



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2024 – 02:36 PM EDT

PDB ID : 1DVA
Title : Crystal Structure of the Complex Between the Peptide Exosite Inhibitor E-76 and Coagulation Factor VIIA
Authors : Eigenbrot, C.; Ultsch, M.H.
Deposited on : 2000-01-20
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 ⓘ 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

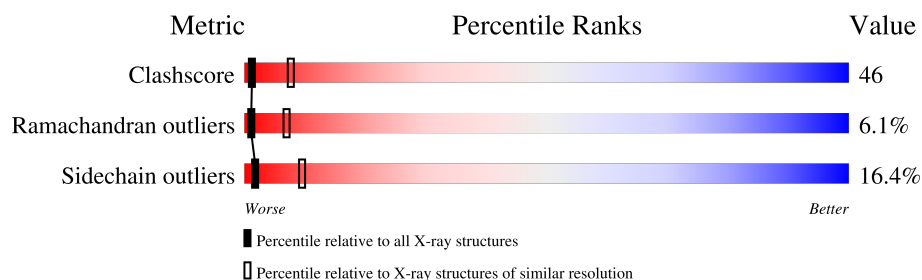
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.


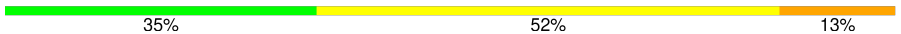
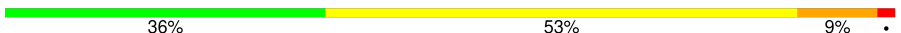

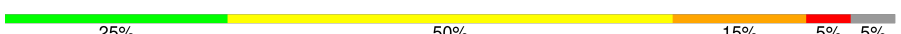
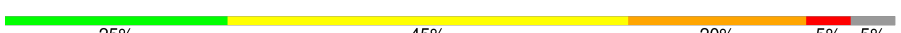

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	254	
1	I	254	
2	L	101	
2	M	101	
3	X	20	
3	Y	20	
4	A	2	

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
9	GLC	M	503	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5917 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 DES-GLA FACTOR VIIA (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	254	Total	C	N	O	S	85	0	0
			1974	1253	351	357	13			
1	I	254	Total	C	N	O	S	118	0	0
			1974	1253	351	357	13			

- Molecule 2 is a protein called DES-GLA FACTOR VIIA (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	101	Total	C	N	O	S	42	0	0
			759	456	130	160	13			
2	M	101	Total	C	N	O	S	116	0	0
			759	456	130	160	13			

- Molecule 3 is a protein called PEPTIDE E-76.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	19	Total	C	N	O	S	0	0	1
			151	95	26	28	2			
3	Y	19	Total	C	N	O	S	0	0	1
			151	95	26	28	2			

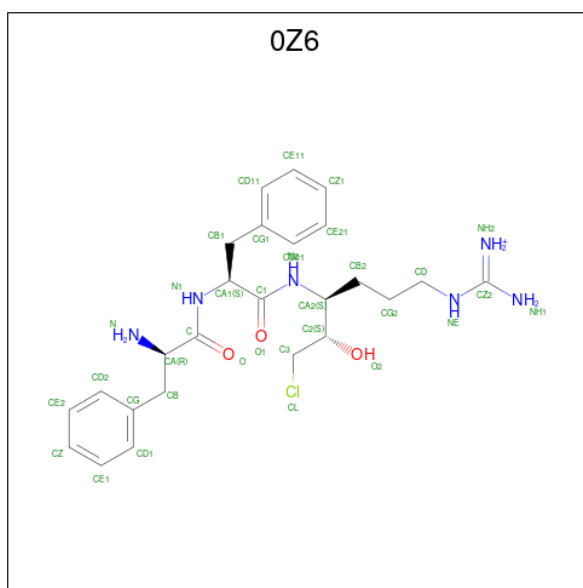
- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	A	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 5 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydro

xyhexan-3-yl]-L-phenylalaninamide (three-letter code: 0Z6) (formula: $C_{25}H_{36}ClN_6O_3$).

