wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:48 PM GMT

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
http://wwpdb.org/validation/2016/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:

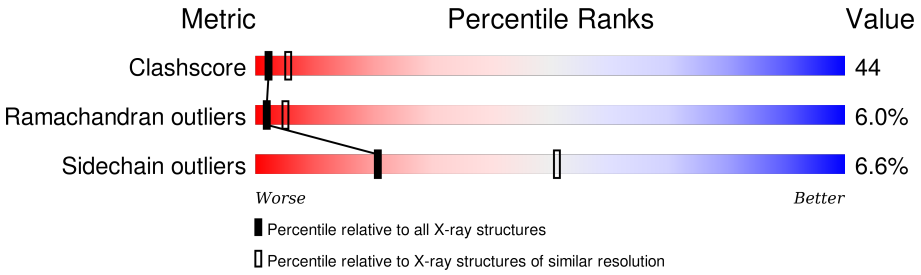
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

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% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	323	43% 47% 7%
3	C	323	42% 47% 8%
3	F	323	42% 50% 6%
3	I	323	41% 49% 7%
3	L	323	40% 50% 7%
4	M	5	20% 60% 20%
4	N	5	20% 60% 20%
4	O	5	40% 40% 20%
4	P	5	60% 20% 20%

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	GAL	H	575	-	-	X	-
5	NH2	M	6	-	-	X	-
5	NH2	P	6	-	-	X	-
6	NDG	D	574	-	-	X	-
6	NDG	K	570	-	-	X	-
6	NDG	N	571	-	-	X	-
7	MAN	H	480	-	-	X	-
7	MAN	H	573	-	-	X	-
7	MAN	P	576	-	-	X	-
8	NAG	C	571	-	-	X	-
8	NAG	E	570	-	-	X	-
8	NAG	F	571	-	-	X	-
8	NAG	H	574	X	-	X	-
8	NAG	I	571	-	-	X	-
8	NAG	L	571	X	-	-	-
9	BMA	E	572	-	-	X	-
9	BMA	E	573	X	-	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	SEE REMARK 999	UNP P02674
D	153	ALA	THR	SEE REMARK 999	UNP P02674
G	153	ALA	THR	SEE REMARK 999	UNP P02674
J	153	ALA	THR	SEE REMARK 999	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			

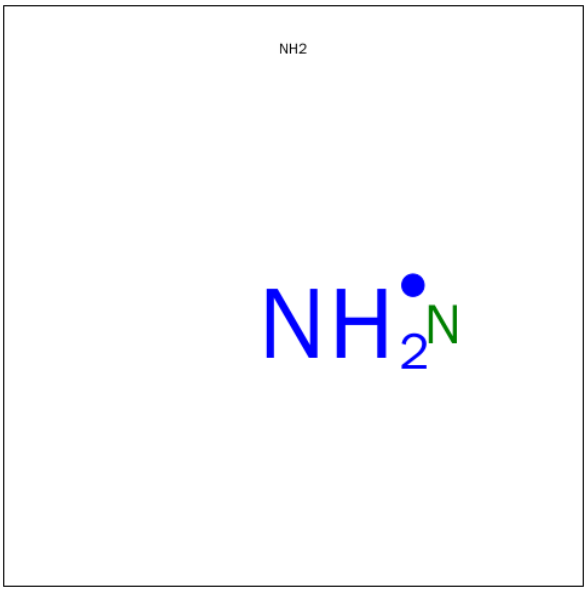
There are 4 discrepancies between the modelled and reference sequences:

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

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

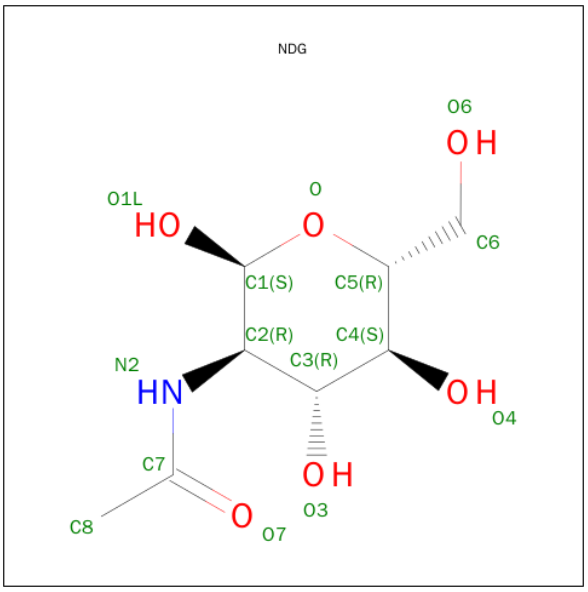
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	4	Total	C	N	O	0	0	0
			32	19	9	4			
4	N	4	Total	C	N	O	0	0	0
			32	19	9	4			
4	O	4	Total	C	N	O	0	0	0
			32	19	9	4			
4	P	4	Total	C	N	O	0	0	0
			32	19	9	4			

- Molecule 5 is AMINO GROUP (three-letter code: NH2) (formula: H_2N).



