W O R L D W I D E
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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jul 31, 2023 – 01:03 AM EDT

PDB ID	:	1FZE
Title	:	CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN
Authors	:	Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on	:	1998-12-23
Resolution	:	3.00 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:

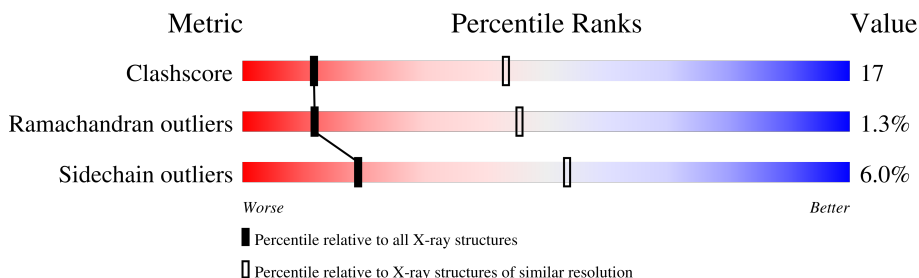|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		1.3%
Sidechain outliers		6.0%

Worse | | *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	47% 41% 5% 7%
1	D	87	55% 33% • 8%
2	B	328	58% 32% • 6%
2	E	328	56% 34% • 6%
3	C	319	63% 29% • 5%
3	F	319	63% 29% • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	470	-	-	X	-
4	NAG	B	471	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11201 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total 668	C 414	N 128	O 123	S 3	0	0	0
1	D	80	Total 660	C 410	N 127	O 120	S 3	0	0	0

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total 2480	C 1549	N 435	O 474	S 22	0	0	0
2	E	308	Total 2473	C 1544	N 434	O 473	S 22	0	0	0

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total 2433	C 1545	N 408	O 468	S 12	0	0	0
3	F	302	Total 2425	C 1539	N 407	O 467	S 12	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

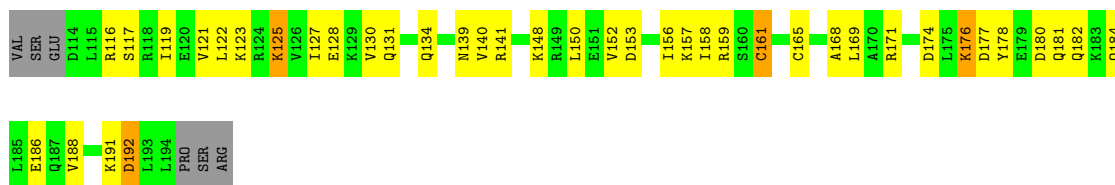| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Ca 2	0	0
5	C	1	Total 1	Ca 1	0	0
5	E	2	Total 2	Ca 2	0	0
5	F	1	Total 1	Ca 1	0	0

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.
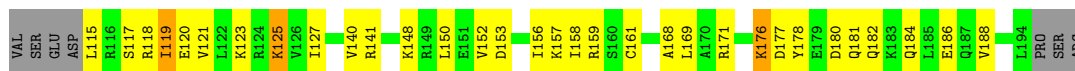
Note EDS was not executed.
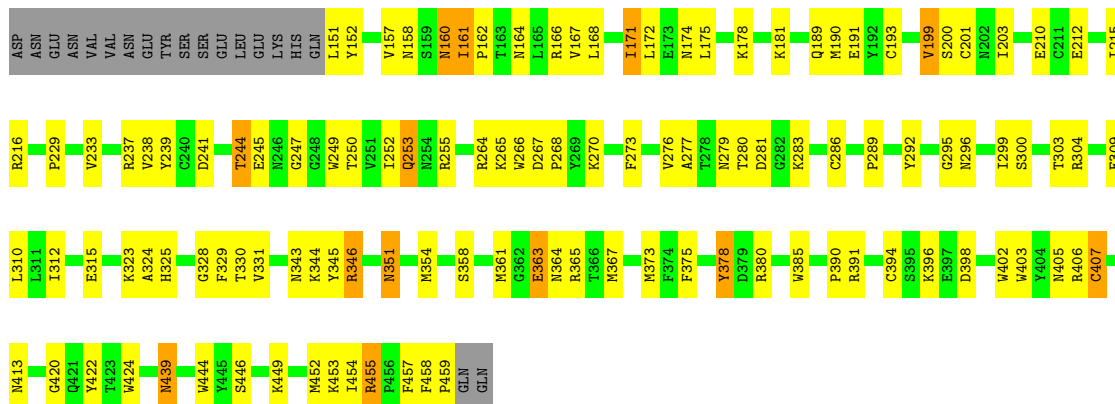
- Molecule 1: FIBRINOGEN
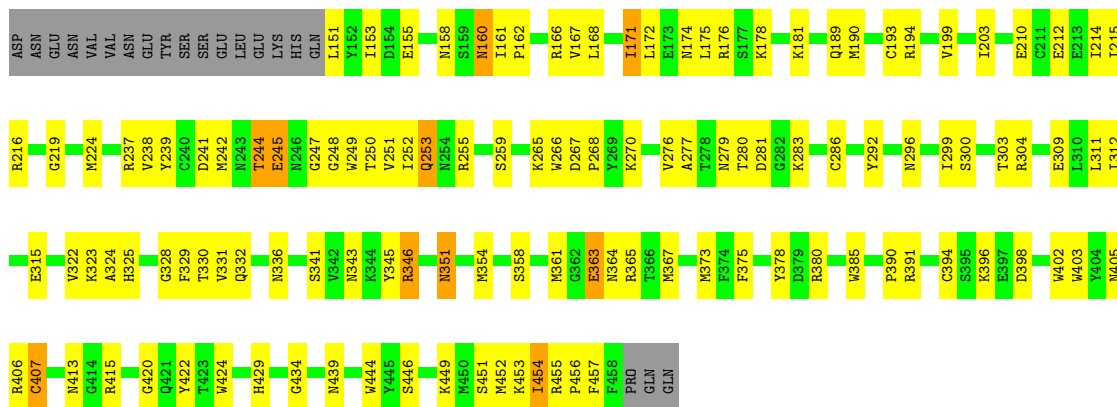
Chain A:

- Molecule 1: FIBRINOGEN

Chain D:

- Molecule 2: FIBRINOGEN

Chain B:

- Molecule 2: FIBRINOGEN

Chain E:

ASP ASN GLU ASN VAL VAL ASN GLU TYR SER SER GLU GLU LEU LYS HIS GLN L151 Y152 I153 D154 E155 N158 S159 N160 I161 P162 R166 V167 L168 I171 L172 E173 N174 L175 R176 S177 K178 K181 Q189 M190 C193 R194 V199 I203 E210 C211 E212 E213 I214 I215

R216 G219 M224 R237 V238 Y239 C240 D241 M242 N243 T244 E245 N246 G247 Q248 W249 T250 V251 I252 Q253 N254 R255 S259 K265 W266 D267 P268 Y269 K270 V276 A277 T278 N279 T280 D281 G282 K283 C286 Y292 N296 I299 S300 T303 R304 E309 L310 L311 I312

E315 V322 K323 A324 H325 G328 F329 T330 V331 Q332 N336 S341 Y342 N343 K344 Y345 R346 N351 M354 S358 M361 G362 E363 N364 R365 T366 M367 M373 F374 F375 Y378 D379 R380 W385 P390 R391 C394 S395 K396 E397 D398 W402 W403 Y404 N405

R406 C407 N413 G414 R415 G420 Q421 Y422 T423 W424 H429 G434 N439 W444 Y445 S446 K449 M450 S451 M452 K453 I454 R455 P456 F457 F458 PRO GLN GLN

• Molecule 3: FIBRINOGEN

Chain C:

63%　　　　29%　　•　5%

LYS MET LEU GLU E92 Y96 E97 A98 S99 I100 H103 D104 I107 Y114 N117 N118 Q119 V122 N123 L131 C135 D141 T142 V143 T149 G150 D152 C153 Q154 S164 G165 L166 Y167 F168 N175 L179 C182 E183 I184 N189 G190 W191 Q195

K196 R197 L198 F204 N207 W208 I209 E225 F226 W227 L228 G229 N230 E231 K232 I236 S237 T238 Q239 I242 L246 R247 V248 E249 L250 E251 D252 W253 T259 A260 D261 M264 F265 K266 K273 Y274 R275 L276 T277 Y278 A279 Y280 F295 F304 T305 S306 H307 Q311

N317 D318 N319 N325 W334 W335 M336 N337 K338 C339 H340 A341 L344 G352 T353 Y354 S355 K356 G362 Y363 D364 N365 K373 T374 R375 W376 Y377 S378 M379 K380 K381 T382 T383 M384 I387 F388 F389 N390 R391 L392 T393 I394 GLY GLU GLY GLN GLN HIS HIS LEU GLY GLY

ALA LYS

• Molecule 3: FIBRINOGEN

Chain F:

63%　　　　29%　　•　5%

LYS MET LEU GLU E92 I93 M94 K95 Y96 H103 I107 I113 N117 N118 V122 K125 E126 K127 V128 A129 G130 L131 C135 D141 T142 V143 T149 G150 K151 D152 C153 Q154 D155 I156 K159 S164 F168 I169 N175 E183 I184 N189 G190 W191 T192

V193 F194 Q195 K196 R197 L198 F204 N207 W208 I209 E225 F226 W227 N230 I236 S237 T238 Q239 I242 L246 R247 V248 E249 L250 E251 D252 W253 T257 S258 T259 M264 F265 K266 K273 Y274 R275 L276 T277 Y278 F295 S300 F303 F304 T305 S306 H307

