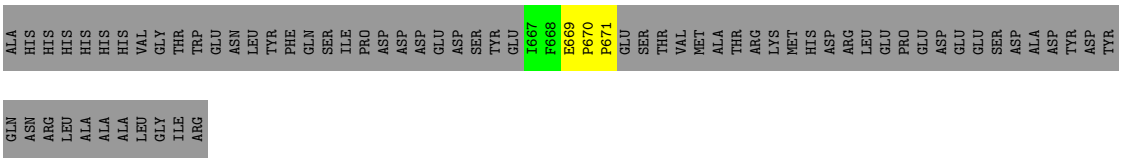




• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER

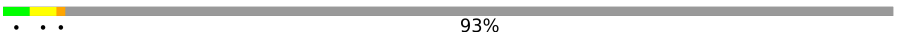
Chain O:

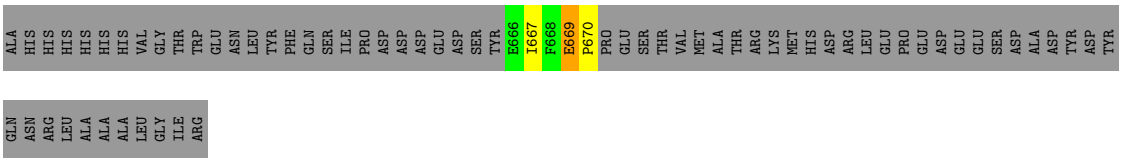




• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER

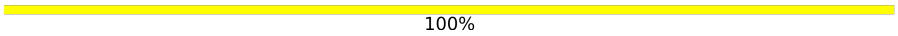
Chain P:





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

Chain I:



• Molecule 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	Depositor
Cell constants a, b, c, α, β, γ	62.24Å 68.23Å 98.97Å 72.57° 84.05° 80.45°	Depositor
Resolution (Å)	61.28 – 2.55 61.28 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.6 (61.28-2.55) 94.6 (61.28-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.279 0.208 , 0.276	Depositor DCC
R_{free} test set	2384 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9477	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0360e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: BGC, NAG, BEN, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.00	0/236	1.01	0/314
1	C	0.85	0/236	0.85	0/314
1	E	0.83	0/236	0.90	0/314
1	G	0.89	0/232	0.97	0/309
2	B	0.86	2/2104 (0.1%)	0.88	0/2838
2	D	0.76	0/2090	0.86	2/2821 (0.1%)
2	F	0.76	0/2100	0.82	0/2836
2	H	0.77	0/2109	0.85	2/2848 (0.1%)
3	M	1.00	0/53	0.85	0/72
3	N	0.92	0/44	0.71	0/60
3	O	0.78	0/44	0.70	0/60
3	P	1.18	0/45	1.27	0/60
All	All	0.80	2/9529 (0.0%)	0.86	4/12846 (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
2	D	0	1
2	F	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	377	TRP	CZ3-CH2	6.19	1.50	1.40
2	B	536	CYS	CB-SG	-5.33	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	525	VAL	CB-CA-C	-6.11	99.80	111.40
2	H	460	ASP	CB-CG-OD1	5.65	123.39	118.30
2	H	402	LEU	CA-CB-CG	5.53	128.01	115.30
2	D	482	CYS	CA-CB-SG	5.30	123.54	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	618	ASP	Peptide
2	F	431	ARG	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	A	234	0	229	1	0
1	C	234	0	229	7	0
1	E	234	0	229	5	0
1	G	230	0	226	3	0
2	B	2045	0	2016	46	0
2	D	2031	0	2006	41	0
2	F	2047	0	2023	53	0
2	H	2056	0	2031	40	0
3	M	51	0	45	0	0
3	N	42	0	39	1	0
3	O	42	0	39	3	0
3	P	44	0	38	9	0
4	I	28	0	25	0	0
4	J	28	0	25	2	0
5	B	14	0	13	2	0
5	D	14	0	13	0	0
6	B	9	0	7	0	0
6	D	9	0	7	0	0
6	F	9	0	7	0	0
6	H	9	0	7	1	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	B	12	0	12	1	0
8	F	12	0	12	0	0
8	H	12	0	12	1	0
9	A	1	0	0	0	0
9	B	11	0	0	0	0
9	C	2	0	0	0	0
9	F	6	0	0	0	0
9	H	3	0	0	0	0
9	N	1	0	0	2	0
All	All	9477	0	9290	202	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 11.

