



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 03:34 PM EST

PDB ID : 1LWU
Title : Crystal structure of fragment D from lamprey fibrinogen complexed with the peptide Gly-His-Arg-Pro-amide
Authors : Yang, Z.; Spraggon, G.; Pandi, L.; Everse, S.J.; Riley, M.; Doolittle, R.F.
Deposited on : 2002-06-03
Resolution : 2.80 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

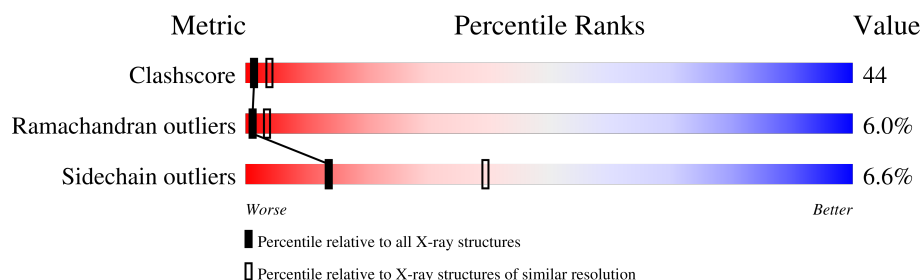
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)


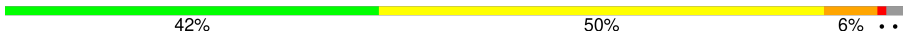



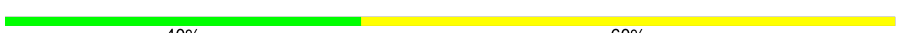



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	25% 48% 9% • 17%
1	D	119	27% 45% 11% • 17%
1	G	119	25% 50% 8% • 17%
1	J	119	27% 45% 10% • 17%
2	B	323	45% 44% 8% ••
2	E	323	45% 44% 8% ••
2	H	323	41% 49% 7% ••
2	K	323	43% 47% 7% ••

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Mol	Chain	Length	Quality of chain
3	C	323	
3	F	323	
3	I	323	
3	L	323	
4	M	5	
4	N	5	
4	O	5	
4	P	5	
5	Q	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BMA	E	502	-	-	X	-
11	GAL	H	507	-	-	X	-
6	NDG	D	301	-	-	X	-
6	NDG	H	506	-	-	X	-
6	NDG	K	501	-	-	X	-
6	NDG	N	101	-	-	X	-
7	MAN	E	503	-	-	X	-
7	MAN	H	503	-	-	X	-
7	MAN	H	505	-	-	X	-
7	MAN	P	101	-	-	X	-
9	NAG	C	501	-	-	X	-
9	NAG	C	502	-	-	X	-
9	NAG	E	501	-	-	X	-
9	NAG	F	502	-	-	X	-
9	NAG	I	502	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24360 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 Fibrinogen alpha-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			833	523	155	152	3			
1	D	99	Total	C	N	O	S	0	0	0
			833	523	155	152	3			
1	G	99	Total	C	N	O	S	0	0	0
			833	523	155	152	3			
1	J	99	Total	C	N	O	S	0	0	0
			833	523	155	152	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	THR	conflict	UNP P02674
D	153	ALA	THR	conflict	UNP P02674
G	153	ALA	THR	conflict	UNP P02674
J	153	ALA	THR	conflict	UNP P02674

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	315	Total	C	N	O	S	0	0	0
			2535	1579	453	482	21			
2	E	315	Total	C	N	O	S	0	0	0
			2535	1579	453	482	21			
2	H	315	Total	C	N	O	S	0	0	0
			2535	1579	453	482	21			
2	K	315	Total	C	N	O	S	0	0	0
			2535	1579	453	482	21			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	317	Total	C	N	O	S	0	0	0
			2599	1642	451	493	13			
3	F	317	Total	C	N	O	S	0	0	0
			2599	1642	451	493	13			
3	I	313	Total	C	N	O	S	0	0	0
			2568	1625	444	486	13			
3	L	313	Total	C	N	O	S	0	0	0
			2568	1625	444	486	13			

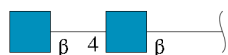
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	PRO	SER	conflict	UNP P04115
F	137	PRO	SER	conflict	UNP P04115
I	137	PRO	SER	conflict	UNP P04115
L	137	PRO	SER	conflict	UNP P04115

- Molecule 4 is a protein called Peptide Ligand Gly-His-Arg-Pro-NH₂.

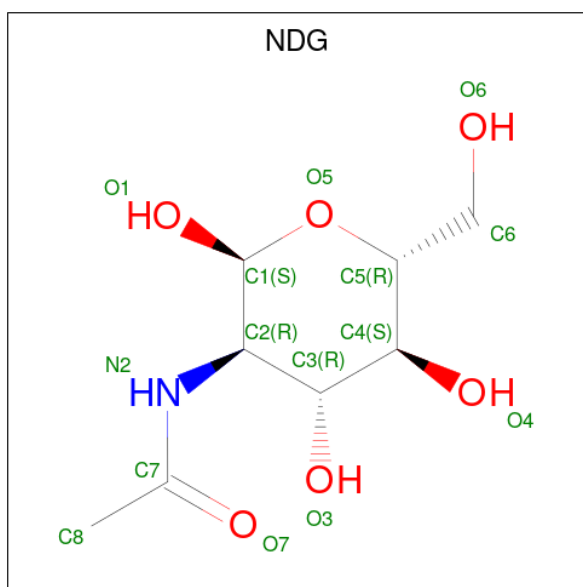
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	5	Total	C	N	O	0	0	1
			33	19	10	4			
4	N	5	Total	C	N	O	0	0	1
			33	19	10	4			
4	O	5	Total	C	N	O	0	0	1
			33	19	10	4			
4	P	5	Total	C	N	O	0	0	1
			33	19	10	4			

