



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

PDB ID : 1FZG
Title : CRYSTAL STRUCTURE OF FRAGMENT D FROM HUMAN FIBRINOGEN WITH THE PEPTIDE LIGAND GLY-HIS-ARG-PRO-AMIDE
Authors : Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on : 1999-01-01
Resolution : 2.50 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 (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

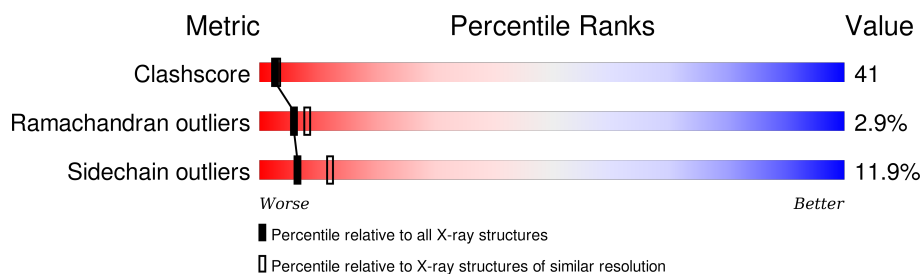
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	
4	M	4	

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Mol	Chain	Length	Quality of chain
4	N	4	
4	S	4	
4	T	4	

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
5	NAG	B	470	-	-	X	-
5	NAG	E	470	-	-	X	-
5	NAG	E	471	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10713 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	67	Total	C	N	O	S	0	0	0
			546	337	103	103	3			
1	D	54	Total	C	N	O	S	0	0	0
			440	269	84	84	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2427	1515	429	461	22			
2	E	296	Total	C	N	O	S	0	0	0
			2376	1484	420	450	22			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2342	1485	396	450	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	T	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	M	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	N	4	Total	C	N	O	0	0	0
			31	19	9	3			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

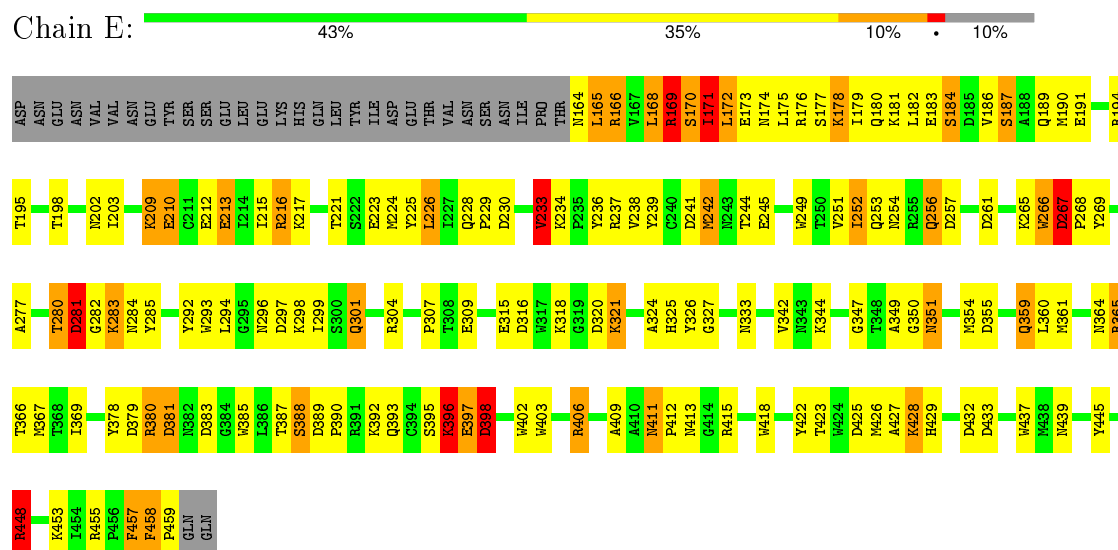
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		
6	C	2	Total	Ca	0	0
			2	2		
6	F	2	Total	Ca	0	0
			2	2		
6	E	2	Total	Ca	0	0
			2	2		

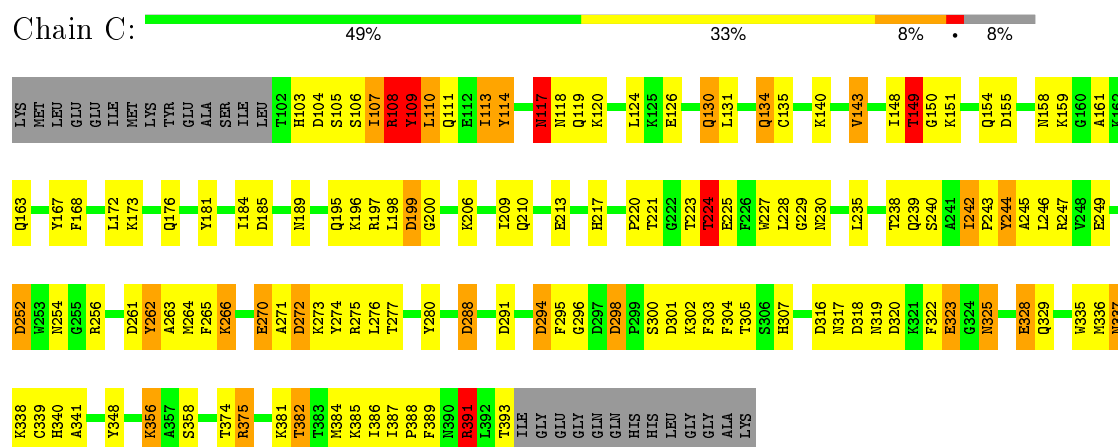
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	31	Total	O	0	0
			31	31		
7	C	20	Total	O	0	0
			20	20		
7	D	3	Total	O	0	0
			3	3		
7	E	29	Total	O	0	0
			29	29		
7	F	23	Total	O	0	0
			23	23		