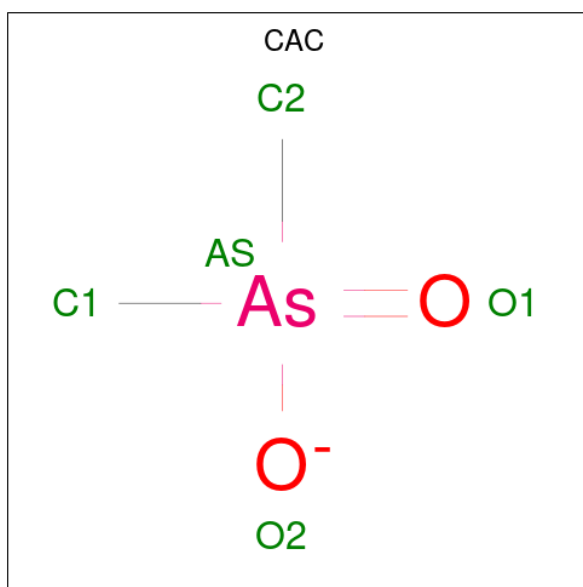


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			34	25	6	3		
5	I	1	Total	C	N	O	0	0
			34	25	6	3		

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

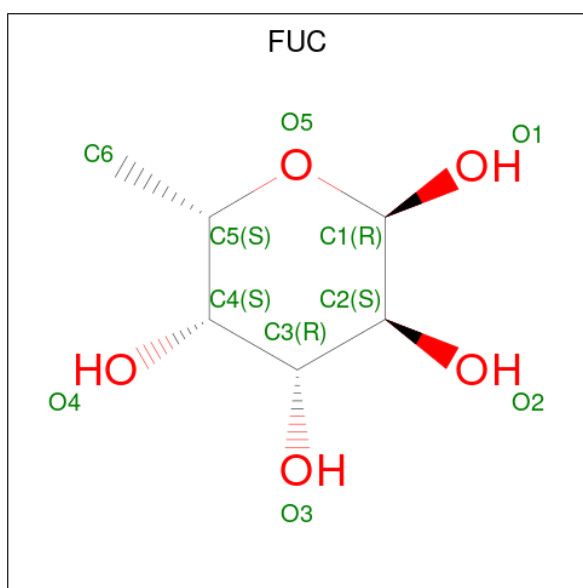
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Ca	0	0
			1	1		
6	L	1	Total	Ca	0	0
			1	1		
6	I	1	Total	Ca	0	0
			1	1		
6	M	1	Total	Ca	0	0
			1	1		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



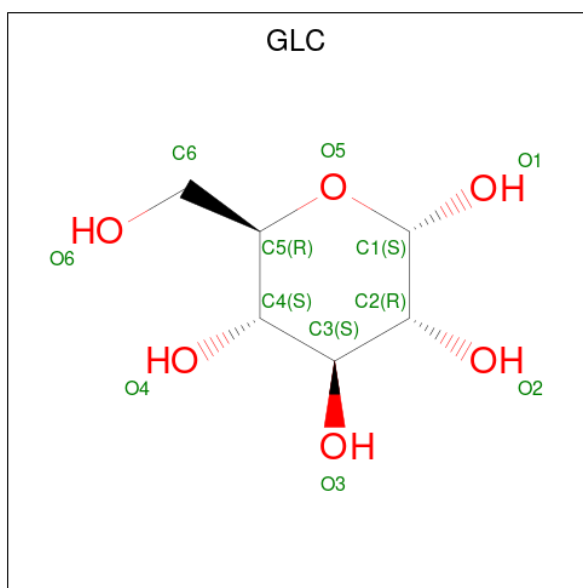
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	H	1	Total	As	C	O	4	0
			5	1	2	2		
7	I	1	Total	As	C	O	4	0
			5	1	2	2		