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



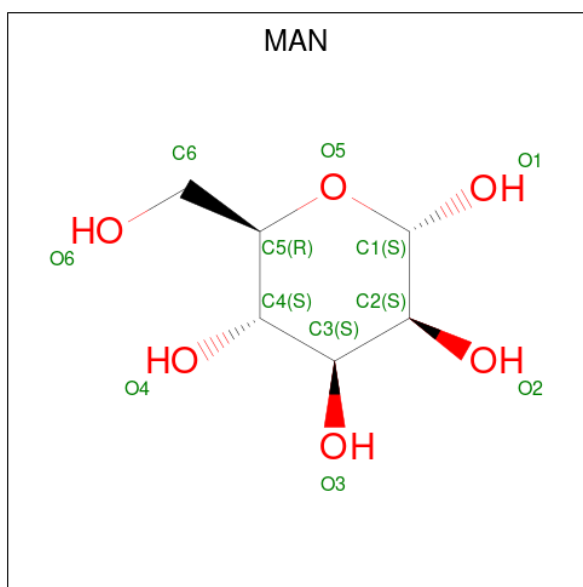
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			15	8	1	6		
6	D	1	Total	C	N	O	0	0
			15	8	1	6		
6	H	1	Total	C	N	O	0	0
			15	8	1	6		
6	H	1	Total	C	N	O	0	0
			15	8	1	6		
6	H	1	Total	C	N	O	0	0
			15	8	1	6		
6	K	1	Total	C	N	O	0	0
			15	8	1	6		
6	M	1	Total	C	N	O	0	0
			15	8	1	6		
6	N	1	Total	C	N	O	0	0
			15	8	1	6		
6	O	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			12	6	6		
7	C	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			12	6	6		
7	F	1	Total	C	O	0	0
			11	6	5		
7	H	1	Total	C	O	0	0
			12	6	6		
7	H	1	Total	C	O	0	0
			12	6	6		
7	J	1	Total	C	O	0	0
			11	6	5		
7	L	1	Total	C	O	0	0
			11	6	5		
7	N	1	Total	C	O	0	0
			12	6	6		
7	P	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

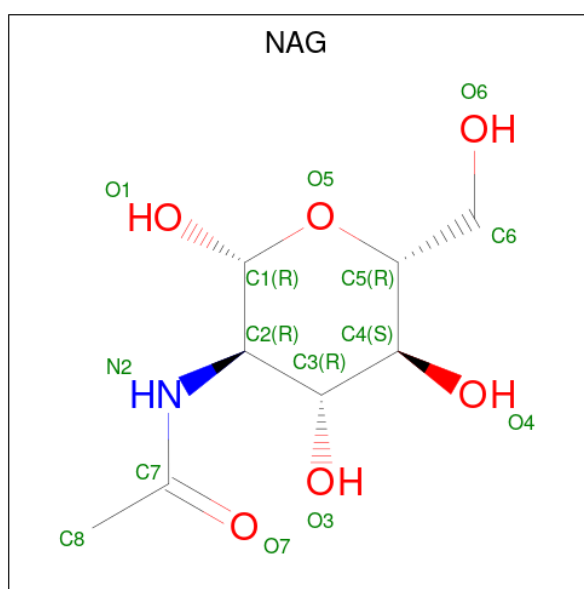
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Ca	0	0
			1	1		
8	F	1	Total	Ca	0	0
			1	1		
8	H	1	Total	Ca	0	0
			1	1		
8	I	1	Total	Ca	0	0
			1	1		
8	K	1	Total	Ca	0	0
			1	1		
8	L	1	Total	Ca	0	0
			1	1		

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



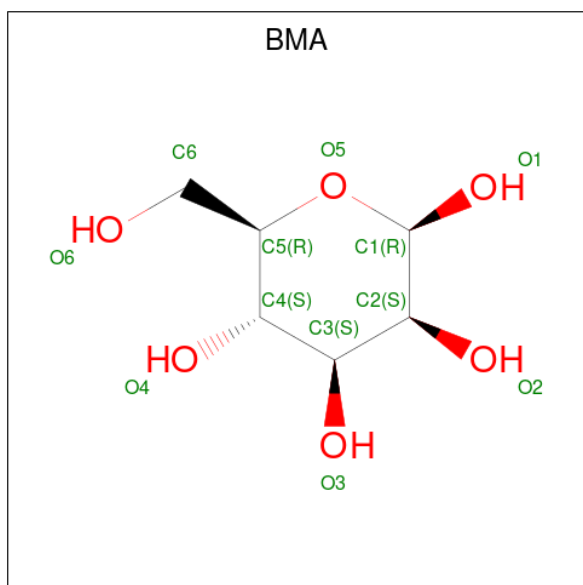
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	E	1	Total	C	N	O	0	0
			15	8	1	6		
9	F	1	Total	C	N	O	0	0
			14	8	1	5		
9	F	1	Total	C	N	O	0	0
			14	8	1	5		

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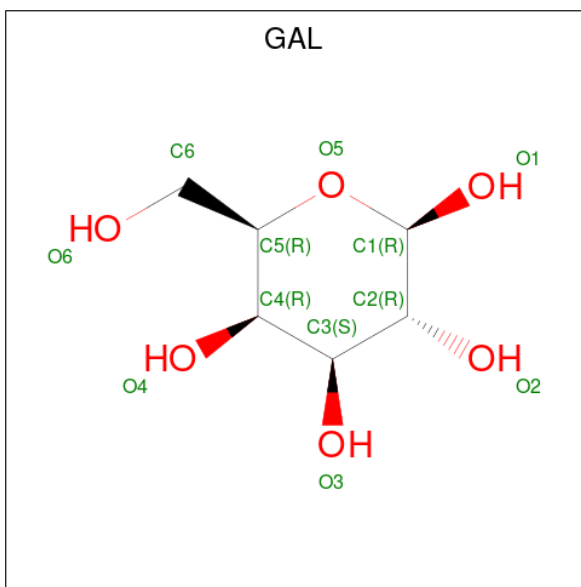
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	1	Total	C	N	O	0	0
			14	8	1	5		
9	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			12	6	6		
10	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 11 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



