



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:52 AM UTC

PDB ID : 1FZB / pdb_00001fzb
Title : CRYSTAL STRUCTURE OF CROSSLINKED 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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

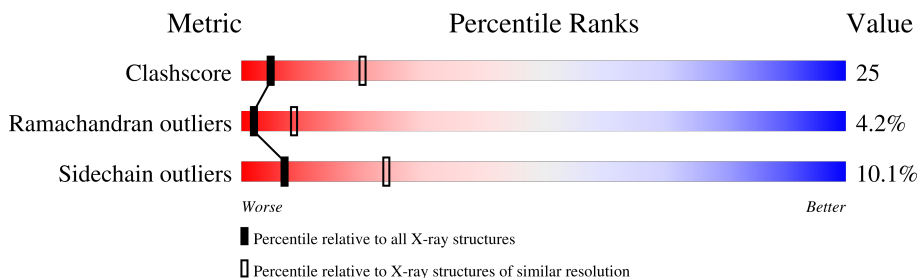
1 Overall quality at a glance

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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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	87	41% 39% 10% • 7%
1	D	87	41% 40% 9% • 7%
2	B	328	44% 41% 8% • 5%
2	E	328	46% 40% 8% • 5%
3	C	319	51% 36% 9% •
3	F	319	54% 35% 7% • •
4	G	4	50% 25% 25%
4	H	4	25% 25% 25% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11417 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	C	N	O	S	0	0	0
			669	413	128	125	3			
1	D	81	Total	C	N	O	S	0	0	0
			669	413	128	125	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	0	0	0
			2508	1566	442	478	22			
2	E	312	Total	C	N	O	S	0	0	0
			2508	1566	442	478	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	311	Total	C	N	O	S	0	0	0
			2493	1581	418	481	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 a protein called PEPTIDE LIGAND GPRG.

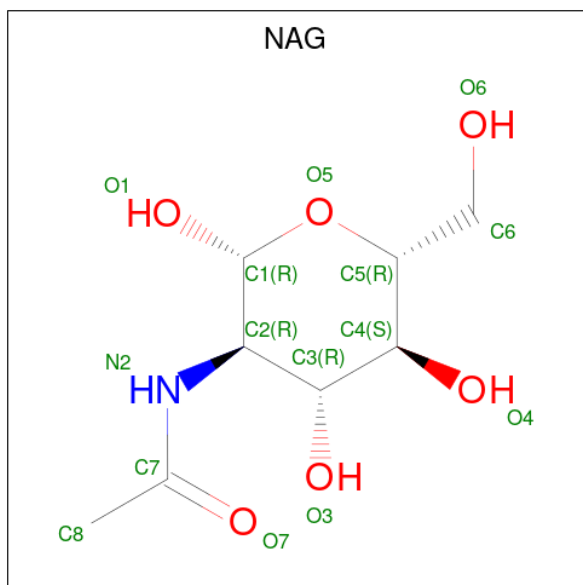
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

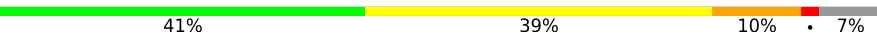
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

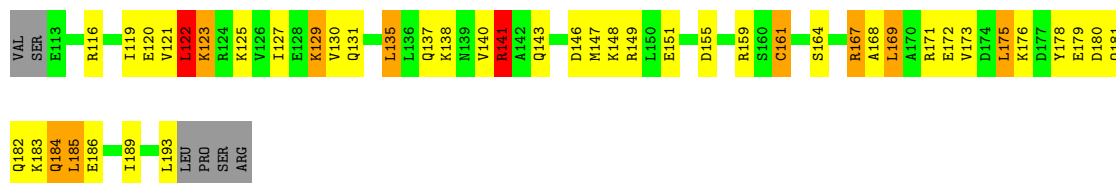
3 Residue-property plots

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.