The worst 5 of 202 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:502:THR:HG22	2:H:525:VAL:HG22	1.31	1.07
2:H:565:GLU:OE1	6:H:2001:BEN:H3	1.73	0.88
2:F:502:THR:HG22	2:F:525:VAL:HG13	1.55	0.87
2:D:541:ARG:HG3	2:D:541:ARG:HH21	1.41	0.83
2:F:502:THR:HG22	2:F:525:VAL:CG1	2.08	0.83

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	A	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
1	C	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
1	E	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
1	G	26/36 (72%)	22 (85%)	4 (15%)	0	100	100
2	B	249/259 (96%)	236 (95%)	11 (4%)	2 (1%)	19	27
2	D	247/259 (95%)	231 (94%)	15 (6%)	1 (0%)	34	46
2	F	246/259 (95%)	233 (95%)	10 (4%)	3 (1%)	13	17
2	H	248/259 (96%)	229 (92%)	16 (6%)	3 (1%)	13	17
3	M	4/71 (6%)	3 (75%)	0	1 (25%)	0	0
3	N	3/71 (4%)	3 (100%)	0	0	100	100
3	O	3/71 (4%)	2 (67%)	1 (33%)	0	100	100
3	P	3/71 (4%)	2 (67%)	0	1 (33%)	0	0
All	All	1110/1464 (76%)	1036 (93%)	63 (6%)	11 (1%)	15	22

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	669	GLU
2	F	458	ASN
2	H	511	TRP
2	H	608	ARG
3	M	671	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	26/31 (84%)	24 (92%)	2 (8%)	13	16
1	C	26/31 (84%)	25 (96%)	1 (4%)	33	45
1	E	26/31 (84%)	24 (92%)	2 (8%)	13	16
1	G	26/31 (84%)	25 (96%)	1 (4%)	33	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	221/225 (98%)	206 (93%)	15 (7%)	16 20
2	D	220/225 (98%)	196 (89%)	24 (11%)	6 6
2	F	221/225 (98%)	205 (93%)	16 (7%)	14 18
2	H	221/225 (98%)	211 (96%)	10 (4%)	27 37
3	M	6/63 (10%)	5 (83%)	1 (17%)	2 2
3	N	5/63 (8%)	5 (100%)	0	100 100
3	O	5/63 (8%)	5 (100%)	0	100 100
3	P	5/63 (8%)	4 (80%)	1 (20%)	1 1
All	All	1008/1276 (79%)	935 (93%)	73 (7%)	14 18

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	604	THR
3	M	672	GLU
2	F	615	LYS
2	H	517	LYS
2	D	433	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\#\|Z\| > 2$
4	NAG	I	1	2,4	14,14,15	0.58	0	17,19,21	2.45	5 (29%)
4	NAG	I	2	4	14,14,15	1.24	1 (7%)	17,19,21	1.20	2 (11%)
4	NAG	J	1	2,4	14,14,15	0.63	0	17,19,21	2.81	7 (41%)
4	NAG	J	2	4	14,14,15	0.65	0	17,19,21	0.96	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	2,4	-	5/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	O5-C1	-4.20	1.37	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1	NAG	C1-O5-C5	6.44	120.92	112.19
4	J	1	NAG	C2-N2-C7	6.35	131.95	122.90
4	I	1	NAG	C2-N2-C7	5.63	130.91	122.90
4	I	1	NAG	C1-O5-C5	5.44	119.56	112.19
4	J	1	NAG	C8-C7-N2	3.79	122.52	116.10