- Molecule 8 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



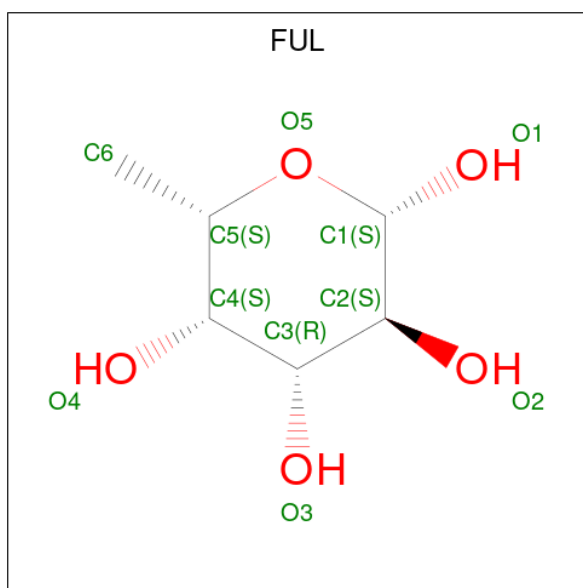
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			10	6	4		
8	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is beta-L-fucopyranose (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	10	0
			10	6	4		

- Molecule 11 is water.

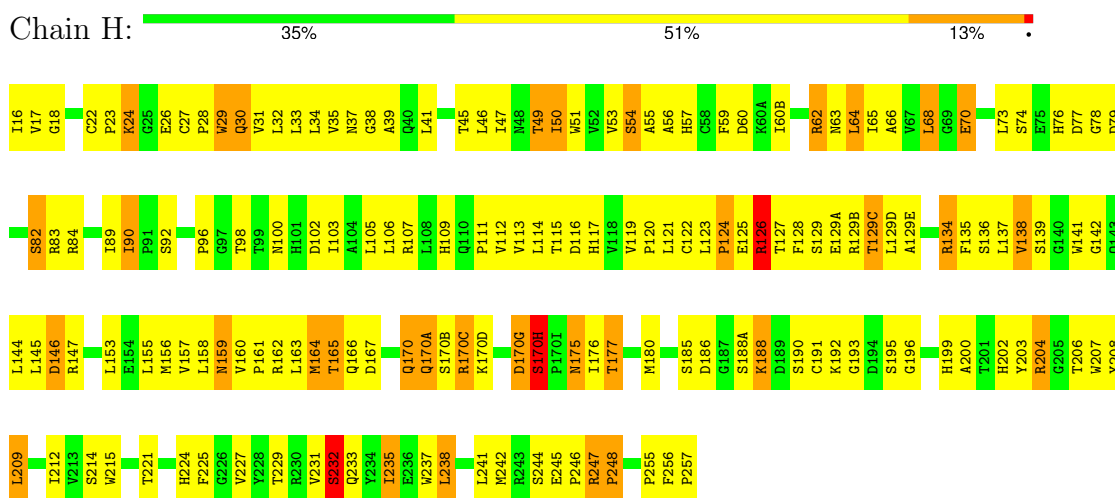
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	3	Total 3	O 3	0	0
11	I	1	Total 1	O 1	0	0

3 Residue-property plots

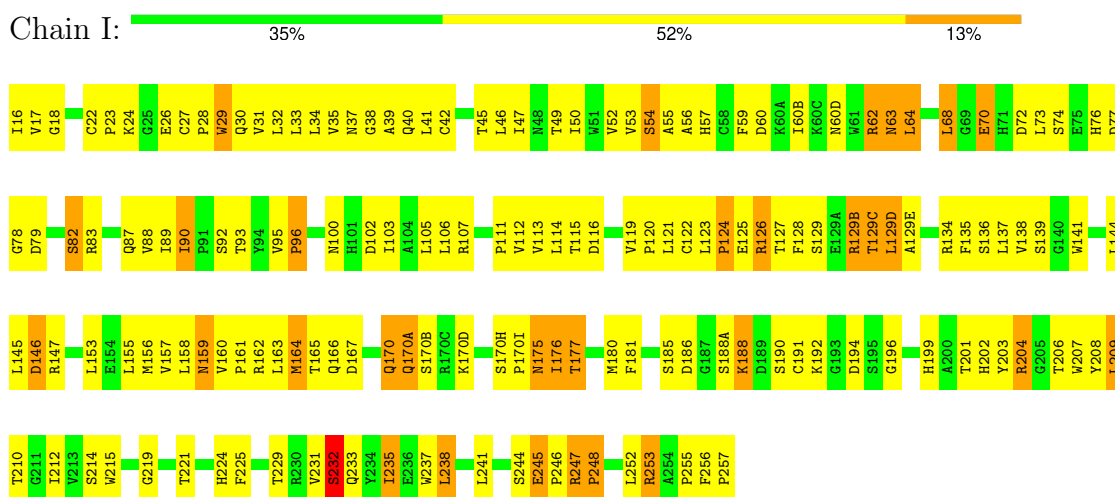
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: DES-GLA FACTOR VIIA (HEAVY CHAIN)