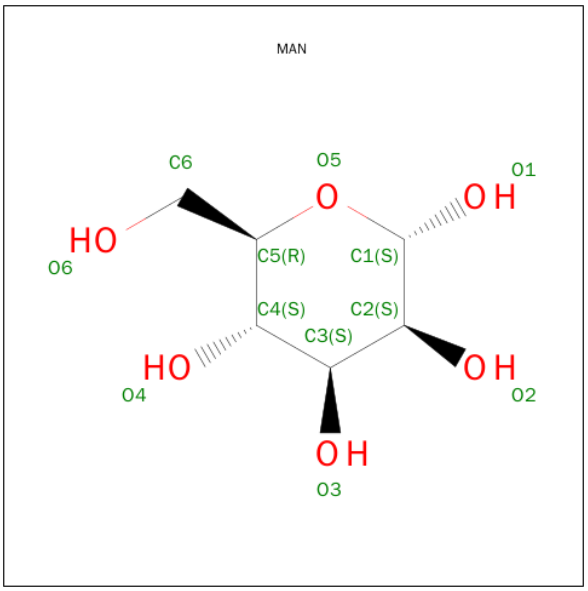
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total N 1 1	0	0
5	N	1	Total N 1 1	0	0
5	O	1	Total N 1 1	0	0
5	P	1	Total N 1 1	0	0

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



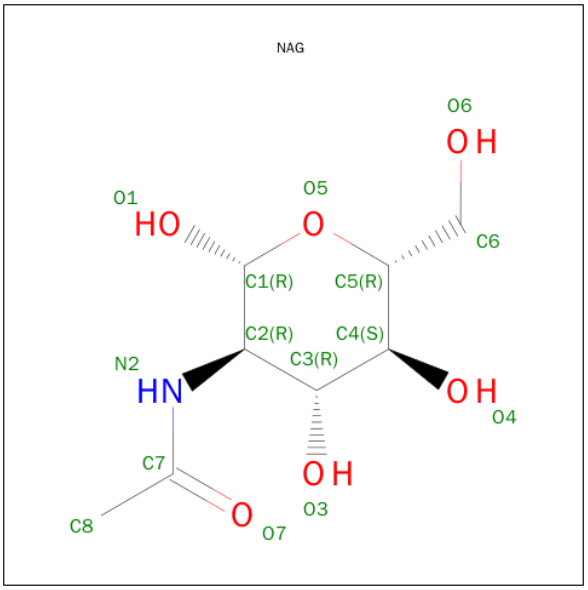
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 12 6 6	0	0
7	H	1	Total C O 12 6 6	0	0
7	N	1	Total C O 12 6 6	0	0
7	H	1	Total C O 12 6 6	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



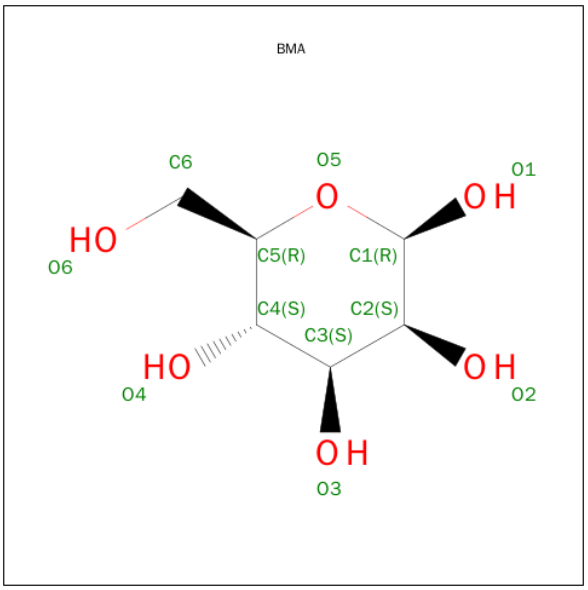
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total C N O 15 8 1 6	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	H	1	Total C N O 15 8 1 6	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0
8	F	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

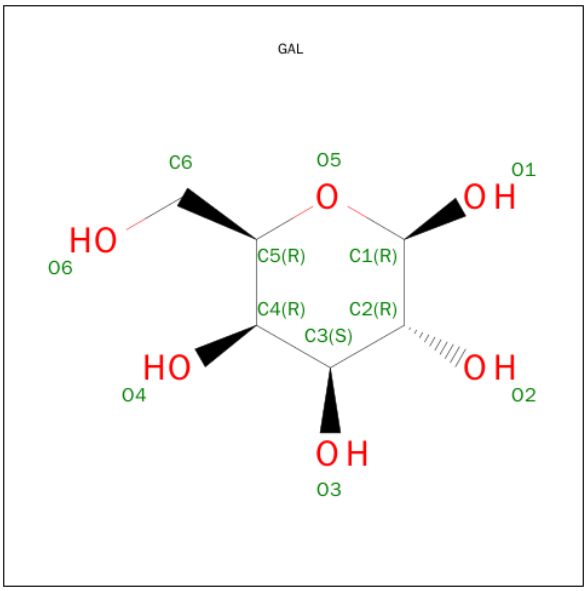
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	1	Total C N O 14 8 1 5	0	0
8	I	1	Total C N O 14 8 1 5	0	0
8	L	1	Total C N O 14 8 1 5	0	0
8	L	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 10 is SUGAR (D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