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

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

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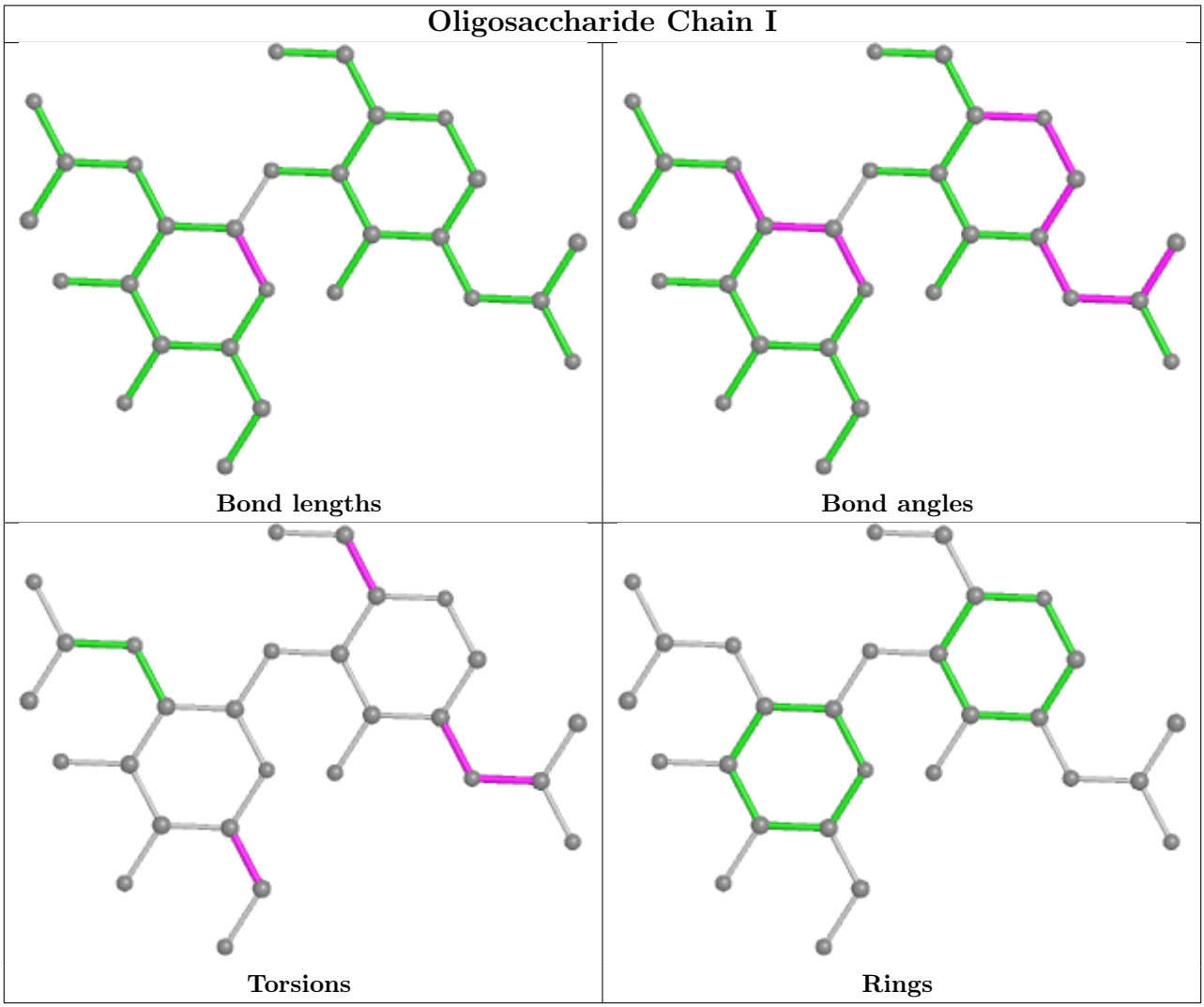
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2

There are no ring outliers.