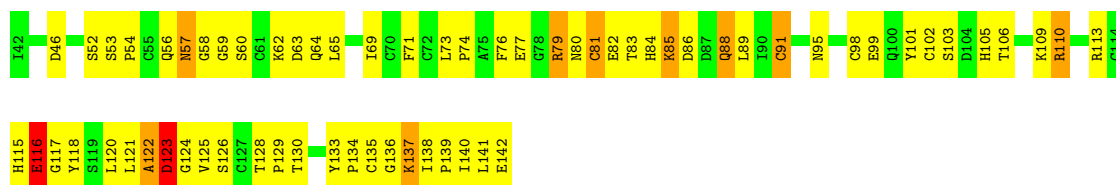


• Molecule 1: DES-GLA FACTOR VIIA (HEAVY CHAIN)

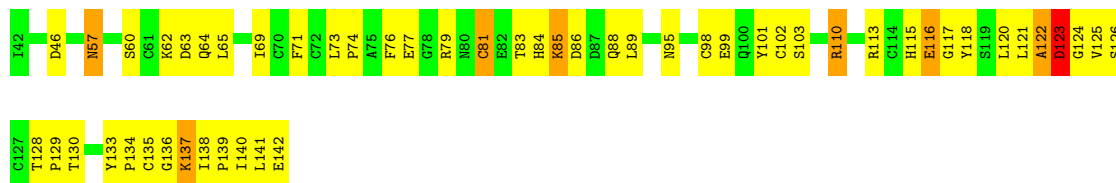


• Molecule 2: DES-GLA FACTOR VIIA (LIGHT CHAIN)





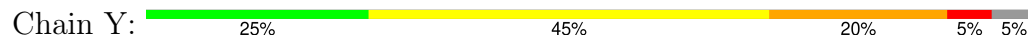
• Molecule 2: DES-GLA FACTOR VIIA (LIGHT CHAIN)



• Molecule 3: PEPTIDE E-76



• Molecule 3: PEPTIDE E-76



• Molecule 4: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



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	70.49Å 55.26Å 111.73Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	97.5 (50.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.225 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5917	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: FUL, CA, GAL, FUC, BGC, ACE, GLC, CAC, OZ6

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	H	0.63	0/2024	0.87	2/2755 (0.1%)
1	I	0.60	0/2024	0.85	1/2755 (0.0%)
2	L	0.53	0/773	0.75	0/1043
2	M	0.55	0/773	0.74	0/1043
3	X	0.76	0/153	1.05	1/209 (0.5%)
3	Y	0.73	0/153	1.04	1/209 (0.5%)
All	All	0.61	0/5900	0.84	5/8014 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1	ALA	N-CA-C	-6.96	92.20	111.00
1	H	170(C)	ARG	N-CA-C	-6.89	92.39	111.00
3	Y	1	ALA	N-CA-C	-6.55	93.31	111.00
1	H	199	HIS	N-CA-C	-5.44	96.32	111.00
1	I	199	HIS	N-CA-C	-5.42	96.36	111.00

There are no chirality outliers.

There are no planarity outliers.

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	H	1974	0	1949	195	0
1	I	1974	0	1949	197	0
2	L	759	0	679	60	0
2	M	759	0	679	48	0
3	X	151	0	132	18	0
3	Y	151	0	132	18	0
4	A	22	0	19	3	0
5	H	34	0	32	4	0
5	I	34	0	32	3	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
7	H	5	0	0	0	0
7	I	5	0	0	0	0
8	L	20	0	20	2	0
9	M	11	0	10	0	0
10	M	10	0	10	0	0
11	H	3	0	0	0	0
11	I	1	0	0	1	0
All	All	5917	0	5643	496	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 46.