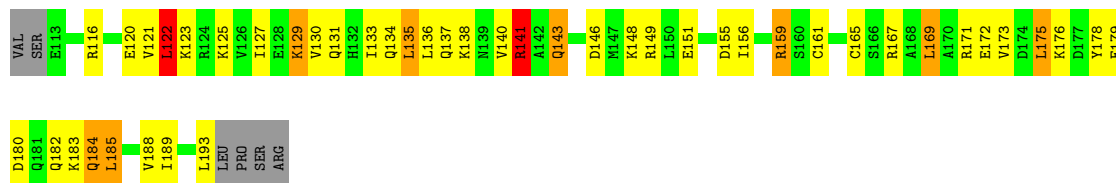
• Molecule 1: FIBRINOGEN

Chain A: 



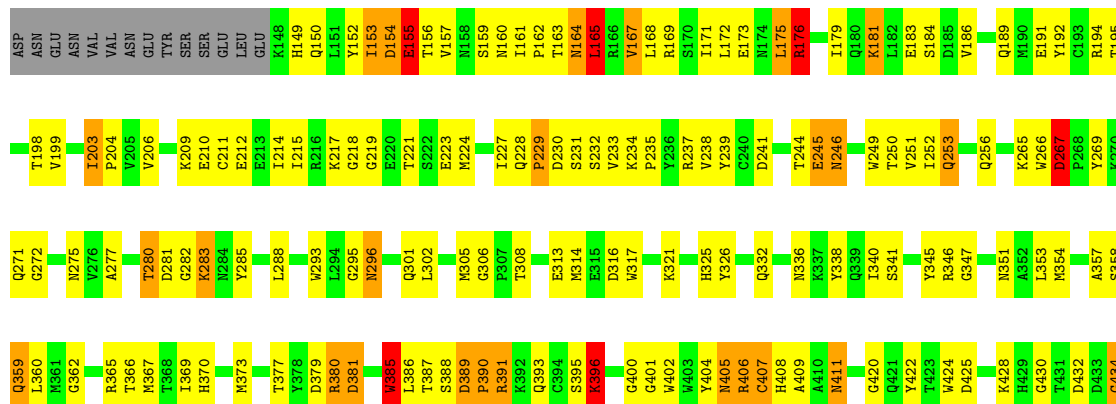
• Molecule 1: FIBRINOGEN

Chain D: 

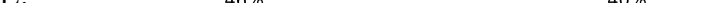


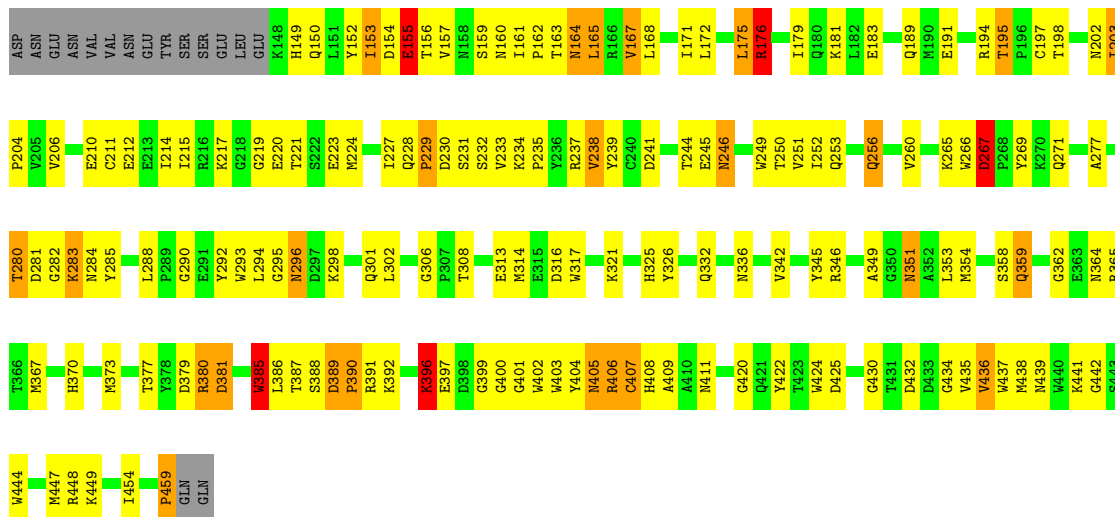
• Molecule 2: FIBRINOGEN

Chain B: 