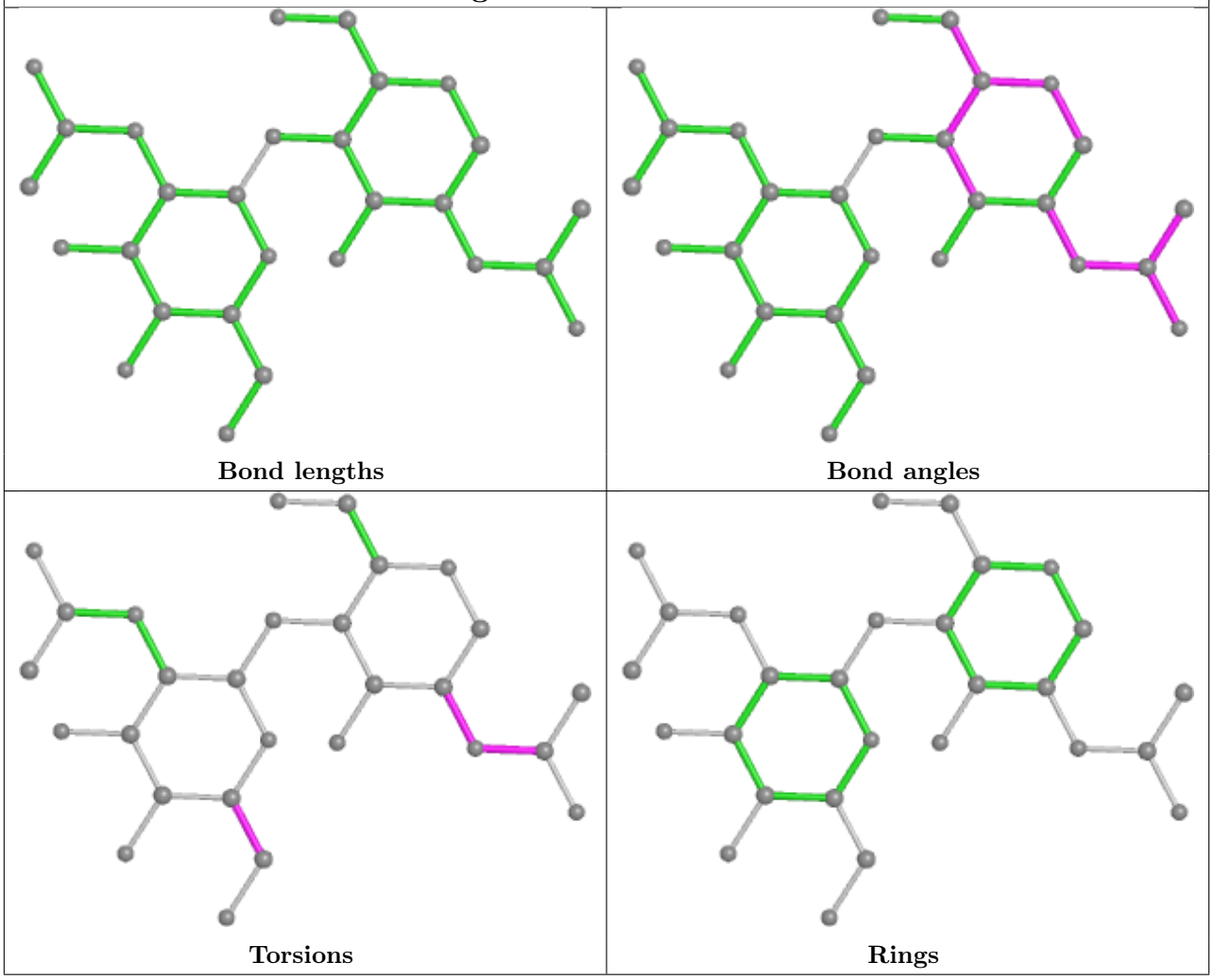
2 monomers are involved in 2 short contacts:

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



5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BGC	H	4201	-	12,12,12	0.82	0	17,17,17	2.98	7 (41%)
6	BEN	H	2001	-	9,9,9	1.29	1 (11%)	7,11,11	1.58	1 (14%)
8	BGC	B	4202	-	12,12,12	0.81	0	17,17,17	1.80	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BEN	B	2001	-	9,9,9	1.60	1 (11%)	7,11,11	0.82	0
5	NAG	D	1416	2	14,14,15	0.70	0	17,19,21	2.60	6 (35%)
5	NAG	B	1416	2	14,14,15	0.69	0	17,19,21	1.76	4 (23%)
8	BGC	F	4203	-	12,12,12	0.95	0	17,17,17	2.90	9 (52%)
6	BEN	F	2001	-	9,9,9	1.29	1 (11%)	7,11,11	0.67	0
6	BEN	D	2001	-	9,9,9	1.75	1 (11%)	7,11,11	1.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BGC	H	4201	-	-	1/2/22/22	0/1/1/1
6	BEN	H	2001	-	-	4/4/4/4	0/1/1/1
8	BGC	B	4202	-	-	2/2/22/22	0/1/1/1
6	BEN	B	2001	-	-	4/4/4/4	0/1/1/1
5	NAG	D	1416	2	-	5/6/23/26	0/1/1/1
5	NAG	B	1416	2	-	3/6/23/26	0/1/1/1
8	BGC	F	4203	-	-	1/2/22/22	0/1/1/1
6	BEN	F	2001	-	-	4/4/4/4	0/1/1/1
6	BEN	D	2001	-	-	4/4/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2001	BEN	C1-C	-4.42	1.39	1.47
6	B	2001	BEN	C1-C	-4.23	1.39	1.47
6	H	2001	BEN	C1-C	-3.34	1.41	1.47
6	F	2001	BEN	C1-C	-2.68	1.42	1.47

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	4203	BGC	C4-C3-C2	-7.36	97.97	110.82
5	D	1416	NAG	C2-N2-C7	7.31	133.31	122.90
8	H	4201	BGC	C4-C3-C2	-6.67	99.19	110.82
8	H	4201	BGC	C1-O5-C5	6.37	125.68	113.66
8	F	4203	BGC	O3-C3-C4	4.22	120.11	110.35

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	4202	BGC	O5-C5-C6-O6
8	B	4202	BGC	C4-C5-C6-O6
5	D	1416	NAG	C4-C5-C6-O6
5	B	1416	NAG	C8-C7-N2-C2
5	B	1416	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	4201	BGC	1	0
6	H	2001	BEN	1	0
8	B	4202	BGC	1	0
5	B	1416	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	29/36 (80%)	-0.16	0 100 100	32, 43, 61, 65	0
1	C	29/36 (80%)	-0.09	0 100 100	34, 50, 68, 79	0
1	E	29/36 (80%)	0.09	1 (3%) 45 52	37, 57, 77, 88	0
1	G	28/36 (77%)	-0.10	0 100 100	33, 50, 76, 85	0
2	B	252/259 (97%)	-0.21	0 100 100	24, 44, 70, 91	0
2	D	250/259 (96%)	-0.04	1 (0%) 92 96	28, 56, 97, 132	0
2	F	252/259 (97%)	-0.12	1 (0%) 92 96	31, 54, 79, 90	0
2	H	254/259 (98%)	-0.19	0 100 100	25, 49, 79, 90	0
3	M	6/71 (8%)	0.26	1 (16%) 1 1	48, 54, 58, 62	1 (16%)
3	N	5/71 (7%)	-0.19	0 100 100	51, 52, 54, 57	0
3	O	5/71 (7%)	-0.11	0 100 100	60, 61, 63, 64	0
3	P	5/71 (7%)	0.11	0 100 100	63, 64, 66, 69	0
All	All	1144/1464 (78%)	-0.13	4 (0%) 94 96	24, 51, 82, 132	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	672	GLU	2.2
1	E	347	LEU	2.2
2	D	541	ARG	2.1
2	F	541	ARG	2.1

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 (i)