The worst 5 of 496 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:H:247:ARG:HG3	1:H:248:PRO:CD	1.82	1.09
1:H:232:SER:HA	1:H:235:ILE:HD11	1.36	1.03
1:H:247:ARG:HG3	1:H:248:PRO:HD2	1.04	1.02
1:I:232:SER:HA	1:I:235:ILE:HD11	1.40	1.00
1:H:247:ARG:CG	1:H:248:PRO:HD2	1.95	0.95

There are no symmetry-related clashes.

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	H	252/254 (99%)	202 (80%)	34 (14%)	16 (6%)	1	6
1	I	252/254 (99%)	200 (79%)	40 (16%)	12 (5%)	2	11
2	L	99/101 (98%)	83 (84%)	8 (8%)	8 (8%)	1	3
2	M	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	1	4
3	X	17/20 (85%)	15 (88%)	1 (6%)	1 (6%)	1	7
3	Y	17/20 (85%)	14 (82%)	2 (12%)	1 (6%)	1	7
All	All	736/750 (98%)	595 (81%)	96 (13%)	45 (6%)	1	7

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	49	THR
1	H	78	GLY
1	H	146	ASP
1	H	170(A)	GLN
2	L	123	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	H	216/216 (100%)	178 (82%)	38 (18%)	1	8
1	I	216/216 (100%)	179 (83%)	37 (17%)	1	8
2	L	88/88 (100%)	77 (88%)	11 (12%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	88/88 (100%)	77 (88%)	11 (12%)	3	17
3	X	16/16 (100%)	12 (75%)	4 (25%)	0	2
3	Y	16/16 (100%)	12 (75%)	4 (25%)	0	2
All	All	640/640 (100%)	535 (84%)	105 (16%)	2	9

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	63	ASN
1	I	159	ASN
2	M	137	LYS
1	I	68	LEU
1	I	126	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	95	ASN
1	I	217	GLN
1	I	60(D)	ASN
1	I	175	ASN
1	I	30	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 ⓘ

2 monosaccharides 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$
4	BGC	A	1	4,2	11,11,12	0.83	0	15,15,17	1.28	1 (6%)
4	GAL	A	2	4	11,11,12	0.96	1 (9%)	15,15,17	0.81	1 (6%)

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	BGC	A	1	4,2	-	0/2/19/22	0/1/1/1
4	GAL	A	2	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	GAL	O5-C5	2.17	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	BGC	C1-C2-C3	3.69	115.02	109.64
4	A	2	GAL	C1-C2-C3	-2.13	106.54	109.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