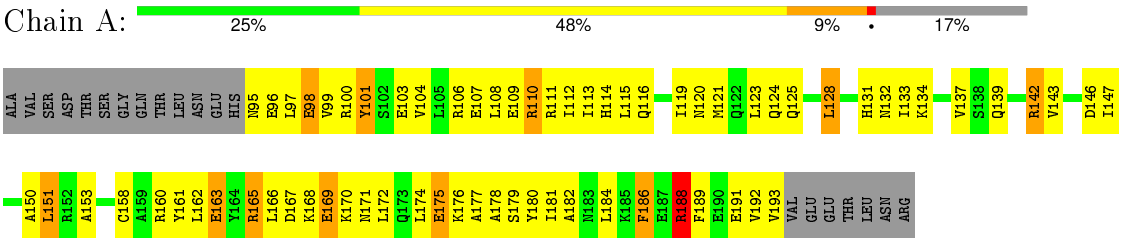
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

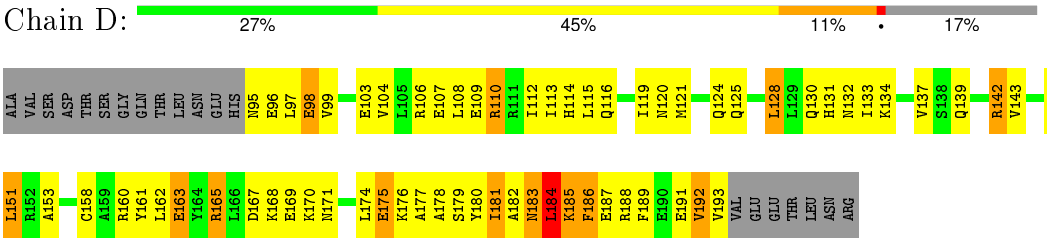
- Molecule 1: Fibrinogen alpha-1 chain

Chain A:



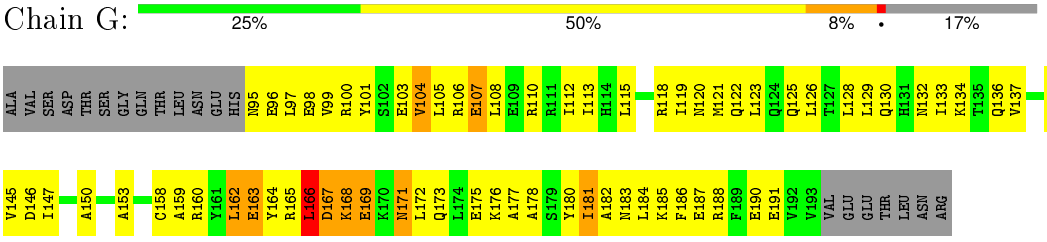
- Molecule 1: Fibrinogen alpha-1 chain

Chain D:



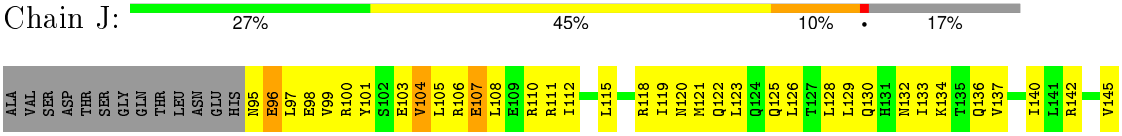
- Molecule 1: Fibrinogen alpha-1 chain

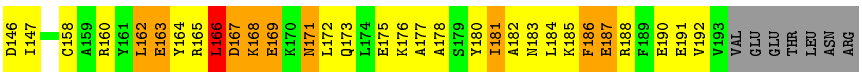
Chain G:



- Molecule 1: Fibrinogen alpha-1 chain

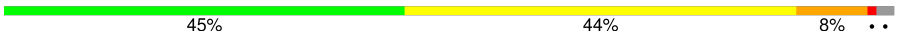
Chain J:

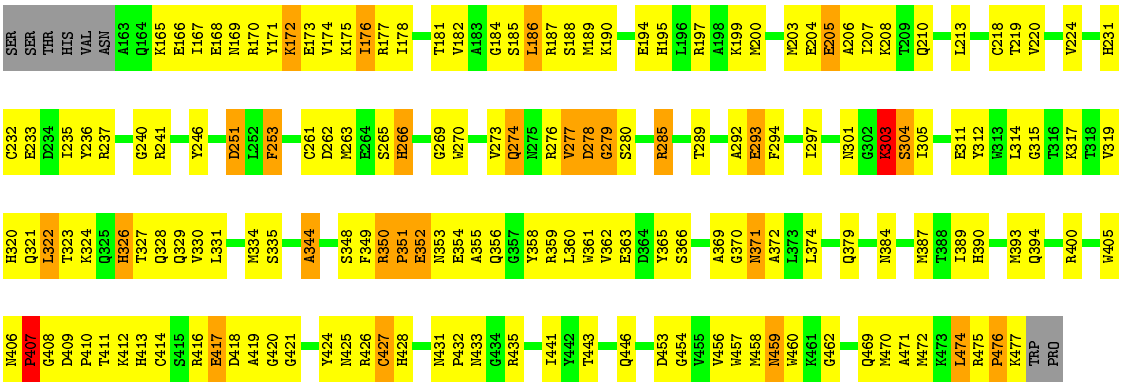




• Molecule 2: Fibrinogen beta chain

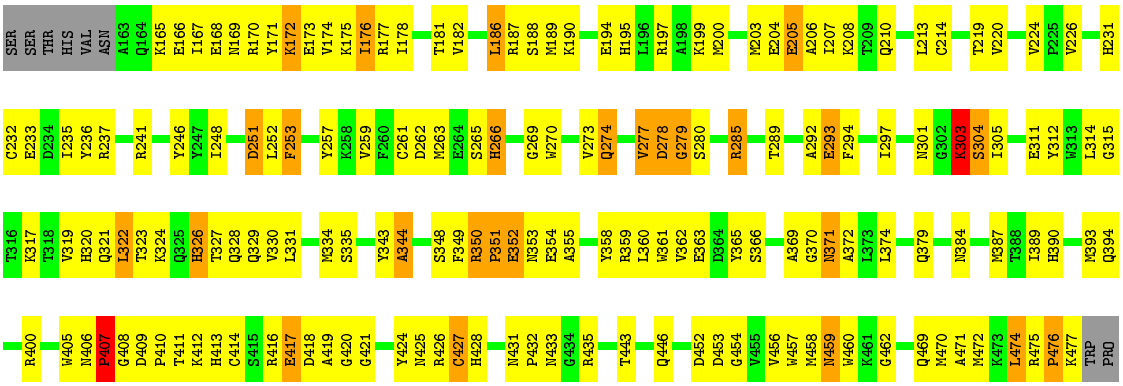
Chain B:





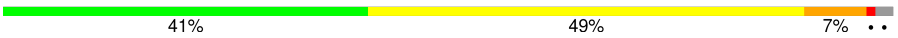
• Molecule 2: Fibrinogen beta chain

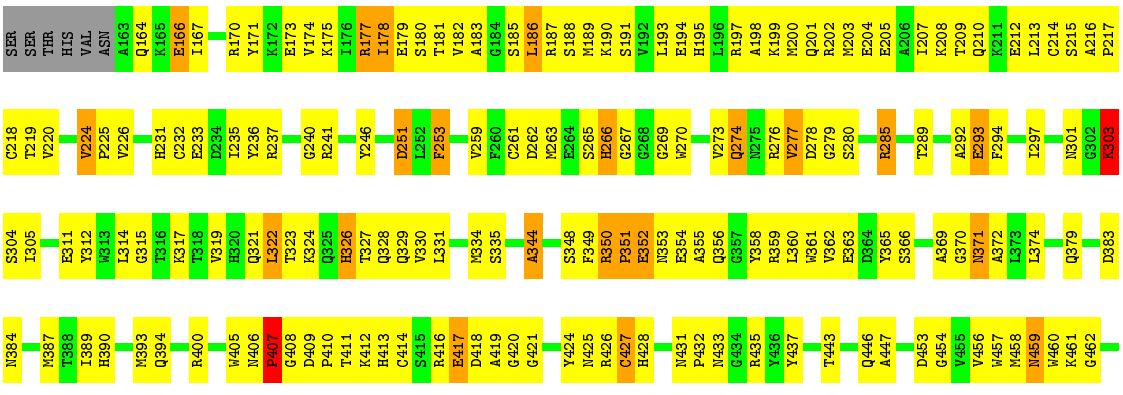
Chain E:

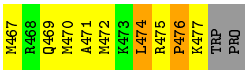


• Molecule 2: Fibrinogen beta chain

Chain H:

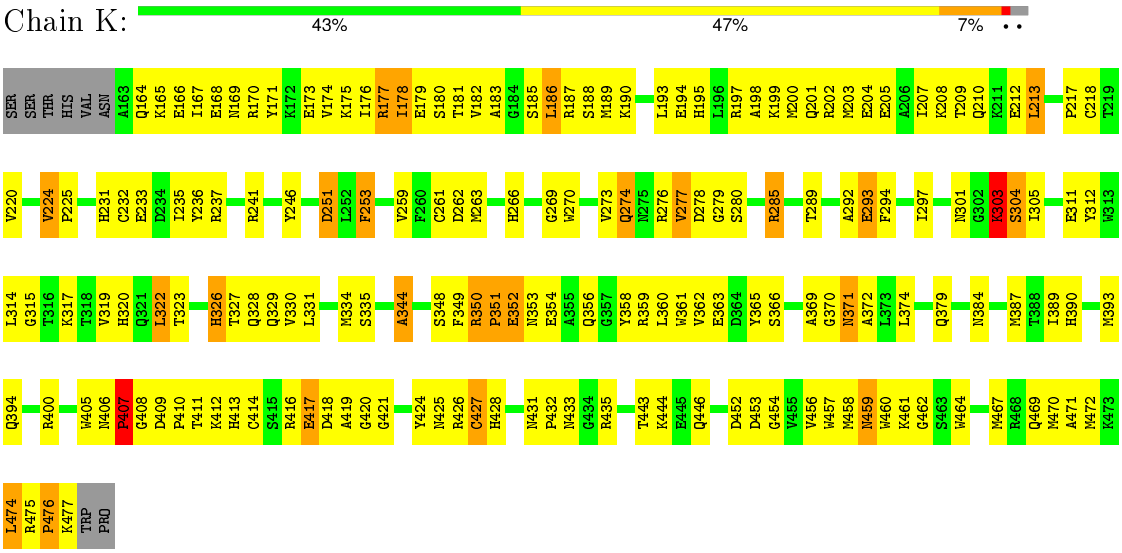






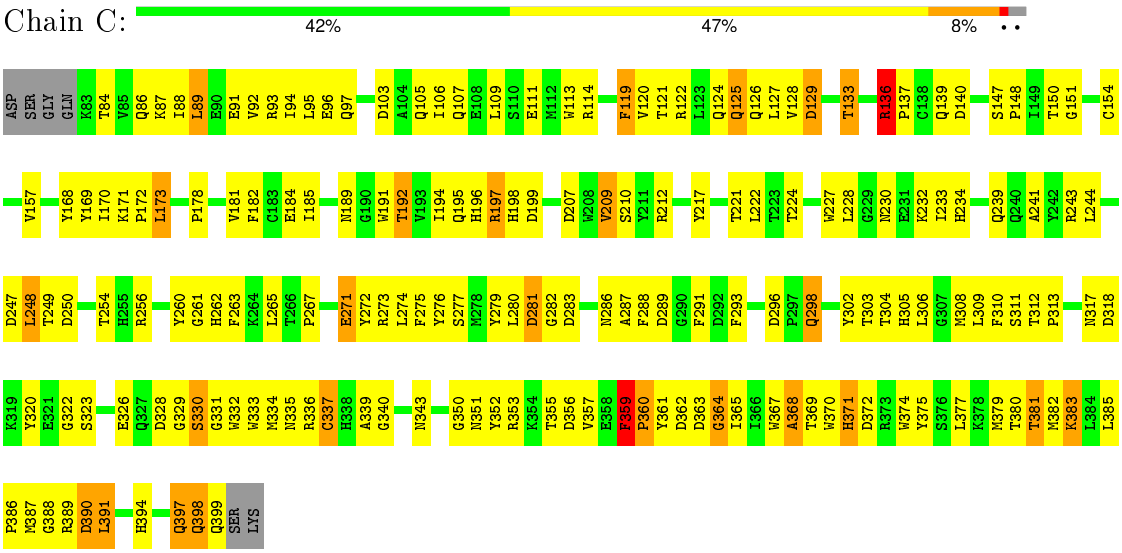
- Molecule 2: Fibrinogen beta chain

Chain K:



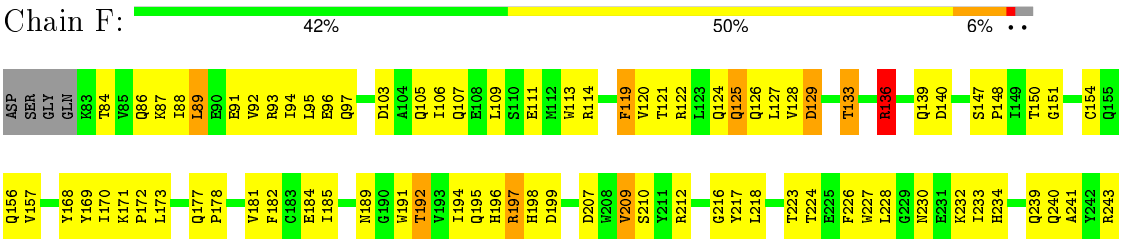
- Molecule 3: Fibrinogen gamma chain

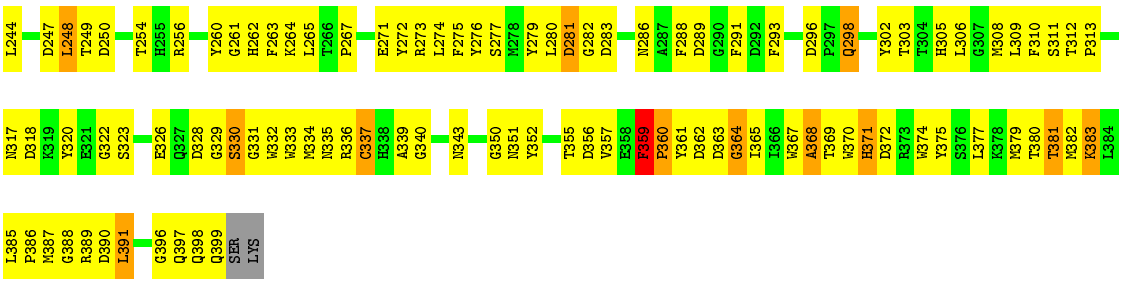
Chain C:



- Molecule 3: Fibrinogen gamma chain

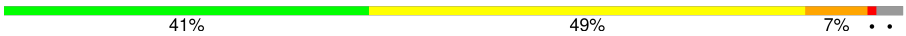
Chain F:

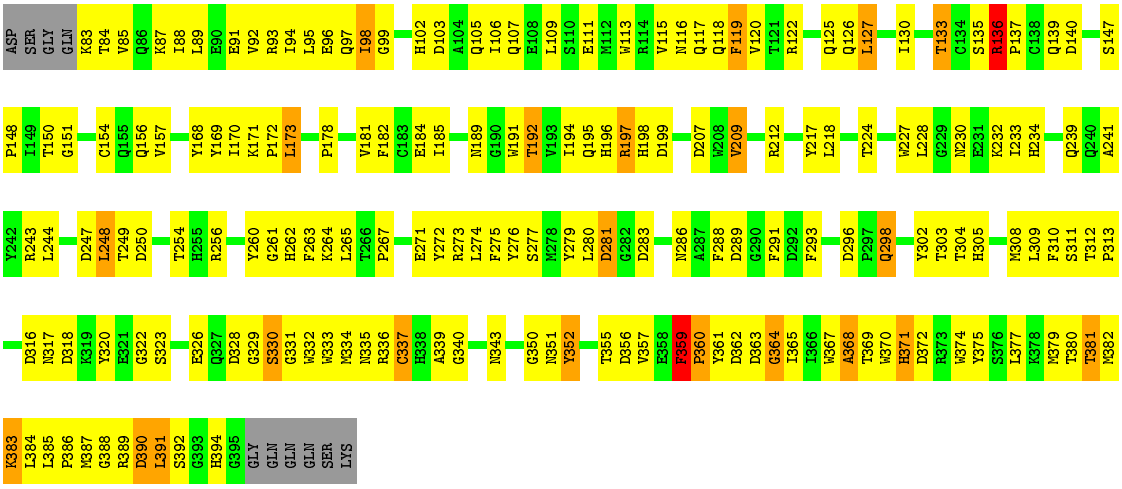




• Molecule 3: Fibrinogen gamma chain

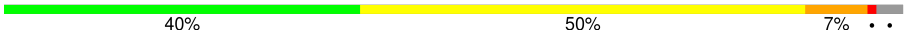
Chain I:

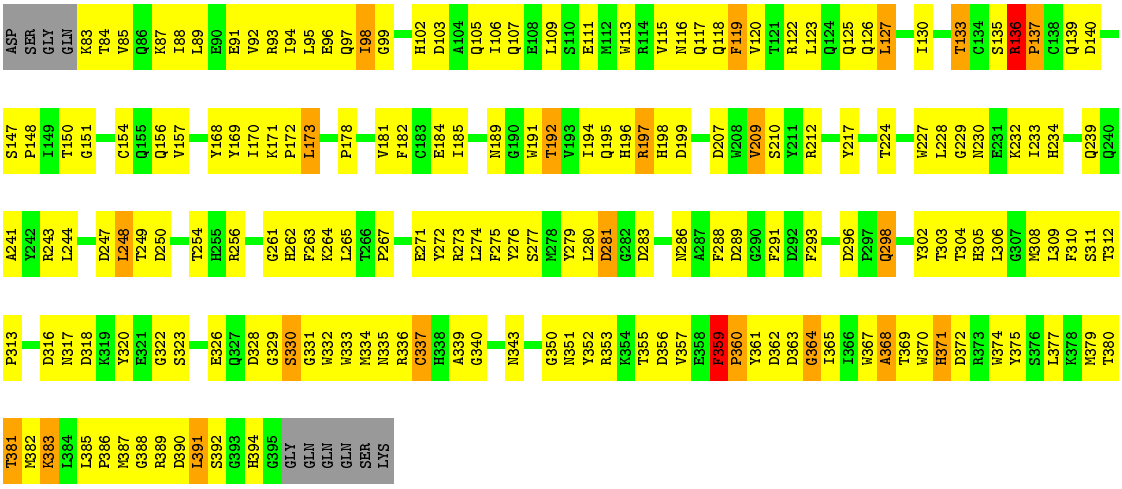




• Molecule 3: Fibrinogen gamma chain

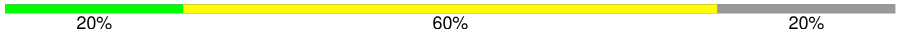
Chain L:





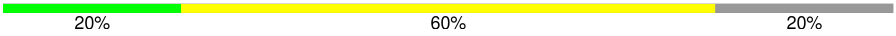
• Molecule 4: Ligand Gly-His-Arg-Pro-NH2

Chain M:



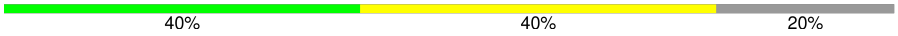
• Molecule 4: Ligand Gly-His-Arg-Pro-NH2

Chain N:



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

Chain O:



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

Chain P:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, NDG, GAL, NH2, MAN