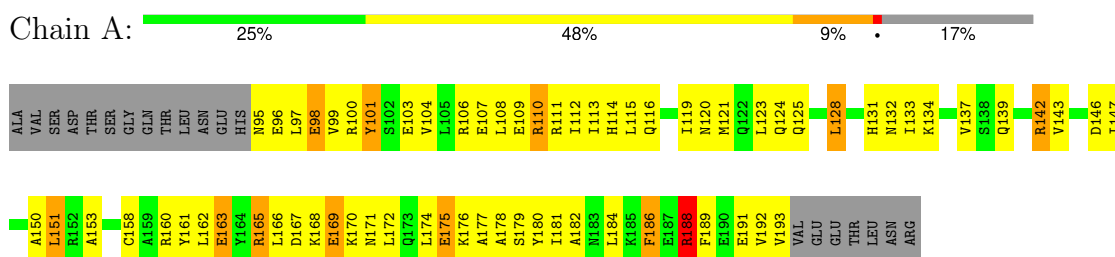
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	O	0	0
			12	6	6		

3 Residue-property plots

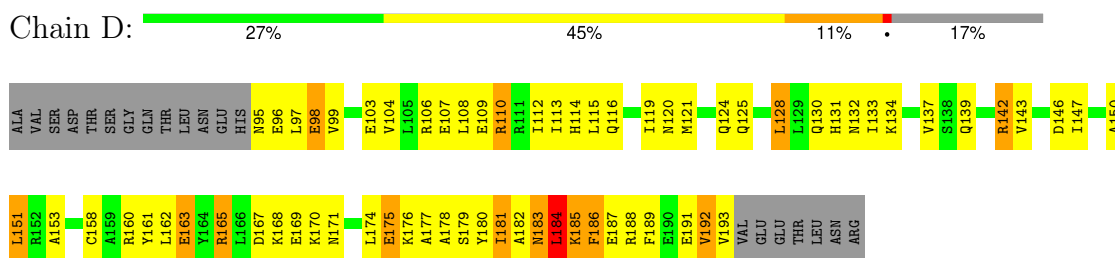
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

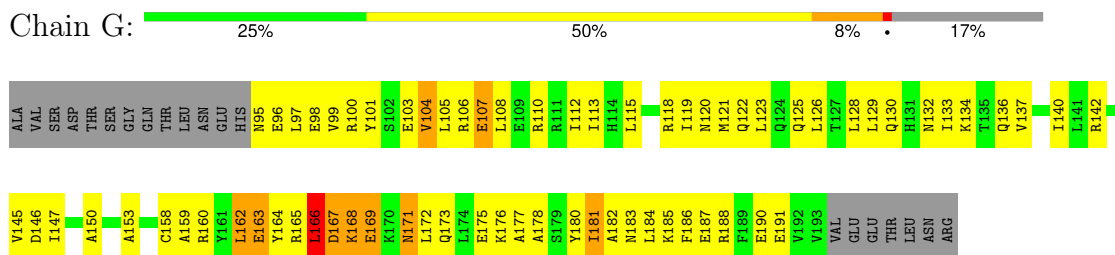
• Molecule 1: Fibrinogen alpha-1 chain



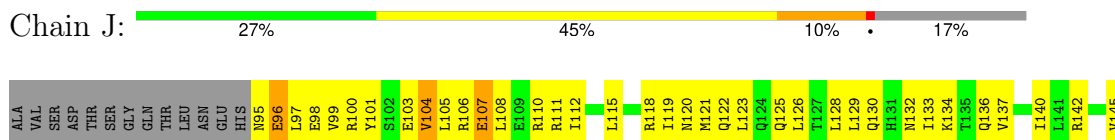
• Molecule 1: Fibrinogen alpha-1 chain

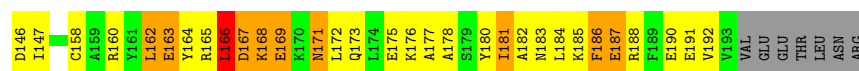


• Molecule 1: Fibrinogen alpha-1 chain



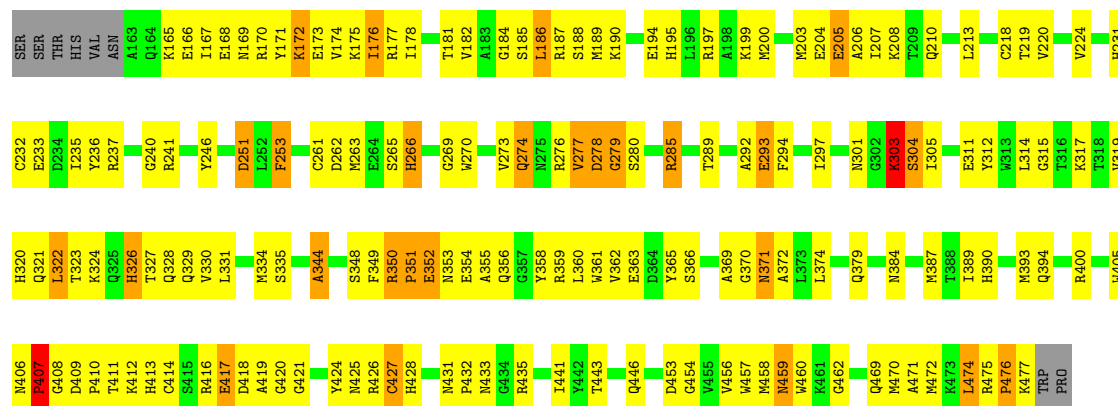
• Molecule 1: Fibrinogen alpha-1 chain





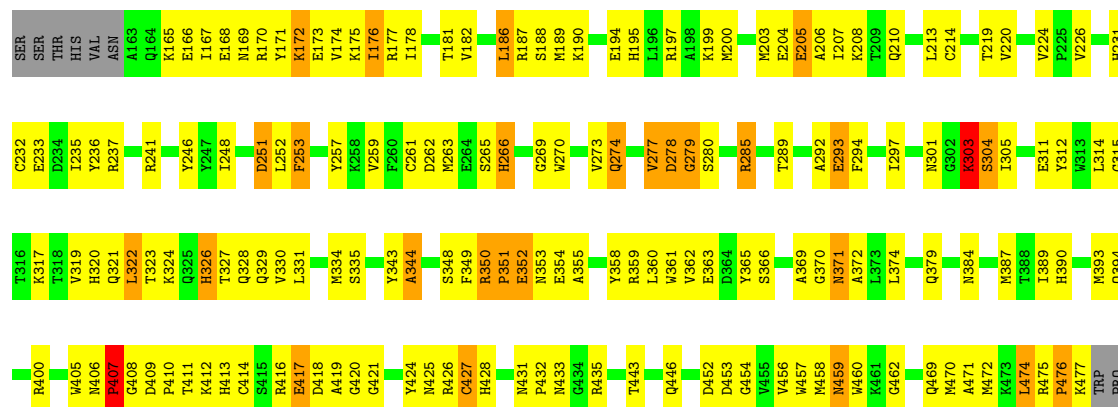
• Molecule 2: Fibrinogen beta chain

Chain B: 45% 44% 8% ..