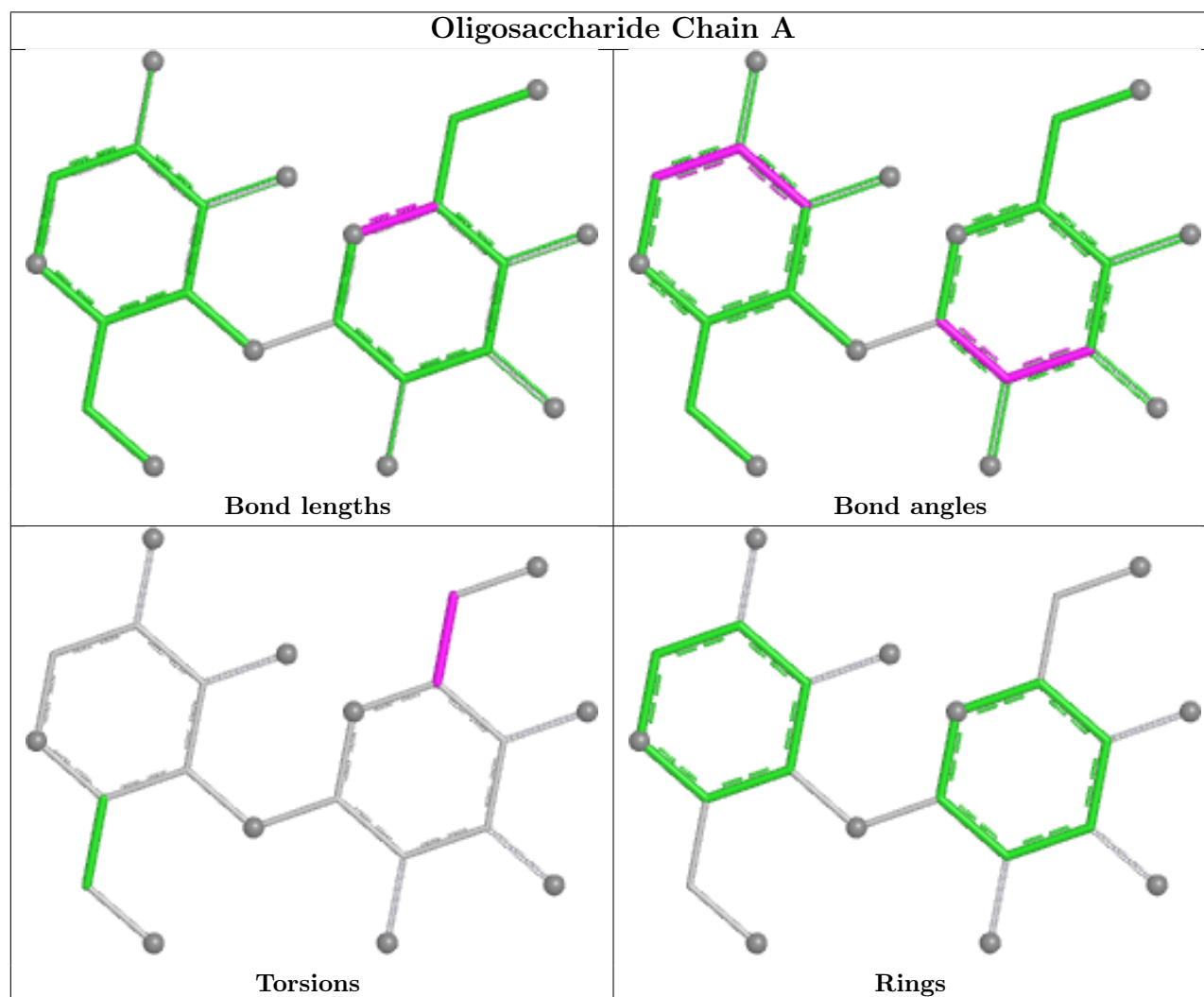
Mol	Chain	Res	Type	Atoms
4	A	2	GAL	O5-C5-C6-O6
4	A	2	GAL	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	GAL	2	0
4	A	1	BGC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
9	GLC	M	503	2	11,11,12	0.83	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FUC	L	504	2	10,10,11	1.22	2 (20%)	14,14,16	1.12	2 (14%)
5	OZ6	H	1	1	34,35,36	1.38	1 (2%)	41,45,46	0.84	3 (7%)
7	CAC	H	310	-	2,4,4	0.52	0	2,6,6	0.32	0
8	FUC	L	506	-	10,10,11	0.81	0	14,14,16	0.59	0
5	OZ6	I	1	1	34,35,36	1.45	1 (2%)	41,45,46	0.96	3 (7%)
10	FUL	M	505	2	10,10,11	0.58	0	14,14,16	0.58	0
7	CAC	I	311	-	2,4,4	0.47	0	2,6,6	0.44	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
9	GLC	M	503	2	1/1/4/5	0/2/19/22	0/1/1/1
8	FUC	L	504	2	-	-	0/1/1/1
5	OZ6	H	1	1	-	5/35/35/37	0/2/2/2
8	FUC	L	506	-	-	-	0/1/1/1
5	OZ6	I	1	1	-	5/35/35/37	0/2/2/2
10	FUL	M	505	2	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	OZ6	O2-C2	-7.74	1.22	1.43
5	H	1	OZ6	O2-C2	-7.71	1.22	1.43
8	L	504	FUC	O5-C5	2.44	1.48	1.43
8	L	504	FUC	C1-C2	-2.16	1.47	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	OZ6	O2-C2-C3	3.19	119.21	109.68
5	I	1	OZ6	CA2-N2-C1	-3.04	117.97	123.25
5	H	1	OZ6	CA2-N2-C1	-2.77	118.42	123.25
5	H	1	OZ6	C2-CA2-N2	2.36	115.18	110.90
8	L	504	FUC	O2-C2-C1	-2.14	104.32	109.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	M	503	GLC	C1