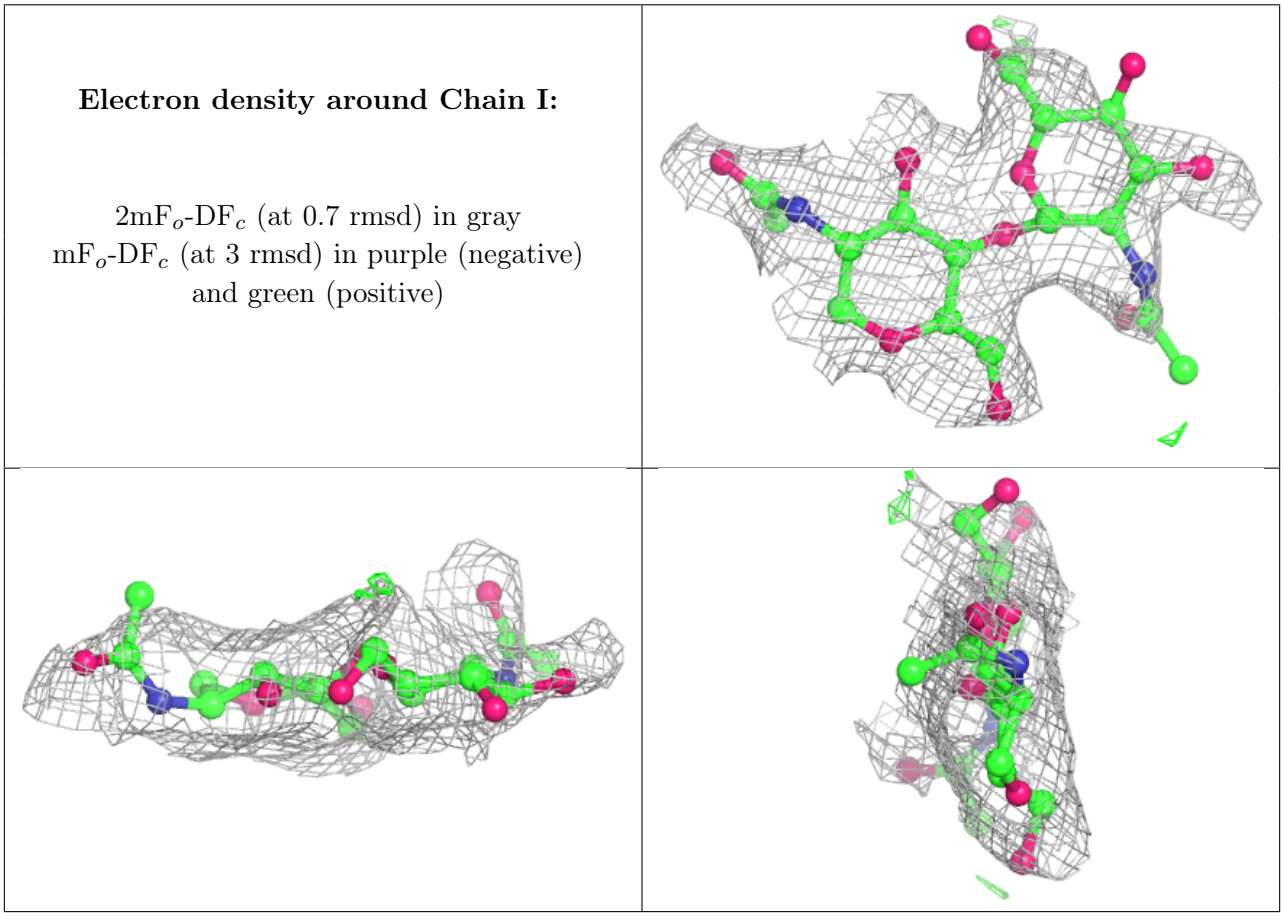
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NAG	J	2	14/15	0.67	0.23	135,142,153,158	0
4	NAG	I	2	14/15	0.78	0.24	129,135,145,148	0
4	NAG	J	1	14/15	0.88	0.16	100,109,122,126	0
4	NAG	I	1	14/15	0.89	0.12	98,106,116,121	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.