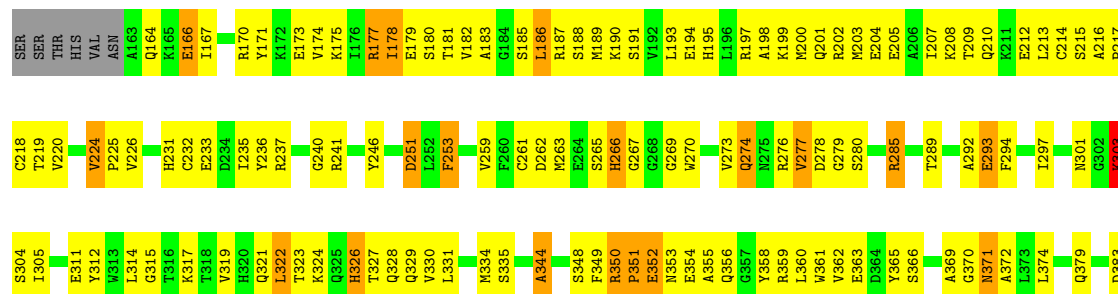
• Molecule 2: Fibrinogen beta chain

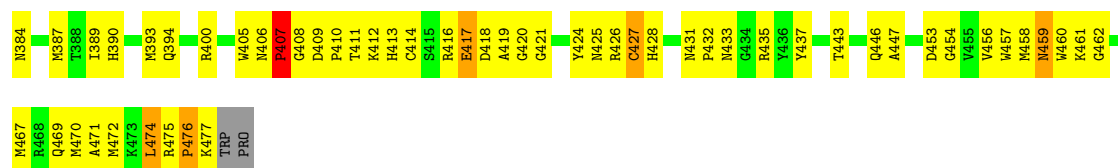
Chain E: 45% 44% 8% ..



• Molecule 2: Fibrinogen beta chain

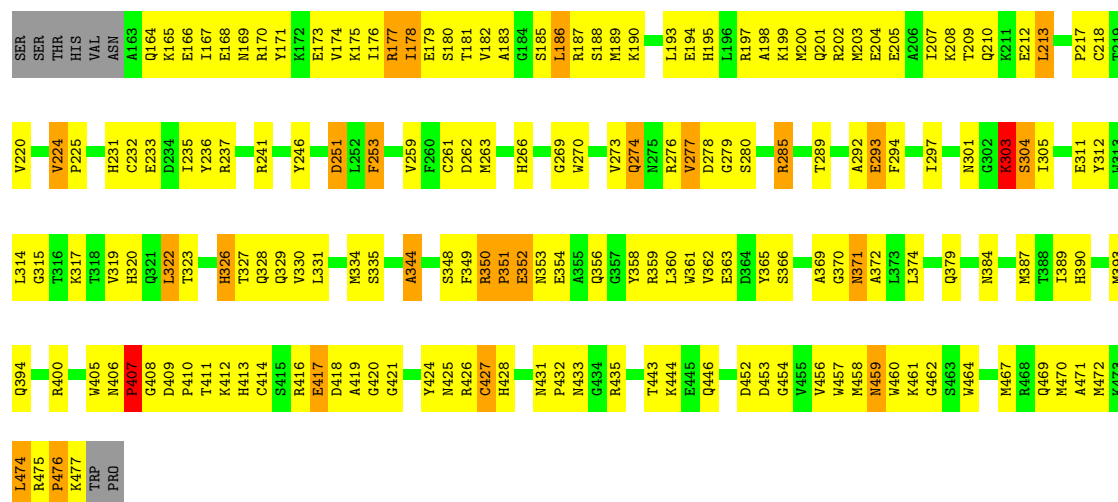
Chain H: 41% 49% 7% ..





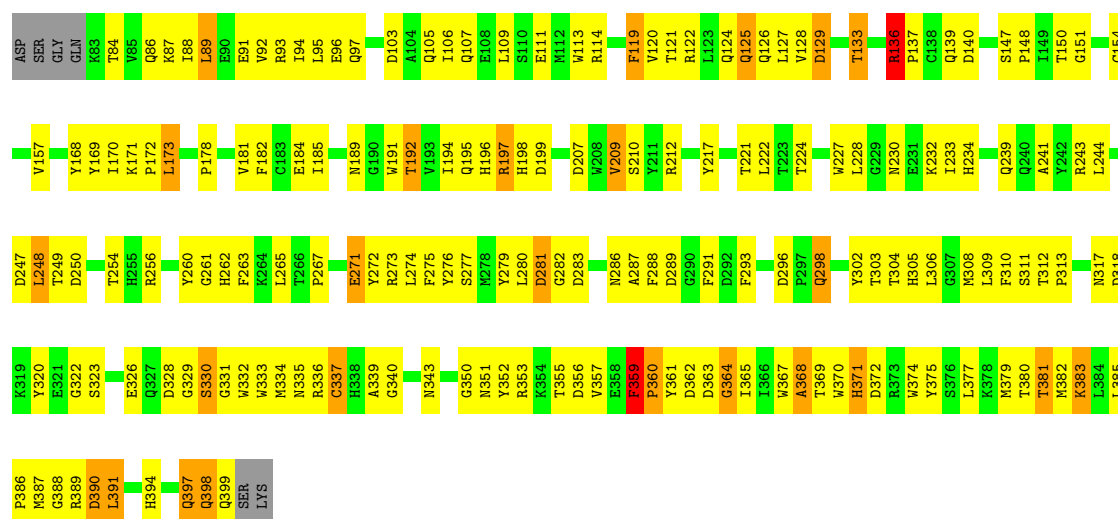
• Molecule 2: Fibrinogen beta chain

Chain K: 43% 47% 7% ..