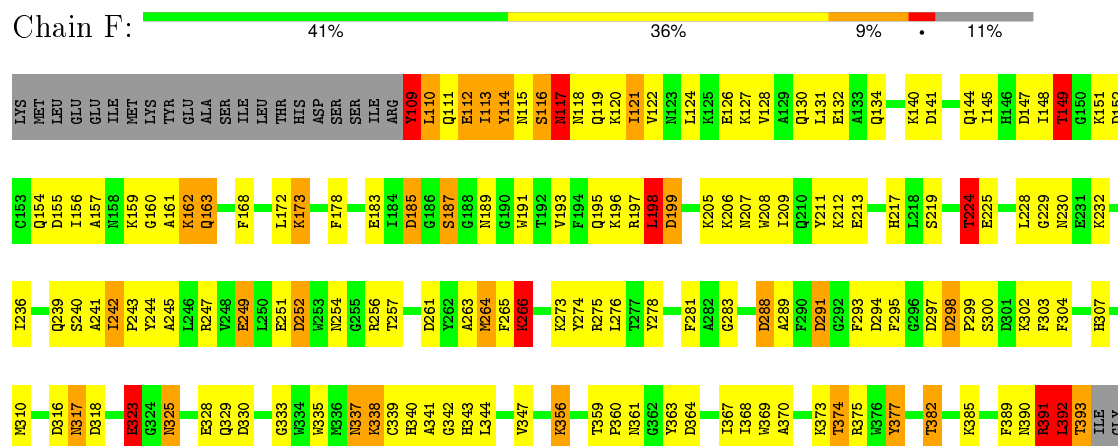
• Molecule 2: FIBRINOGEN



• Molecule 3: FIBRINOGEN



• Molecule 3: FIBRINOGEN

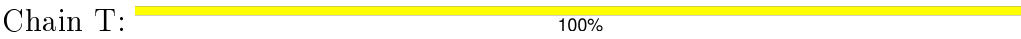


GLU
GLY
GLN
HIS
LEU
GLY
ALA
LYS

● Molecule 4: FIBRINOGEN



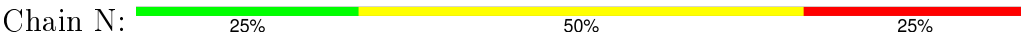
● Molecule 4: FIBRINOGEN



● Molecule 4: FIBRINOGEN



● Molecule 4: FIBRINOGEN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.80 Å 149.40 Å 234.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	88.5 (30.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.233 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10713	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	0.72	0/547	2.37	20/730 (2.7%)
1	D	0.73	0/440	2.68	21/586 (3.6%)
2	B	0.95	2/2489 (0.1%)	2.25	110/3363 (3.3%)
2	E	0.86	1/2437 (0.0%)	2.24	92/3290 (2.8%)
3	C	0.86	2/2407 (0.1%)	2.02	71/3256 (2.2%)
3	F	0.77	1/2351 (0.0%)	1.89	57/3180 (1.8%)
4	M	1.13	0/32	4.00	3/42 (7.1%)
4	N	0.84	0/32	4.64	2/42 (4.8%)
4	S	1.04	0/32	4.51	4/42 (9.5%)
4	T	0.83	0/32	1.68	0/42
All	All	0.85	6/10799 (0.1%)	2.18	380/14573 (2.6%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	GLY	N-CA	8.02	1.58	1.46
2	E	350	GLY	N-CA	7.45	1.57	1.46
3	C	229	GLY	N-CA	7.23	1.56	1.46
3	F	229	GLY	N-CA	6.59	1.55	1.46
2	B	395	SER	CB-OG	-5.82	1.34	1.42

The worst 5 of 380 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	448	ARG	CD-NE-CZ	35.69	173.56	123.60
1	D	162	ARG	CD-NE-CZ	34.21	171.49	123.60
4	N	3	ARG	CD-NE-CZ	27.48	162.08	123.60
2	E	455	ARG	NE-CZ-NH2	-23.33	108.63	120.30
1	A	159	ARG	NE-CZ-NH1	22.89	131.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	427	ALA	Mainchain

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	546	0	573	106	0
1	D	440	0	456	108	0
2	B	2427	0	2295	163	0
2	E	2376	0	2243	214	0
3	C	2342	0	2188	143	6
3	F	2287	0	2136	223	5
4	M	31	0	32	5	0
4	N	31	0	32	9	0
4	S	31	0	32	7	0
4	T	31	0	32	6	0
5	B	28	0	25	10	0
5	E	28	0	25	11	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	1	0	0	0	0
7	B	31	0	0	10	0
7	C	20	0	0	2	0
7	D	3	0	0	2	0
7	E	29	0	0	8	0
7	F	23	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10713	0	10069	841	6

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 41.