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(^{o})	Ideal(^{o})
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 (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	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	207	0
2	E	2535	0	2364	202	0
2	H	2535	0	2364	248	0
2	K	2535	0	2364	232	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	32	0	32	5	0
4	N	32	0	32	5	0
4	O	32	0	32	4	0
4	P	32	0	32	2	0
5	M	1	0	0	2	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	2	0
6	B	15	0	15	4	0
6	D	15	0	15	10	0
6	H	30	0	30	10	0
6	K	15	0	15	9	0
6	M	15	0	15	5	0
6	N	15	0	15	25	0
6	O	15	0	15	4	0
7	B	12	0	12	3	0
7	C	11	0	10	2	0
7	F	11	0	10	4	0
7	H	24	0	24	26	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	C	28	0	26	8	0
8	E	15	0	15	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	28	0	26	8	0
8	H	15	0	15	23	0
8	I	28	0	26	7	0
8	L	28	0	26	4	0
9	E	24	0	24	33	0
9	H	12	0	12	1	0
10	H	12	0	12	11	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
All	All	24360	0	23099	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)
9:E:572:BMA:C5	6:N:571:NDG:H8C1	1.68	1.21
8:I:571:NAG:O3	7:J:572:MAN:C1	1.91	1.18
1:A:188:ARG:HD2	1:A:188:ARG:H	1.07	1.18
7:H:480:MAN:O6	7:H:573:MAN:H62	1.39	1.18
9:E:572:BMA:H62	9:E:573:BMA: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%)	2 5
1	D	97/119 (82%)	75 (77%)	13 (13%)	9 (9%)	1 1
1	G	97/119 (82%)	75 (77%)	13 (13%)	9 (9%)	1 1
1	J	97/119 (82%)	74 (76%)	14 (14%)	9 (9%)	1 1
2	B	313/323 (97%)	265 (85%)	29 (9%)	19 (6%)	2 5
2	E	313/323 (97%)	268 (86%)	26 (8%)	19 (6%)	2 5
2	H	313/323 (97%)	260 (83%)	35 (11%)	18 (6%)	2 5
2	K	313/323 (97%)	261 (83%)	32 (10%)	20 (6%)	2 4
3	C	315/323 (98%)	259 (82%)	38 (12%)	18 (6%)	2 6
3	F	315/323 (98%)	259 (82%)	39 (12%)	17 (5%)	2 7
3	I	311/323 (96%)	255 (82%)	41 (13%)	15 (5%)	3 9
3	L	311/323 (96%)	256 (82%)	40 (13%)	15 (5%)	3 9
4	M	2/5 (40%)	1 (50%)	1 (50%)	0	100 100
4	N	2/5 (40%)	1 (50%)	1 (50%)	0	100 100
4	O	2/5 (40%)	2 (100%)	0	0	100 100
4	P	2/5 (40%)	1 (50%)	1 (50%)	0	100 100
All	All	2900/3080 (94%)	2386 (82%)	340 (12%)	174 (6%)	2 5

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 (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	92/110 (84%)	83 (90%)	9 (10%)	10	28
1	D	92/110 (84%)	83 (90%)	9 (10%)	10	28
1	G	92/110 (84%)	88 (96%)	4 (4%)	35	70
1	J	92/110 (84%)	87 (95%)	5 (5%)	27	60
2	B	266/274 (97%)	249 (94%)	17 (6%)	22	52
2	E	266/274 (97%)	249 (94%)	17 (6%)	22	52
2	H	266/274 (97%)	248 (93%)	18 (7%)	20	49
2	K	266/274 (97%)	249 (94%)	17 (6%)	22	52
3	C	276/281 (98%)	258 (94%)	18 (6%)	21	52
3	F	276/281 (98%)	259 (94%)	17 (6%)	23	54
3	I	273/281 (97%)	253 (93%)	20 (7%)	17	44
3	L	273/281 (97%)	255 (93%)	18 (7%)	21	51
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%)	21	51