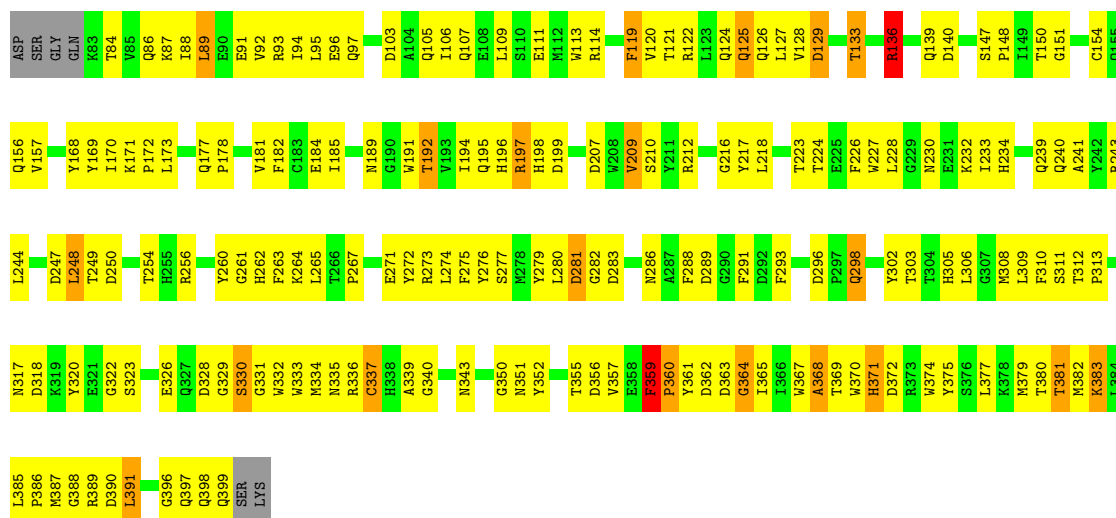
• Molecule 3: Fibrinogen gamma chain

Chain C: 42% 47% 8% ..

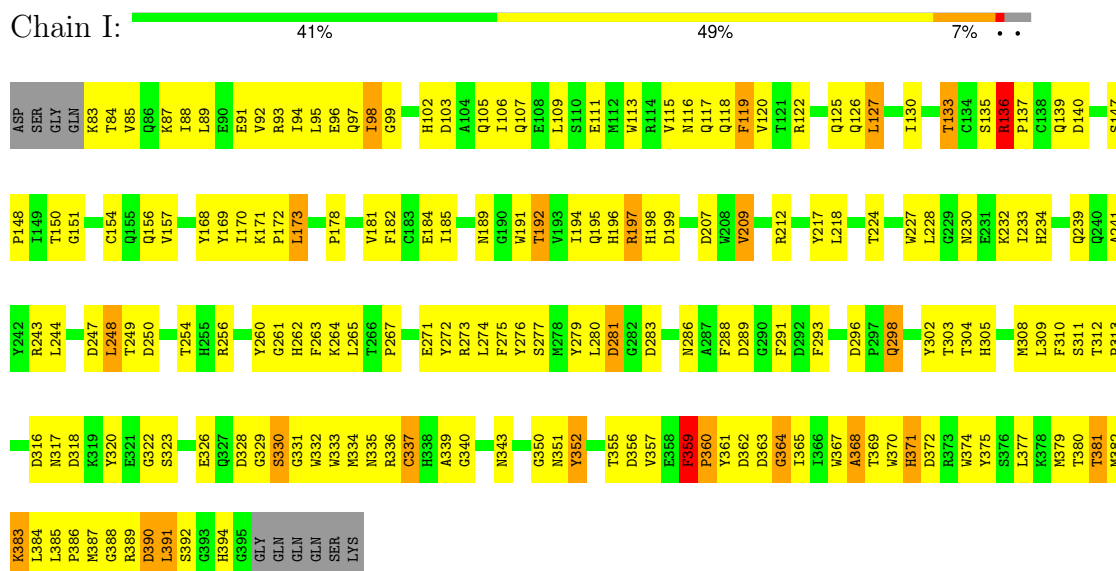


• Molecule 3: Fibrinogen gamma chain

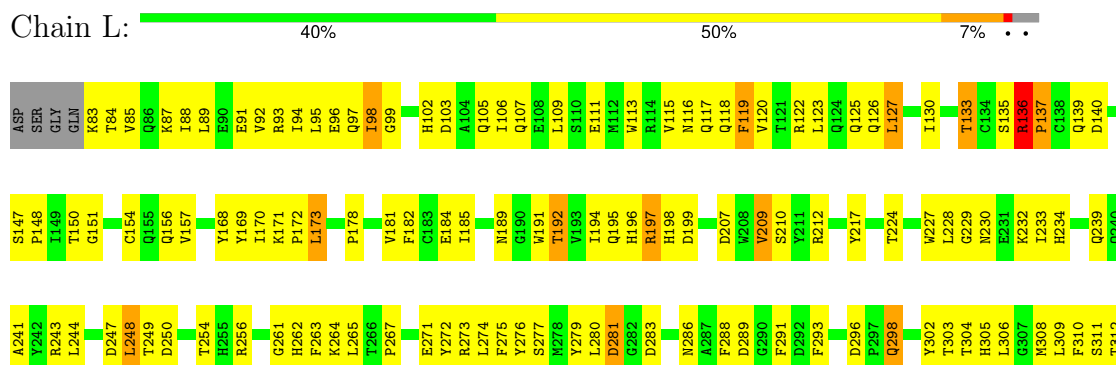
Chain F: 42% 50% 6% ..