5 of 10 torsion outliers are listed below:

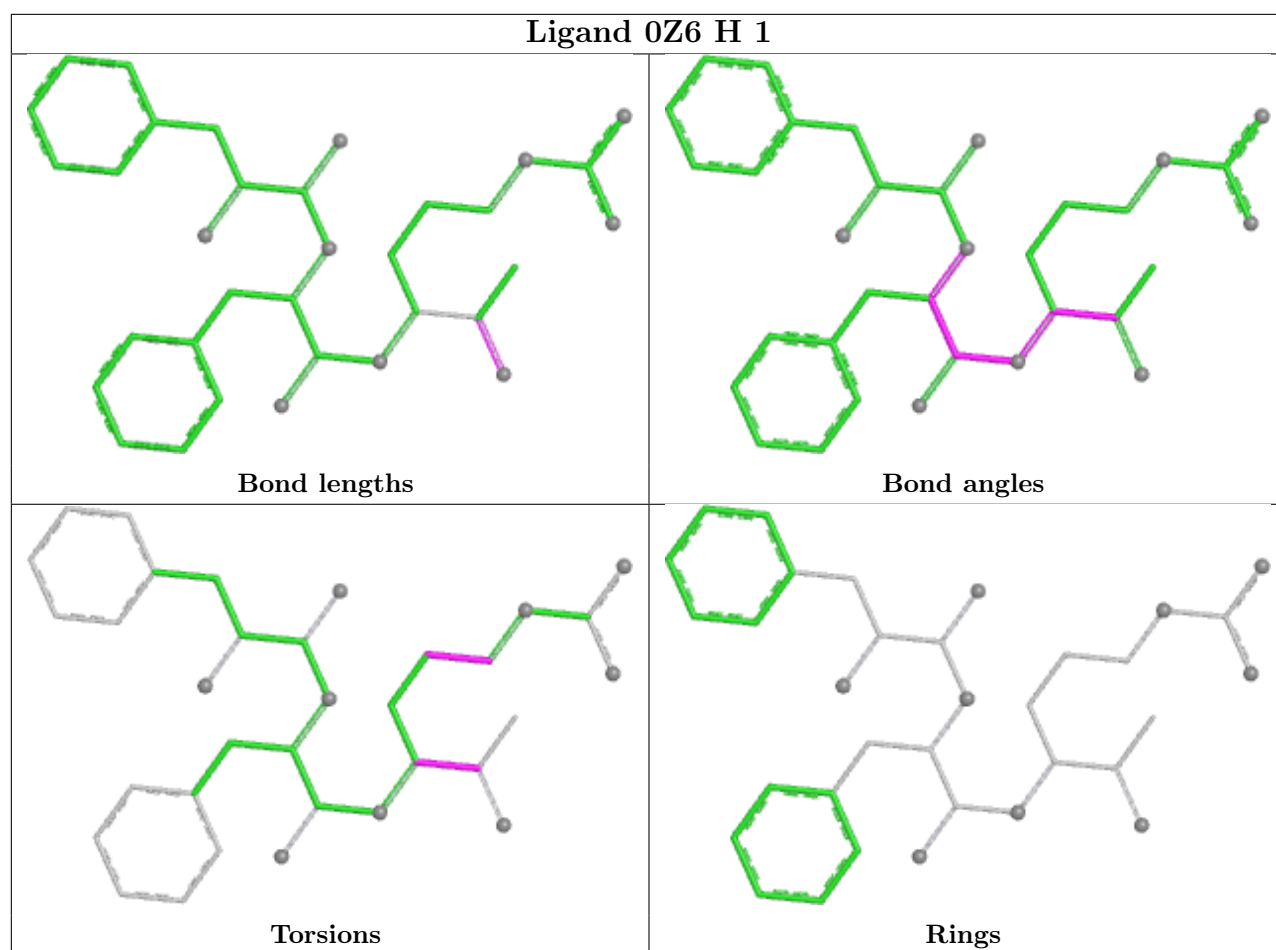
Mol	Chain	Res	Type	Atoms
5	I	1	0Z6	C3-C2-CA2-N2
5	H	1	0Z6	NE-CD-CG2-CB2
5	I	1	0Z6	NE-CD-CG2-CB2
5	H	1	0Z6	C3-C2-CA2-N2
5	I	1	0Z6	C3-C2-CA2-CB2