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

Mol	Chain	Res	Type
3	F	192	THR
2	H	209	THR
3	L	133	THR
3	F	209	VAL
3	F	381	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	240	GLN
2	H	231	HIS
3	L	196	HIS
3	F	298	GLN
1	G	124	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 43 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 31 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	B	570	-	15,15,15	0.38	0	17,21,21	0.54	0
7	MAN	B	572	-	12,12,12	0.43	0	17,17,17	0.45	0
8	NAG	C	570	8,3	14,14,15	1.23	1 (7%)	15,19,21	1.35	3 (20%)
8	NAG	C	571	8	14,14,15	1.27	1 (7%)	15,19,21	1.17	1 (6%)
7	MAN	C	572	-	11,11,12	1.14	1 (9%)	14,15,17	2.63	4 (28%)
6	NDG	D	574	-	15,15,15	0.46	0	17,21,21	0.52	0
8	NAG	E	570	-	15,15,15	0.63	0	17,21,21	1.00	1 (5%)
9	BMA	E	572	-	12,12,12	0.56	0	17,17,17	0.67	0
9	BMA	E	573	-	12,12,12	0.46	0	17,17,17	0.39	0
8	NAG	F	570	8,3	14,14,15	1.23	1 (7%)	15,19,21	1.35	3 (20%)
8	NAG	F	571	8,7	14,14,15	1.28	1 (7%)	15,19,21	1.16	1 (6%)
7	MAN	F	572	8	11,11,12	1.13	1 (9%)	14,15,17	2.63	4 (28%)
7	MAN	H	480	-	12,12,12	0.45	0	17,17,17	0.39	0
6	NDG	H	570	-	15,15,15	0.49	0	17,21,21	0.73	0
6	NDG	H	571	-	15,15,15	0.46	0	17,21,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BMA	H	572	-	12,12,12	0.53	0	17,17,17	0.43	0
7	MAN	H	573	-	12,12,12	0.46	0	17,17,17	0.39	0
8	NAG	H	574	-	15,15,15	0.46	0	17,21,21	0.52	0
10	GAL	H	575	-	12,12,12	0.95	0	17,17,17	0.68	0
8	NAG	I	570	8,3	14,14,15	1.23	1 (7%)	15,19,21	1.35	3 (20%)
8	NAG	I	571	8	14,14,15	1.27	1 (7%)	15,19,21	1.17	1 (6%)
7	MAN	J	572	-	11,11,12	1.13	1 (9%)	14,15,17	2.62	4 (28%)
6	NDG	K	570	-	15,15,15	0.69	0	17,21,21	0.68	0
8	NAG	L	570	8,3	14,14,15	1.23	1 (7%)	15,19,21	1.34	3 (20%)
8	NAG	L	571	8	14,14,15	1.28	1 (7%)	15,19,21	1.16	1 (6%)
7	MAN	L	572	-	11,11,12	1.12	1 (9%)	14,15,17	2.63	4 (28%)
6	NDG	M	571	-	15,15,15	0.49	0	17,21,21	0.53	0
6	NDG	N	571	-	15,15,15	0.41	0	17,21,21	0.65	0
7	MAN	N	576	-	12,12,12	0.45	0	17,17,17	0.40	0
6	NDG	O	571	-	15,15,15	0.58	0	17,21,21	0.50	0
7	MAN	P	576	-	12,12,12	0.45	0	17,17,17	0.40	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	B	570	-	-	0/6/26/26	0/1/1/1
7	MAN	B	572	-	-	0/2/22/22	0/1/1/1
8	NAG	C	570	8,3	-	0/6/23/26	0/1/1/1
8	NAG	C	571	8	-	0/6/23/26	0/1/1/1
7	MAN	C	572	-	-	0/2/19/22	0/1/1/1
6	NDG	D	574	-	-	0/6/26/26	0/1/1/1
8	NAG	E	570	-	-	0/6/26/26	0/1/1/1
9	BMA	E	572	-	-	0/2/22/22	0/1/1/1
9	BMA	E	573	-	1/1/5/5	0/2/22/22	0/1/1/1
8	NAG	F	570	8,3	-	0/6/23/26	0/1/1/1
8	NAG	F	571	8,7	-	0/6/23/26	0/1/1/1
7	MAN	F	572	8	-	0/2/19/22	0/1/1/1
7	MAN	H	480	-	-	0/2/22/22	0/1/1/1
6	NDG	H	570	-	-	0/6/26/26	0/1/1/1
6	NDG	H	571	-	-	0/6/26/26	0/1/1/1
9	BMA	H	572	-	-	0/2/22/22	0/1/1/1
7	MAN	H	573	-	-	0/2/22/22	0/1/1/1
8	NAG	H	574	-	1/1/6/7	0/6/26/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GAL	H	575	-	-	0/2/22/22	0/1/1/1
8	NAG	I	570	8,3	-	0/6/23/26	0/1/1/1
8	NAG	I	571	8	-	0/6/23/26	0/1/1/1
7	MAN	J	572	-	-	0/2/19/22	0/1/1/1
6	NDG	K	570	-	-	0/6/26/26	0/1/1/1
8	NAG	L	570	8,3	-	0/6/23/26	0/1/1/1
8	NAG	L	571	8	1/1/5/7	0/6/23/26	0/1/1/1
7	MAN	L	572	-	-	0/2/19/22	0/1/1/1
6	NDG	M	571	-	-	0/6/26/26	0/1/1/1
6	NDG	N	571	-	-	0/6/26/26	0/1/1/1
7	MAN	N	576	-	-	0/2/22/22	0/1/1/1
6	NDG	O	571	-	-	0/6/26/26	0/1/1/1
7	MAN	P	576	-	-	0/2/22/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	570	NAG	O7-C7	-4.02	1.13	1.23
8	C	570	NAG	O7-C7	-4.00	1.13	1.23
8	F	570	NAG	O7-C7	-4.00	1.13	1.23
8	L	570	NAG	O7-C7	-3.99	1.14	1.23
8	F	571	NAG	O7-C7	-3.64	1.14	1.23

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	572	MAN	O3-C3-C2	-2.53	105.42	110.00
7	J	572	MAN	O3-C3-C2	-2.53	105.43	110.00
7	L	572	MAN	O3-C3-C2	-2.51	105.46	110.00
7	F	572	MAN	O3-C3-C2	-2.51	105.47	110.00
8	F	570	NAG	C6-C5-C4	-2.29	107.37	113.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	573	BMA	C1
8	L	571	NAG	C1
8	H	574	NAG	C1

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 130 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	570	NDG	4	0
7	B	572	MAN	3	0
8	C	570	NAG	6	0
8	C	571	NAG	8	0
7	C	572	MAN	2	0
6	D	574	NDG	10	0
8	E	570	NAG	9	0
9	E	572	BMA	23	0
9	E	573	BMA	13	0
8	F	570	NAG	4	0
8	F	571	NAG	8	0
7	F	572	MAN	4	0
7	H	480	MAN	15	0
6	H	570	NDG	4	0
6	H	571	NDG	6	0
9	H	572	BMA	1	0
7	H	573	MAN	14	0
8	H	574	NAG	23	0
10	H	575	GAL	11	0
8	I	570	NAG	5	0
8	I	571	NAG	7	0
7	J	572	MAN	2	0
6	K	570	NDG	9	0
8	L	570	NAG	2	0
8	L	571	NAG	4	0
7	L	572	MAN	2	0
6	M	571	NDG	5	0
6	N	571	NDG	25	0
7	N	576	MAN	1	0
6	O	571	NDG	4	0
7	P	576	MAN	8	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.