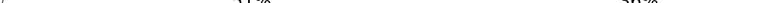


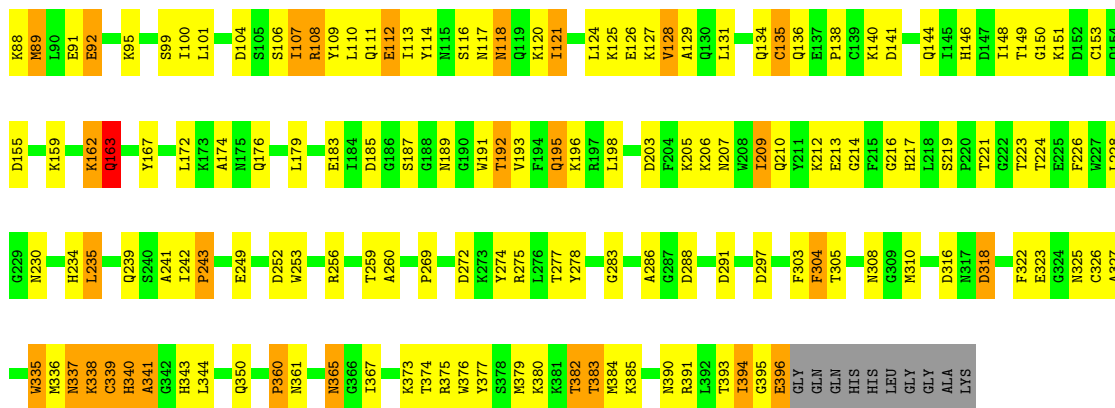
- Molecule 2: FIBRINOGEN

Chain E:  46% 40% 8% 5%



- Molecule 3: FIBRINOGEN

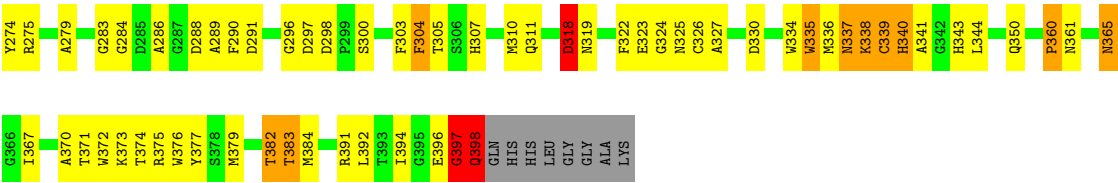
Chain C:  51% 36% 9% .



- Molecule 3: FIBRINOGEN

Chain F: 54% 35% 7% . .

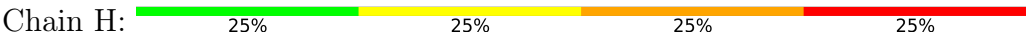




• Molecule 4: PEPTIDE LIGAND GPRG



• Molecule 4: PEPTIDE LIGAND GPRG



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	93.82Å 95.50Å 113.76Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	88.8 (30.00-2.90)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.241 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11417	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: NAG, CA

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	1/670 (0.1%)	1.10	4/892 (0.4%)
1	D	0.84	1/670 (0.1%)	1.12	4/892 (0.4%)
2	B	0.79	2/2572 (0.1%)	1.22	39/3475 (1.1%)
2	E	0.82	3/2572 (0.1%)	1.21	34/3475 (1.0%)
3	C	0.72	2/2546 (0.1%)	1.17	19/3440 (0.6%)
3	F	0.70	4/2559 (0.2%)	1.09	20/3457 (0.6%)
4	G	0.60	0/31	0.86	0/40
4	H	0.96	0/31	1.04	0/40
All	All	0.76	13/11651 (0.1%)	1.16	120/15711 (0.8%)