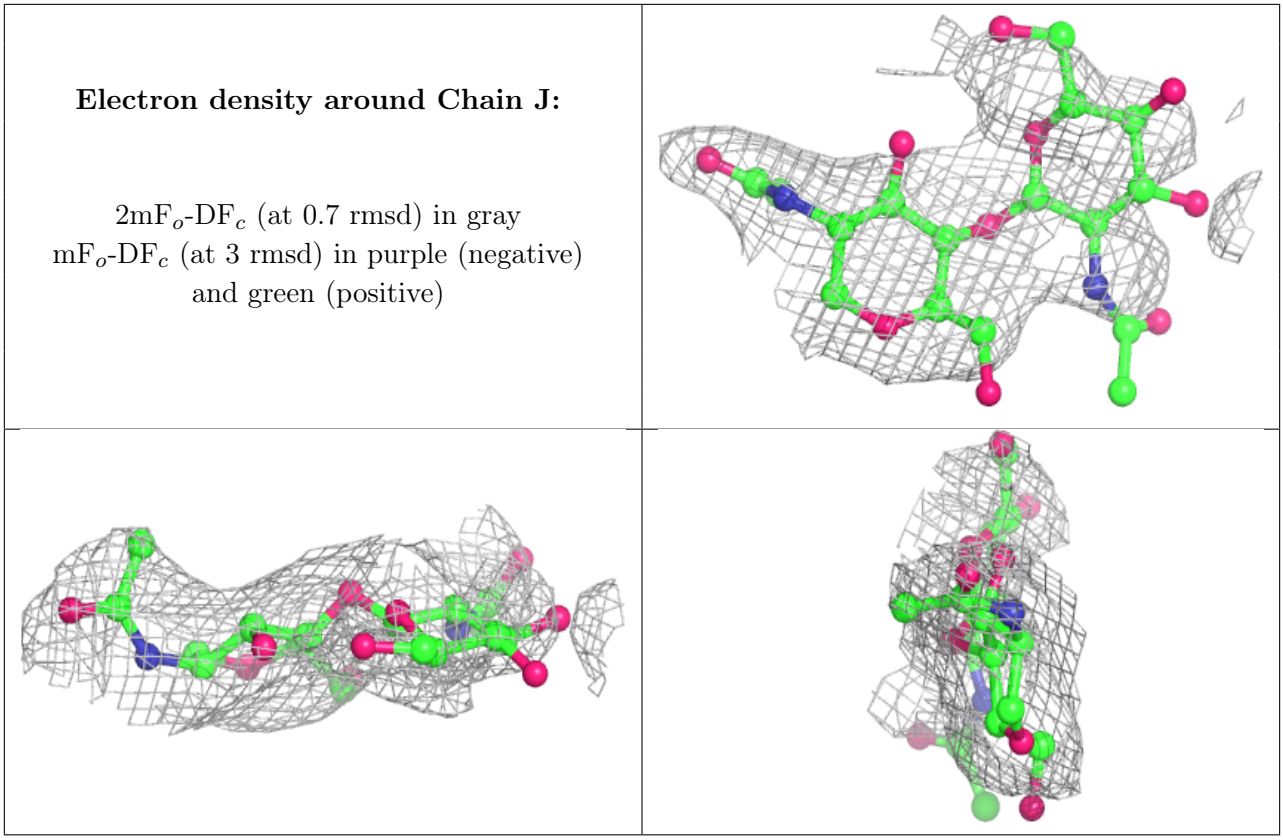
Electron density around Chain I:

$2mF_o$-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
5	NAG	B	1416	14/15	0.84	0.17	92,101,110,112	0
8	BGC	B	4202	12/12	0.84	0.25	136,139,143,144	0
8	BGC	F	4203	12/12	0.84	0.27	93,98,109,111	0
5	NAG	D	1416	14/15	0.87	0.24	127,133,141,147	0
7	NA	B	1500	1/1	0.88	0.17	49,49,49,49	0
7	NA	D	1500	1/1	0.89	0.09	28,28,28,28	0
7	NA	C	3200	1/1	0.90	0.11	65,65,65,65	0
8	BGC	H	4201	12/12	0.90	0.20	77,84,88,92	0
7	NA	G	1501	1/1	0.92	0.09	50,50,50,50	0
7	NA	H	1500	1/1	0.93	0.13	48,48,48,48	0
7	NA	F	1500	1/1	0.94	0.08	42,42,42,42	0
6	BEN	D	2001	9/9	0.97	0.16	42,45,47,48	0
6	BEN	F	2001	9/9	0.97	0.18	41,43,44,45	0
6	BEN	B	2001	9/9	0.97	0.16	38,41,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NA	B	1501	1/1	0.97	0.28	50,50,50,50	0
6	BEN	H	2001	9/9	0.98	0.17	33,36,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.