Q311 F312 S313 N317 D318 N319 N325 W334 W335 M336 N337 K338 C339 H340 A341 L344 G352 T353 Y354 S355 K356 D364 N365 K373 T374 R375 W376 Y377 S378 M379 K380 K381 T382 T383 M384 K385 I386 I387 P388 F389 N390 T393 ILE GLY GLU GLY GLN GLN HIS HIS LEU GLY

GLY ALA LYS

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.00Å 48.60Å 166.40Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	96.7 (30.00-3.00)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.251 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11201	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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: CA, NAG

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	0.33	0/669	0.56	0/891
1	D	0.35	0/661	0.58	0/880
2	B	0.37	0/2543	0.64	0/3437
2	E	0.37	0/2535	0.64	0/3425
3	C	0.37	0/2499	0.60	0/3379
3	F	0.37	0/2491	0.60	1/3368 (0.0%)
All	All	0.37	0/11398	0.61	1/15380 (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	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	338	LYS	N-CA-C	-5.13	97.15	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	378	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	E	378	TYR	Sidechain

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	668	0	717	34	4
1	D	660	0	713	27	4
2	B	2480	0	2344	99	19
2	E	2473	0	2337	96	10
3	C	2433	0	2285	78	6
3	F	2425	0	2274	68	15
4	B	28	0	26	10	0
4	E	28	0	26	1	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	11201	0	10722	381	29

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 17.

The worst 5 of 381 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LEU:HA	1:D:118:ARG:HD3	1.38	1.00
1:A:140:VAL:HG11	2:B:171:ILE:HD11	1.52	0.91
1:A:161:CYS:HA	3:C:135:CYS:HB3	1.56	0.86
4:B:470:NAG:H3	4:B:471:NAG:C4	2.03	0.86
4:B:470:NAG:H3	4:B:471:NAG:H4	1.58	0.86

The worst 5 of 29 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:ARG:NH2	3:F:126:GLU:CB[2_656]	0.22	1.98
3:C:123:ASN:OD1	2:E:390:PRO:CB[2_656]	0.83	1.37
2:B:390:PRO:C	3:F:130:GLN:OE1[2_656]	1.06	1.14
2:B:390:PRO:CA	3:F:130:GLN:OE1[2_656]	1.15	1.05
2:B:390:PRO:CB	3:F:130:GLN:CD[2_656]	1.36	0.84

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	79/87 (91%)	71 (90%)	8 (10%)	0	100	100
1	D	78/87 (90%)	72 (92%)	5 (6%)	1 (1%)	12	45
2	B	307/328 (94%)	271 (88%)	31 (10%)	5 (2%)	9	40
2	E	306/328 (93%)	272 (89%)	29 (10%)	5 (2%)	9	40
3	C	301/319 (94%)	260 (86%)	36 (12%)	5 (2%)	9	39
3	F	300/319 (94%)	261 (87%)	37 (12%)	2 (1%)	22	60
All	All	1371/1468 (93%)	1207 (88%)	146 (11%)	18 (1%)	12	45

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	THR
3	C	339	CYS
3	C	393	THR
2	E	244	THR
3	F	339	CYS

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	76/82 (93%)	68 (90%)	8 (10%)	7	27
1	D	75/82 (92%)	69 (92%)	6 (8%)	12	40
2	B	267/286 (93%)	252 (94%)	15 (6%)	21	56
2	E	266/286 (93%)	253 (95%)	13 (5%)	25	61
3	C	256/267 (96%)	241 (94%)	15 (6%)	19	54
3	F	255/267 (96%)	240 (94%)	15 (6%)	19	54
All	All	1195/1270 (94%)	1123 (94%)	72 (6%)	19	53

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	117	ASN
3	F	390	ASN
3	F	152	ASP
3	F	304	PHE
3	C	135	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	390	ASN
2	E	253	GLN
3	F	239	GLN
1	D	184	GLN
2	E	189	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	NAG	E	470	-	14,14,15	0.43	0	17,19,21	0.70	1 (5%)
4	NAG	E	471	-	14,14,15	0.42	0	17,19,21	0.64	0
4	NAG	B	471	-	14,14,15	0.44	0	17,19,21	0.52	0
4	NAG	B	470	-	14,14,15	0.44	0	17,19,21	0.69	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	E	470	-	-	2/6/23/26	0/1/1/1
4	NAG	E	471	-	-	3/6/23/26	0/1/1/1
4	NAG	B	471	-	-	3/6/23/26	0/1/1/1
4	NAG	B	470	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	470	NAG	C2-N2-C7	-2.02	120.03	122.90

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	471	NAG	O5-C5-C6-O6
4	B	471	NAG	C4-C5-C6-O6
4	E	471	NAG	O5-C5-C6-O6
4	E	470	NAG	O5-C5-C6-O6
4	E	471	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	471	NAG	1	0
4	B	471	NAG	10	0
4	B	470	NAG	9	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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.