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	E	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	459	PRO	C-O	17.55	1.58	1.23
2	B	175	LEU	C-N	-16.50	1.11	1.34
1	D	193	LEU	C-O	15.23	1.54	1.23
2	E	175	LEU	C-N	-15.13	1.13	1.34
2	B	459	PRO	C-O	15.02	1.53	1.23

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	396	GLU	CA-C-O	-25.65	77.20	120.80
3	F	136	GLN	N-CA-C	-11.49	101.52	114.62
3	C	136	GLN	N-CA-C	-11.48	101.54	114.62
1	D	193	LEU	CA-C-O	-11.40	101.43	120.80
2	E	159	SER	N-CA-C	-10.33	102.84	114.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	292	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	669	0	712	44	0
1	D	669	0	712	54	0
2	B	2508	0	2371	147	0
2	E	2508	0	2372	138	0
3	C	2480	0	2333	133	0
3	F	2493	0	2344	109	0
4	G	30	0	32	0	0
4	H	30	0	32	7	0
5	B	14	0	13	1	0
5	E	14	0	13	6	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
All	All	11417	0	10934	568	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 25.

The worst 5 of 568 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:C	3:C:396:GLU:CA	1.77	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLU:CA	3:C:396:GLU:O	1.82	1.22
2:E:389:ASP:HB3	2:E:390:PRO:HD2	1.38	1.05
2:B:389:ASP:HB3	2:B:390:PRO:HD2	1.37	1.02
3:C:209:ILE:H	3:C:209:ILE:HD12	1.25	0.98

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	79/87 (91%)	72 (91%)	5 (6%)	2 (2%)	4	17
1	D	79/87 (91%)	72 (91%)	5 (6%)	2 (2%)	4	17
2	B	310/328 (94%)	263 (85%)	33 (11%)	14 (4%)	2	8
2	E	310/328 (94%)	258 (83%)	39 (13%)	13 (4%)	2	9
3	C	307/319 (96%)	264 (86%)	33 (11%)	10 (3%)	3	13
3	F	309/319 (97%)	257 (83%)	38 (12%)	14 (4%)	2	8
4	G	2/4 (50%)	0	0	2 (100%)	0	0
4	H	2/4 (50%)	0	0	2 (100%)	0	0
All	All	1398/1476 (95%)	1186 (85%)	153 (11%)	59 (4%)	2	9

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	149	HIS
2	B	280	THR
2	B	391	ARG
2	B	407	CYS
3	C	89	MET

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%)	62 (82%)	14 (18%)	1	6
1	D	76/82 (93%)	62 (82%)	14 (18%)	1	6
2	B	270/286 (94%)	246 (91%)	24 (9%)	9	28
2	E	270/286 (94%)	246 (91%)	24 (9%)	9	28
3	C	261/267 (98%)	239 (92%)	22 (8%)	10	31
3	F	262/267 (98%)	239 (91%)	23 (9%)	9	29
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1221/1276 (96%)	1098 (90%)	123 (10%)	7	24

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	382	THR
3	F	243	PRO
1	D	175	LEU
3	F	209	ILE
3	F	383	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	134	GLN
3	F	176	GLN
3	F	325	ASN
3	C	176	GLN
3	C	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
5	NAG	B	1	-	14,14,15	0.45	0	17,19,21	0.68	0
5	NAG	E	1	-	14,14,15	0.50	0	17,19,21	0.67	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
5	NAG	B	1	-	-	3/6/23/26	0/1/1/1
5	NAG	E	1	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C3-C2-N2-C7
5	B	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	NAG	1	0
5	E	1	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	F	1
2	E	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	397:GLY	C	398:GLN	N	1.19
1	E	175:LEU	C	176:ARG	N	1.13
1	B	175:LEU	C	176:ARG	N	1.11

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.