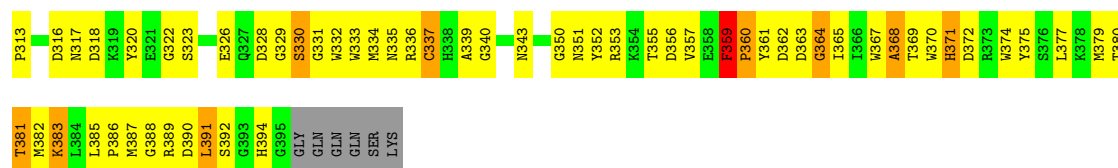


• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain





- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2

Chain M: 20% 80%



- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2

Chain N: 40% 60%



- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2

Chain O: 60% 40%



- Molecule 4: Peptide Ligand Gly-His-Arg-Pro-NH2

Chain P: 60% 40%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 100%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.73Å 47.65Å 244.65Å 88.81° 97.23° 86.17°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	87.9 (20.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24360	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, GAL, CA, NAG, NDG, MAN, 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	A	0.38	0/840	0.66	0/1126
1	D	0.36	0/840	0.67	0/1126
1	G	0.35	0/840	0.58	0/1126
1	J	0.35	0/840	0.59	0/1126
2	B	0.43	0/2602	0.69	1/3517 (0.0%)
2	E	0.46	0/2602	0.71	1/3517 (0.0%)
2	H	0.42	0/2602	0.69	1/3517 (0.0%)
2	K	0.43	0/2602	0.69	1/3517 (0.0%)
3	C	0.39	0/2671	0.64	2/3616 (0.1%)
3	F	0.39	0/2671	0.62	1/3616 (0.0%)
3	I	0.38	0/2640	0.64	1/3575 (0.0%)
3	L	0.39	0/2640	0.64	2/3575 (0.1%)
4	M	0.51	0/33	0.55	0/43
4	N	0.57	0/33	0.78	0/43
4	O	0.46	0/33	0.61	0/43
4	P	0.48	0/33	0.58	0/43
All	All	0.41	0/24522	0.66	10/33126 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	136	ARG	C-N-CD	-8.41	102.10	120.60
3	F	136	ARG	C-N-CD	-6.86	105.50	120.60
3	I	136	ARG	C-N-CD	-6.69	105.89	120.60
2	E	421	GLY	N-CA-C	-5.84	98.49	113.10
3	L	136	ARG	C-N-CD	-5.79	107.87	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	833	0	864	126	0
1	D	833	0	864	94	0
1	G	833	0	864	114	0
1	J	833	0	864	137	0
2	B	2535	0	2364	206	0
2	E	2535	0	2364	202	0
2	H	2535	0	2364	248	0
2	K	2535	0	2364	230	0
3	C	2599	0	2427	209	0
3	F	2599	0	2428	205	0
3	I	2568	0	2401	226	0
3	L	2568	0	2401	232	0
4	M	33	0	32	7	0
4	N	33	0	32	5	0
4	O	33	0	32	4	0
4	P	33	0	32	4	0
5	Q	28	0	26	5	0
6	B	15	0	12	3	0
6	D	15	0	12	9	0
6	H	45	0	36	31	0
6	K	15	0	12	7	0
6	M	15	0	12	5	0
6	N	15	0	12	25	0
6	O	15	0	12	2	0
7	B	12	0	12	3	0
7	C	11	0	10	2	0
7	E	12	0	12	12	0
7	F	11	0	10	5	0
7	H	24	0	24	27	0
7	J	11	0	10	2	0
7	L	11	0	10	2	0
7	N	12	0	12	1	0
7	P	12	0	12	8	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
9	C	28	0	26	9	0
9	E	15	0	15	9	0
9	F	28	0	26	11	0
9	I	28	0	26	8	0
10	E	12	0	12	23	0
10	H	12	0	12	1	0
11	H	12	0	12	10	0
All	All	24360	0	23072	2079	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 44.

The worst 5 of 2079 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)
10:E:502:BMA:C5	6:N:101:NDG:H8C1	1.68	1.21
9:I:502:NAG:O3	7:J:301:MAN:C1	1.91	1.18
1:A:188:ARG:H	1:A:188:ARG:HD2	1.07	1.18
7:H:503:MAN:O6	7:H:505:MAN:H62	1.39	1.18
10:E:502:BMA:H62	7:E:503:MAN:H62	1.16	1.15

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	97/119 (82%)	74 (76%)	17 (18%)	6 (6%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	97/119 (82%)	75 (77%)	13 (13%)	9 (9%)	0	1
1	G	97/119 (82%)	75 (77%)	13 (13%)	9 (9%)	0	1
1	J	97/119 (82%)	74 (76%)	14 (14%)	9 (9%)	0	1
2	B	313/323 (97%)	265 (85%)	29 (9%)	19 (6%)	1	3
2	E	313/323 (97%)	268 (86%)	26 (8%)	19 (6%)	1	3
2	H	313/323 (97%)	260 (83%)	35 (11%)	18 (6%)	1	4
2	K	313/323 (97%)	261 (83%)	32 (10%)	20 (6%)	1	3
3	C	315/323 (98%)	259 (82%)	38 (12%)	18 (6%)	1	4
3	F	315/323 (98%)	259 (82%)	39 (12%)	17 (5%)	1	5
3	I	311/323 (96%)	255 (82%)	41 (13%)	15 (5%)	2	6
3	L	311/323 (96%)	256 (82%)	40 (13%)	15 (5%)	2	6
4	M	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
4	N	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
4	O	3/5 (60%)	3 (100%)	0	0	100	100
4	P	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	2904/3080 (94%)	2389 (82%)	341 (12%)	174 (6%)	1	3

5 of 174 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
2	B	277	VAL
2	B	293	GLU
3	C	337	CYS
3	C	357	VAL

5.3.2 Protein sidechains ⓘ

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	92/110 (84%)	83 (90%)	9 (10%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	92/110 (84%)	83 (90%)	9 (10%)	6	21
1	G	92/110 (84%)	88 (96%)	4 (4%)	25	57
1	J	92/110 (84%)	87 (95%)	5 (5%)	18	48
2	B	266/274 (97%)	249 (94%)	17 (6%)	14	41
2	E	266/274 (97%)	249 (94%)	17 (6%)	14	41
2	H	266/274 (97%)	248 (93%)	18 (7%)	13	38
2	K	266/274 (97%)	249 (94%)	17 (6%)	14	41
3	C	276/281 (98%)	258 (94%)	18 (6%)	14	40
3	F	276/281 (98%)	259 (94%)	17 (6%)	15	43
3	I	273/281 (97%)	253 (93%)	20 (7%)	11	34
3	L	273/281 (97%)	255 (93%)	18 (7%)	14	39
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	3 (100%)	0	100	100
4	O	3/3 (100%)	3 (100%)	0	100	100
4	P	3/3 (100%)	3 (100%)	0	100	100
All	All	2542/2672 (95%)	2373 (93%)	169 (7%)	14	39

