



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:42 am GMT

PDB ID : 1FZA
Title : CRYSTAL STRUCTURE OF FIBRINOGEN FRAGMENT D
Authors : Spraggon, G.; Everse, S.J.; Doolittle, R.F.
Deposited on : 1997-08-05
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

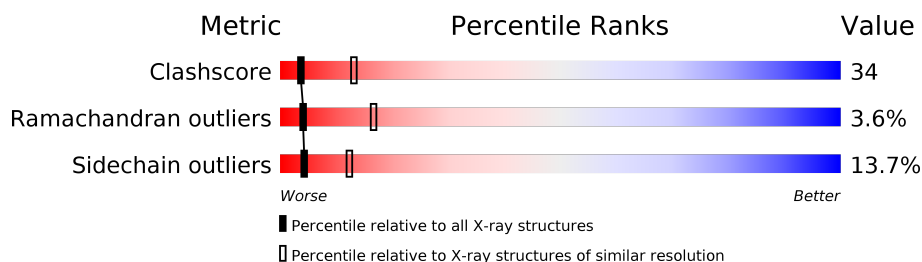
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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 $\leq 5\%$. 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	87	
1	D	87	
2	B	328	
2	E	328	
3	C	319	
3	F	319	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11418 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	85	Total	C	N	O	S	0	0	0
			697	432	132	130	3			
1	D	85	Total	C	N	O	S	0	0	0
			697	432	132	130	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	313	Total	C	N	O	S	0	0	0
			2517	1571	444	480	22			
2	E	313	Total	C	N	O	S	0	0	0
			2517	1571	444	480	22			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	309	Total	C	N	O	S	0	0	0
			2480	1574	415	478	13			
3	F	309	Total	C	N	O	S	0	0	0
			2480	1574	415	478	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	LYS	ILE	CONFLICT	UNP P02679
F	88	LYS	ILE	CONFLICT	UNP P02679

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

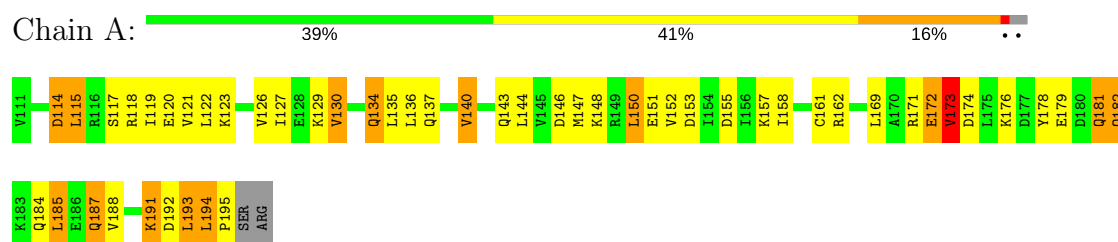
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

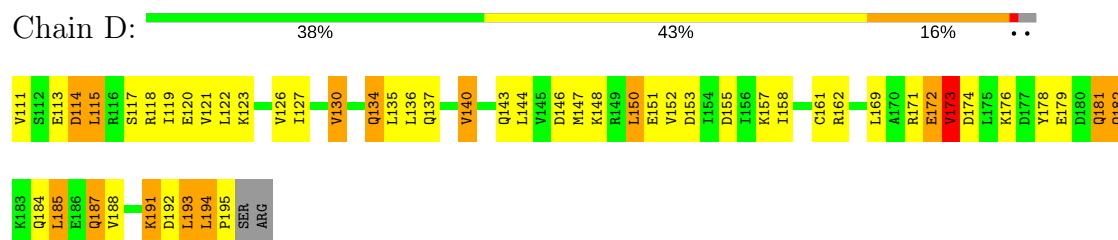
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