The worst 5 of 841 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:LEU:HD11	3:F:114:TYR:CD2	1.31	1.59
3:C:104:ASP:HA	3:C:107:ILE:CD1	1.33	1.53
2:E:171:ILE:CG2	2:E:172:LEU:CD2	1.86	1.50
2:E:171:ILE:CG2	2:E:172:LEU:HD23	1.08	1.49
3:F:109:TYR:N	3:F:112:GLU:CB	1.78	1.46

The worst 5 of 6 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:374:THR:OG1	3:F:328:GLU:OE2[4_466]	1.16	1.04
3:C:375:ARG:NH2	3:F:361:ASN:OD1[4_466]	1.42	0.78
3:C:375:ARG:N	7:F:426:HOH:O[4_466]	1.52	0.68
3:C:374:THR:OG1	3:F:328:GLU:CD[4_466]	1.80	0.40
3:C:295:PHE:O	3:F:329:GLN:OE1[4_466]	2.01	0.19

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	65/87 (75%)	52 (80%)	6 (9%)	7 (11%)	0 0
1	D	52/87 (60%)	39 (75%)	8 (15%)	5 (10%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	301/328 (92%)	273 (91%)	19 (6%)	9 (3%)	5	7
2	E	294/328 (90%)	262 (89%)	23 (8%)	9 (3%)	5	7
3	C	290/319 (91%)	265 (91%)	24 (8%)	1 (0%)	46	68
3	F	283/319 (89%)	261 (92%)	16 (6%)	6 (2%)	9	14
4	M	2/4 (50%)	2 (100%)	0	0	100	100
4	N	2/4 (50%)	2 (100%)	0	0	100	100
4	S	2/4 (50%)	2 (100%)	0	0	100	100
4	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1293/1484 (87%)	1160 (90%)	96 (7%)	37 (3%)	6	8

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	190	ALA
2	B	169	ARG
2	B	171	ILE
2	B	281	ASP

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	62/82 (76%)	46 (74%)	16 (26%)	0	1
1	D	50/82 (61%)	40 (80%)	10 (20%)	1	3
2	B	261/286 (91%)	226 (87%)	35 (13%)	5	9
2	E	254/286 (89%)	231 (91%)	23 (9%)	12	22
3	C	246/267 (92%)	223 (91%)	23 (9%)	11	21
3	F	239/267 (90%)	214 (90%)	25 (10%)	8	16
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	S	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	T	3/3 (100%)	3 (100%)	0	100	100
All	All	1124/1282 (88%)	990 (88%)	134 (12%)	6	12

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	163	GLN
1	D	138	LYS
3	F	323	GLU
3	C	242	ILE
3	C	328	GLU

Some 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	325	ASN
2	E	271	GLN
3	F	307	HIS
3	C	329	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 ⓘ

4 carbohydrates 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	B	470	2,5	14,14,15	1.19	1 (7%)	15,19,21	4.36	6 (40%)
5	NAG	B	471	5	14,14,15	1.52	2 (14%)	15,19,21	4.06	4 (26%)
5	NAG	E	470	2,5	14,14,15	1.29	1 (7%)	15,19,21	1.84	4 (26%)
5	NAG	E	471	5	14,14,15	1.36	2 (14%)	15,19,21	2.09	4 (26%)

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	B	470	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	471	5	-	0/6/23/26	0/1/1/1
5	NAG	E	470	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	471	5	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	471	NAG	O7-C7	-3.77	1.14	1.23
5	E	470	NAG	O7-C7	-3.73	1.14	1.23
5	B	470	NAG	O7-C7	-3.27	1.15	1.23
5	B	471	NAG	O7-C7	-3.04	1.16	1.23
5	E	471	NAG	C2-N2	2.64	1.51	1.46

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	471	NAG	C1-O5-C5	-13.34	95.31	112.25
5	B	470	NAG	C4-C3-C2	-8.37	98.21	111.23
5	B	470	NAG	O4-C4-C3	-7.65	93.12	110.34
5	E	471	NAG	C1-O5-C5	-5.46	105.32	112.25
5	B	470	NAG	C2-N2-C7	-4.75	116.94	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	10	0
5	B	471	NAG	4	0
5	E	470	NAG	11	0
5	E	471	NAG	10	0

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.