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	136	ARG
2	K	322	LEU
3	I	248	LEU
1	J	166	LEU
2	K	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	274	GLN
2	K	371	ASN
3	L	189	ASN
2	E	384	ASN
2	E	379	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

2 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
5	NAG	Q	1	5,3	14,14,15	1.29	1 (7%)	17,19,21	1.32	3 (17%)
5	NAG	Q	2	5	14,14,15	1.33	2 (14%)	17,19,21	1.11	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Q	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	1	NAG	O7-C7	-4.15	1.14	1.23
5	Q	2	NAG	O7-C7	-3.75	1.14	1.23
5	Q	2	NAG	C2-N2	2.10	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	1	NAG	C3-C4-C5	2.40	114.58	110.23
5	Q	1	NAG	C6-C5-C4	-2.28	107.41	113.02
5	Q	1	NAG	C1-O5-C5	2.26	115.22	112.19
5	Q	2	NAG	C1-O5-C5	2.20	115.14	112.19

There are no chirality outliers.

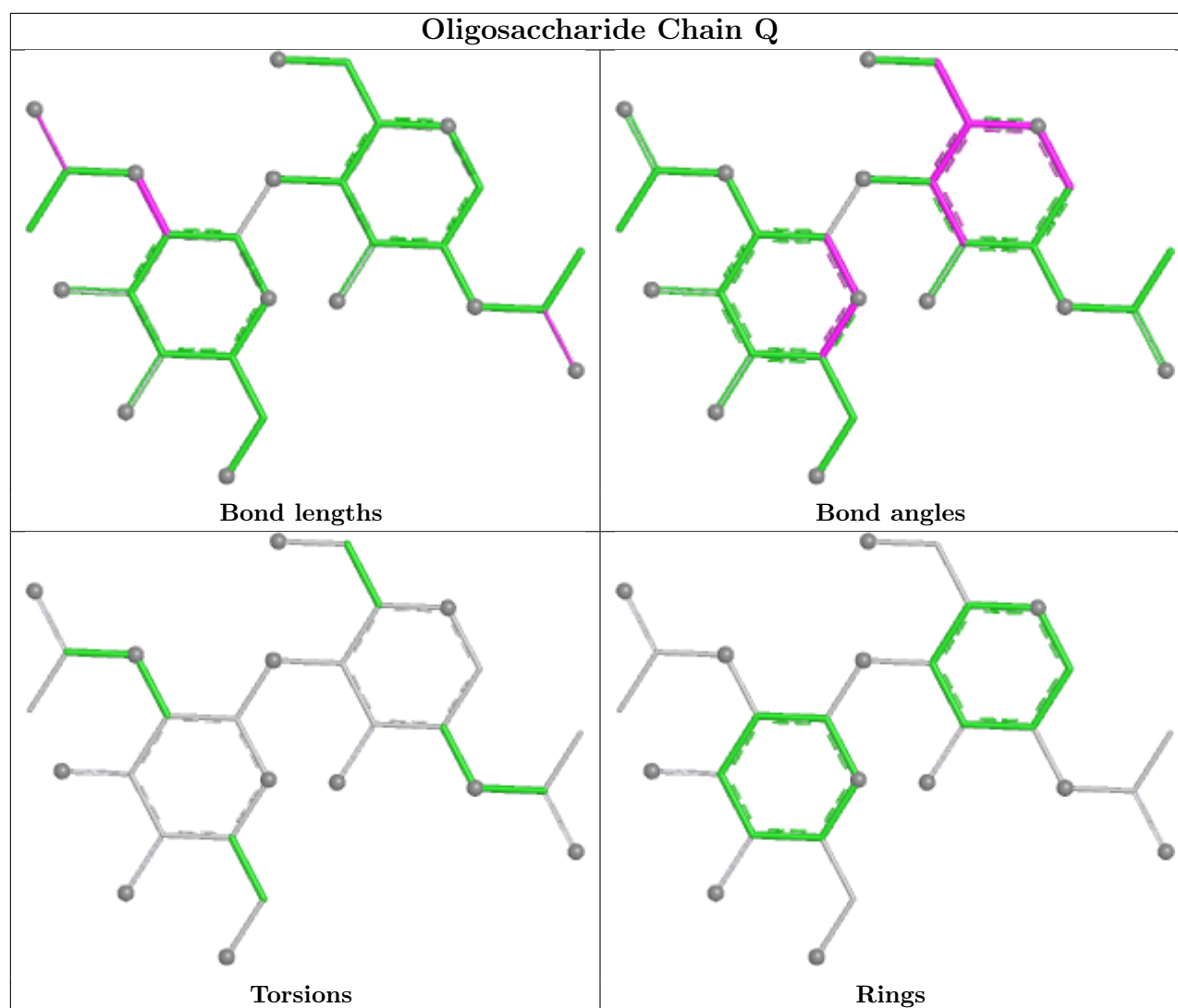
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	1	NAG	3	0
5	Q	2	NAG	5	0