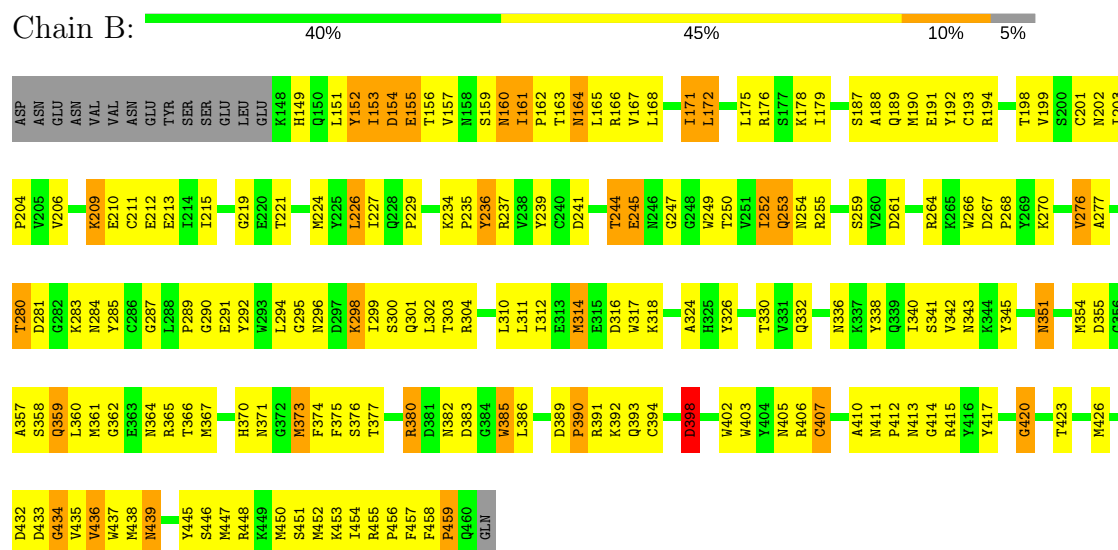
• Molecule 1: FIBRINOGEN



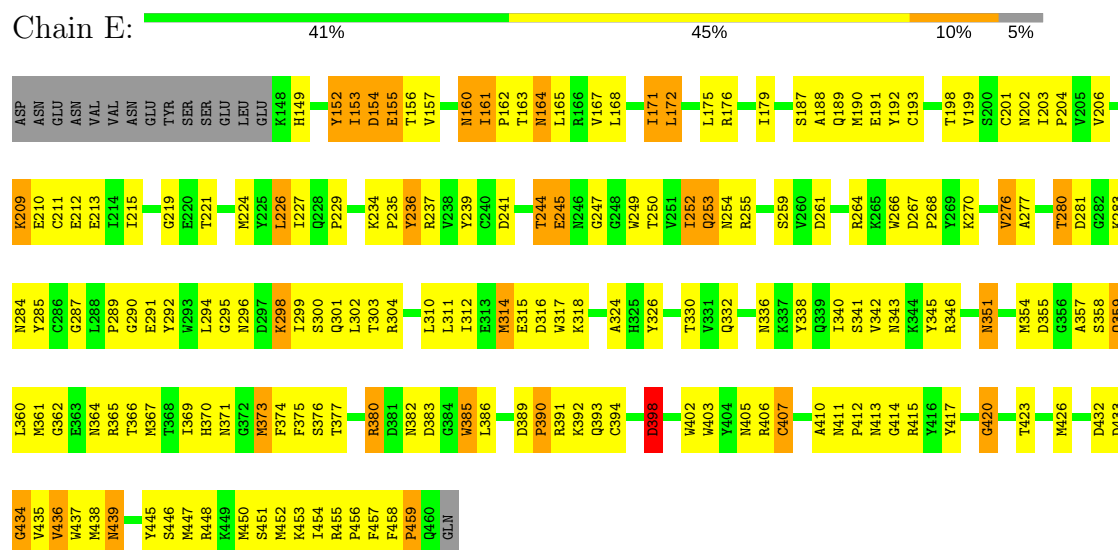
• Molecule 1: FIBRINOGEN



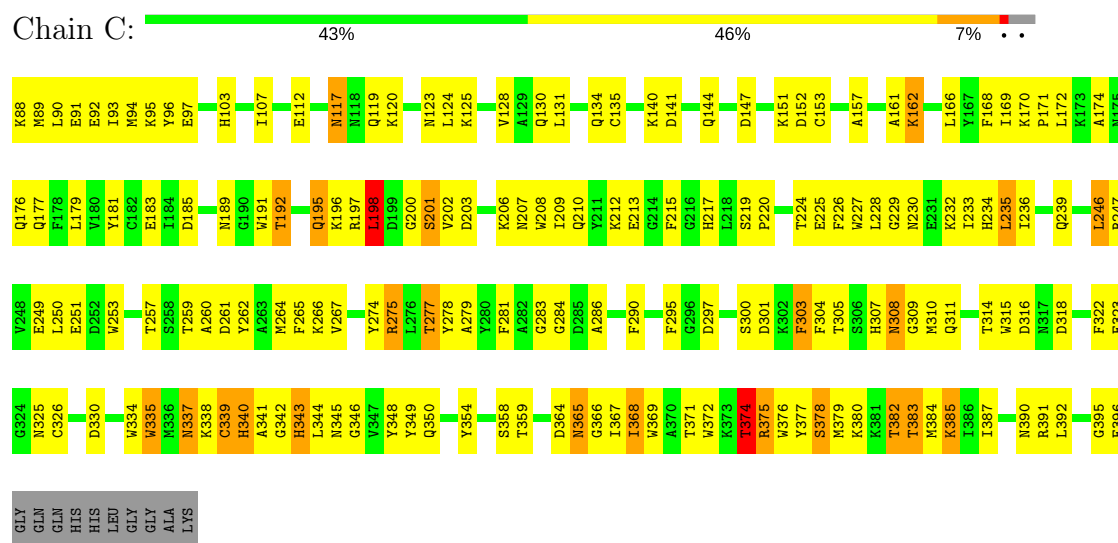
• Molecule 2: FIBRINOGEN



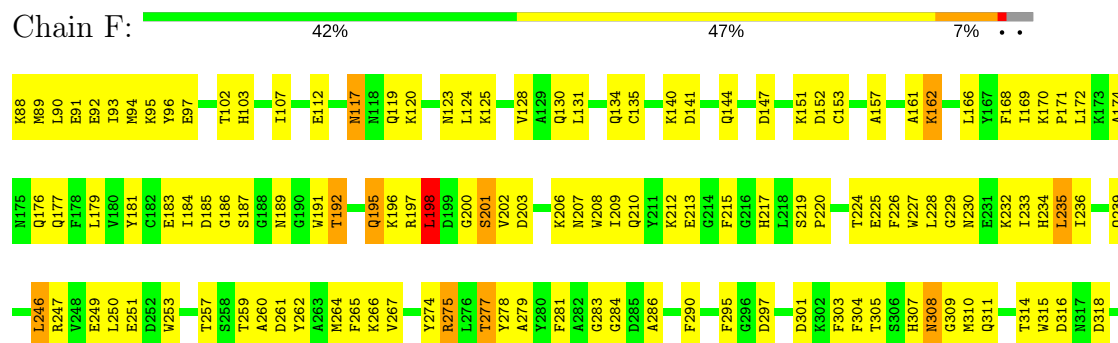
• Molecule 2: FIBRINOGEN



• Molecule 3: FIBRINOGEN



• Molecule 3: FIBRINOGEN



E396	F322
GLY	F323
GLN	G324
GLN	N325
HIS	N326
HIS	D330
LEU	M331
GLY	W334
GLY	N335
ALA	K336
LYS	R337
	K338
	C339
	H340
	A341
	G342
	H343
	L344
	N345
	G346
	V347
	Y348
	Y349
	Q350
	Y354
	S358
	T359
	D364
	N365
	G366
	I367
	L368
	W369
	A370
	T371
	W372
	K373
	T374
	R375
	W376
	Y377
	S378
	M379
	K380
	K381
	T382
	T383
	M384
	K385
	L386
	L387
	N390
	R391
	C395