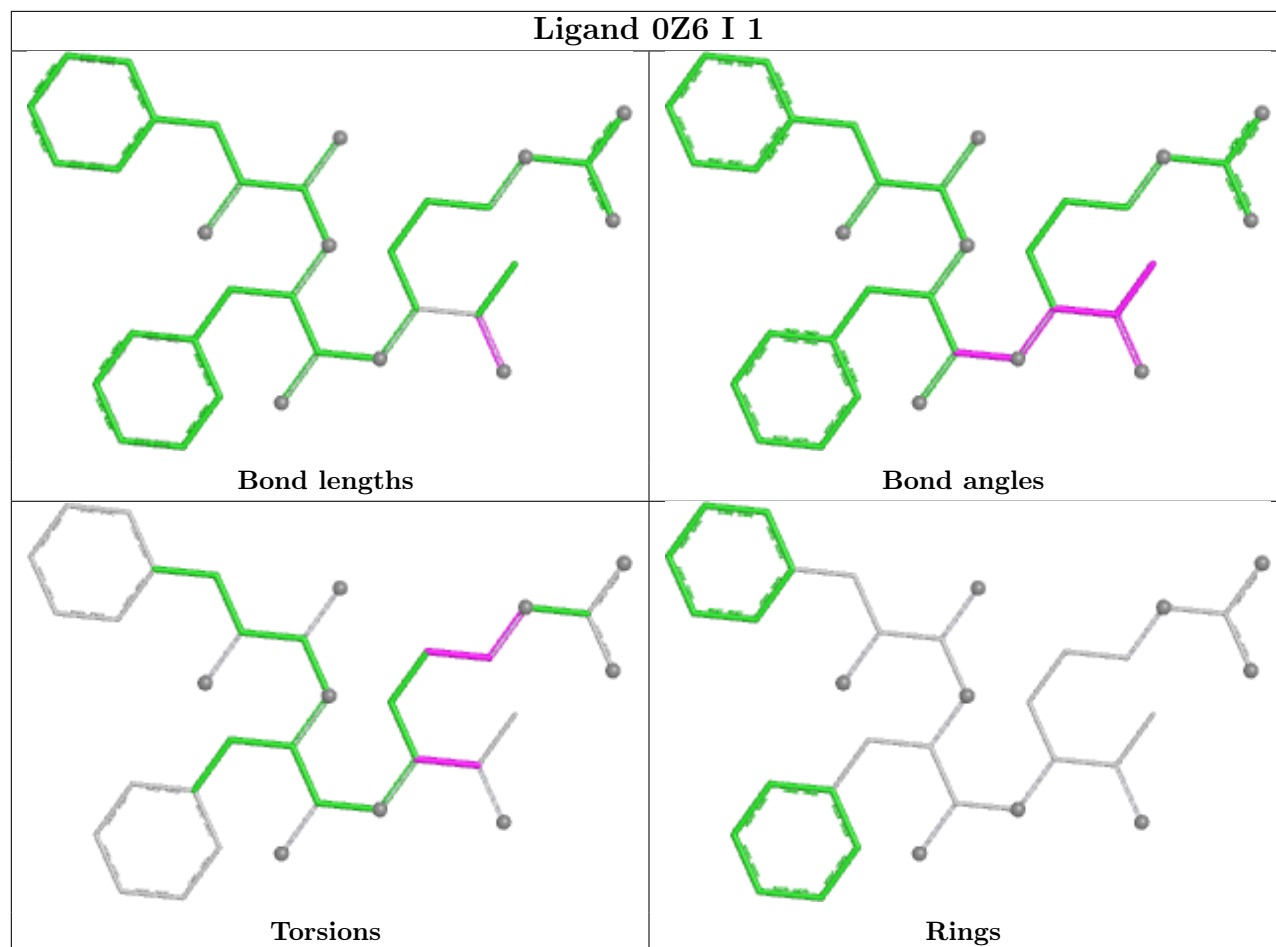
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	504	FUC	2	0
5	H	1	0Z6	4	0
5	I	1	0Z6	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 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.