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



5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 8 are monoatomic - leaving 29 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	NDG	N	101	-	15,15,15	0.41	0	21,21,21	0.62	0
6	NDG	K	501	-	15,15,15	0.71	0	21,21,21	0.90	1 (4%)
7	MAN	L	501	-	11,11,12	1.12	1 (9%)	15,15,17	2.15	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	H	503	-	12,12,12	0.44	0	17,17,17	0.36	0
6	NDG	H	506	-	15,15,15	0.47	0	21,21,21	0.67	0
9	NAG	E	501	-	15,15,15	0.65	0	21,21,21	1.18	3 (14%)
7	MAN	N	102	-	12,12,12	0.44	0	17,17,17	0.37	0
6	NDG	B	501	-	15,15,15	0.38	0	21,21,21	0.61	0
7	MAN	P	101	-	12,12,12	0.44	0	17,17,17	0.36	0
6	NDG	D	301	-	15,15,15	0.47	0	21,21,21	0.66	0
9	NAG	I	502	-	14,14,15	1.32	2 (14%)	17,19,21	1.12	1 (5%)
11	GAL	H	507	-	12,12,12	0.96	0	17,17,17	0.63	0
9	NAG	F	501	3	14,14,15	1.29	1 (7%)	17,19,21	1.33	3 (17%)
9	NAG	I	501	3	14,14,15	1.29	1 (7%)	17,19,21	1.33	3 (17%)
10	BMA	E	502	-	12,12,12	0.55	0	17,17,17	0.64	0
9	NAG	C	501	3	14,14,15	1.29	1 (7%)	17,19,21	1.33	3 (17%)
7	MAN	E	503	-	12,12,12	0.44	0	17,17,17	0.37	0
6	NDG	M	101	-	15,15,15	0.51	0	21,21,21	0.53	0
7	MAN	J	301	-	11,11,12	1.12	1 (9%)	15,15,17	2.15	3 (20%)
6	NDG	O	101	-	15,15,15	0.59	0	21,21,21	0.60	0
7	MAN	C	503	-	11,11,12	1.13	1 (9%)	15,15,17	2.15	3 (20%)
9	NAG	F	502	-	14,14,15	1.34	2 (14%)	17,19,21	1.11	1 (5%)
7	MAN	F	503	-	11,11,12	1.13	1 (9%)	15,15,17	2.16	4 (26%)
7	MAN	H	505	-	12,12,12	0.44	0	17,17,17	0.36	0
9	NAG	C	502	-	14,14,15	1.33	2 (14%)	17,19,21	1.12	1 (5%)
6	NDG	H	502	-	15,15,15	0.47	0	21,21,21	0.66	0
6	NDG	H	501	-	15,15,15	0.48	0	21,21,21	0.77	0
10	BMA	H	504	-	12,12,12	0.54	0	17,17,17	0.38	0
7	MAN	B	502	-	12,12,12	0.45	0	17,17,17	0.44	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	NDG	N	101	-	-	5/6/26/26	0/1/1/1
6	NDG	K	501	-	-	6/6/26/26	0/1/1/1
7	MAN	L	501	-	-	0/2/19/22	0/1/1/1
7	MAN	H	503	-	-	1/2/22/22	0/1/1/1
6	NDG	H	506	-	-	6/6/26/26	0/1/1/1
9	NAG	E	501	-	-	4/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	N	102	-	-	1/2/22/22	0/1/1/1
6	NDG	B	501	-	-	4/6/26/26	0/1/1/1
7	MAN	P	101	-	-	1/2/22/22	0/1/1/1
6	NDG	D	301	-	-	6/6/26/26	0/1/1/1
9	NAG	I	502	-	-	0/6/23/26	0/1/1/1
11	GAL	H	507	-	-	0/2/22/22	0/1/1/1
9	NAG	F	501	3	-	0/6/23/26	0/1/1/1
9	NAG	I	501	3	-	0/6/23/26	0/1/1/1
10	BMA	E	502	-	-	2/2/22/22	0/1/1/1
9	NAG	C	501	3	-	0/6/23/26	0/1/1/1
7	MAN	E	503	-	-	1/2/22/22	0/1/1/1
6	NDG	M	101	-	-	5/6/26/26	0/1/1/1
7	MAN	J	301	-	-	0/2/19/22	0/1/1/1
6	NDG	O	101	-	-	4/6/26/26	0/1/1/1
7	MAN	C	503	-	-	0/2/19/22	0/1/1/1
9	NAG	F	502	-	-	0/6/23/26	0/1/1/1
7	MAN	F	503	-	-	0/2/19/22	0/1/1/1
7	MAN	H	505	-	-	1/2/22/22	0/1/1/1
9	NAG	C	502	-	-	0/6/23/26	0/1/1/1
6	NDG	H	502	-	-	6/6/26/26	0/1/1/1
6	NDG	H	501	-	-	4/6/26/26	0/1/1/1
10	BMA	H	504	-	-	0/2/22/22	0/1/1/1
7	MAN	B	502	-	-	2/2/22/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	501	NAG	O7-C7	-4.18	1.13	1.23
9	C	501	NAG	O7-C7	-4.16	1.13	1.23
9	F	501	NAG	O7-C7	-4.16	1.13	1.23
9	F	502	NAG	O7-C7	-3.79	1.14	1.23
9	C	502	NAG	O7-C7	-3.76	1.14	1.23

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	503	MAN	C1-O5-C5	5.91	120.10	112.19
7	L	501	MAN	C1-O5-C5	5.90	120.09	112.19
7	C	503	MAN	C1-O5-C5	5.89	120.08	112.19
7	J	301	MAN	C1-O5-C5	5.86	120.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	301	MAN	O5-C1-C2	4.14	120.67	110.79

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	NDG	C1-C2-N2-C7
6	B	501	NDG	C8-C7-N2-C2
6	B	501	NDG	O7-C7-N2-C2
6	D	301	NDG	C1-C2-N2-C7
6	D	301	NDG	C8-C7-N2-C2

There are no ring outliers.

29 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	101	NDG	25	0
6	K	501	NDG	7	0
7	L	501	MAN	2	0
7	H	503	MAN	15	0
6	H	506	NDG	23	0
9	E	501	NAG	9	0
7	N	102	MAN	1	0
6	B	501	NDG	3	0
7	P	101	MAN	8	0
6	D	301	NDG	9	0
9	I	502	NAG	8	0
11	H	507	GAL	10	0
9	F	501	NAG	6	0
9	I	501	NAG	6	0
10	E	502	BMA	23	0
9	C	501	NAG	7	0
7	E	503	MAN	12	0
6	M	101	NDG	5	0
7	J	301	MAN	2	0
6	O	101	NDG	2	0
7	C	503	MAN	2	0
9	F	502	NAG	11	0
7	F	503	MAN	5	0
7	H	505	MAN	15	0
9	C	502	NAG	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	502	NDG	6	0
6	H	501	NDG	2	0
10	H	504	BMA	1	0
7	B	502	MAN	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.