4 Data and refinement statistics

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	107.72Å 48.08Å 167.56Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	87.1 (30.00-2.90)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.263 , 0.363	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11418	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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	0.56	0/699	0.75	0/933
1	D	0.56	0/699	0.75	0/933
2	B	0.57	0/2581	0.84	1/3487 (0.0%)
2	E	0.57	0/2581	0.84	1/3487 (0.0%)
3	C	0.51	0/2546	0.71	0/3440
3	F	0.51	0/2546	0.71	0/3440
All	All	0.55	0/11652	0.77	2/15720 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	247	GLY	N-CA-C	-5.09	100.39	113.10
2	B	247	GLY	N-CA-C	-5.07	100.43	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	236	TYR	Sidechain
2	E	236	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	697	0	744	51	0
1	D	697	0	744	50	3
2	B	2517	0	2380	176	4
2	E	2517	0	2380	180	0
3	C	2480	0	2333	180	3
3	F	2480	0	2332	180	4
4	B	14	0	13	2	0
4	E	14	0	13	3	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
All	All	11418	0	10939	764	7

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 34.

The worst 5 of 764 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)
3:C:396:GLU:HA	3:F:187:SER:N	1.59	1.18
1:A:194:LEU:HB3	1:A:195:PRO:HD3	1.33	1.07
3:C:396:GLU:HA	3:F:186:GLY:C	1.74	1.07
1:D:194:LEU:HB3	1:D:195:PRO:HD3	1.33	1.05
3:C:310:MET:SD	3:C:337:ASN:HB2	1.97	1.05

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:303:PHE:CD2	3:F:277:THR:CG2[2_746]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:303:PHE:CE2	3:F:277:THR:CG2[2_746]	1.65	0.55
2:B:159:SER:CB	1:D:114:ASP:OD1[2_545]	1.85	0.35
2:B:162:PRO:CG	1:D:113:GLU:OE1[2_545]	1.93	0.27
3:C:300:SER:CB	3:F:275:ARG:NH1[2_746]	2.06	0.14

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	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	2	10
1	D	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	2	10
2	B	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	3	14
2	E	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	3	14
3	C	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	5	21
3	F	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	5	21
All	All	1402/1468 (96%)	1118 (80%)	234 (17%)	50 (4%)	4	17

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
2	B	245	GLU
2	B	280	THR
2	B	398	ASP
2	B	420	GLY

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	80/82 (98%)	62 (78%)	18 (22%)	1	3
1	D	80/82 (98%)	62 (78%)	18 (22%)	1	3
2	B	271/286 (95%)	237 (88%)	34 (12%)	5	16
2	E	271/286 (95%)	237 (88%)	34 (12%)	5	16
3	C	261/267 (98%)	229 (88%)	32 (12%)	5	16
3	F	261/267 (98%)	229 (88%)	32 (12%)	5	16
All	All	1224/1270 (96%)	1056 (86%)	168 (14%)	4	12

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	365	ASN
1	D	173	VAL
3	F	337	ASN
3	C	375	ARG
1	D	130	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	329	GLN
2	E	160	ASN
3	F	317	ASN
3	C	337	ASN
1	D	137	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	1	-	14,14,15	0.55	0	15,19,21	0.75	0
4	NAG	E	1	-	14,14,15	0.54	0	15,19,21	0.74	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	B	1	-	-	0/6/23/26	0/1/1/1
4	NAG	E	1	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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
4	B	1	NAG	2	0
4	E	1	NAG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.