



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:21 PM UTC

PDB ID : 1PPF / pdb\_00001ppf  
Title : X-RAY CRYSTAL STRUCTURE OF THE COMPLEX OF HUMAN LEUKOCYTE ELASTASE (PMN ELASTASE) AND THE THIRD DOMAIN OF THE TURKEY OVOMUCOID INHIBITOR  
Authors : Bode, W.; Wei, A-Z.  
Deposited on : 1991-10-24  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)  
Xtrriage (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

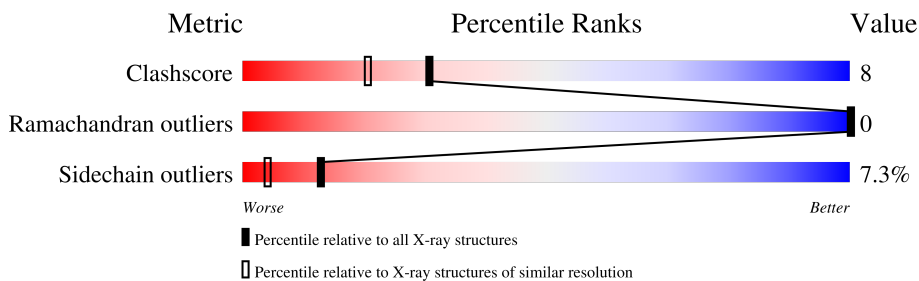
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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  $\geq 3$ , 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	E	218	56% (green), 33% (yellow), 11% (orange/red)
2	I	56	71% (green), 21% (yellow), 5% (orange/red)
3	A	8	75% (yellow), 25% (orange/red)
4	B	8	50% (yellow), 38% (orange/red), 12% (red)

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
4	NAG	B	5	X	-	-	-
4	GLC	B	6	X	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 2518 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.

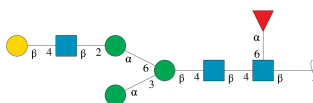
- Molecule 1 is a protein called HUMAN LEUKOCYTE ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	218	1636	1026	316	283	11	20	0	0

- Molecule 2 is a protein called TURKEY OVOMUCOID INHIBITOR (OMTKY3).

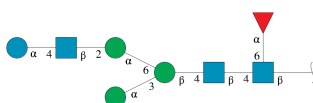
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	56	418	258	70	84	6	4	0	0

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	A	8	96	54	3	39	50	0	0

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	8	96	54	3	39	50	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	210	Total	O	0	0
			210	210		
5	I	62	Total	O	0	0
			62	62		

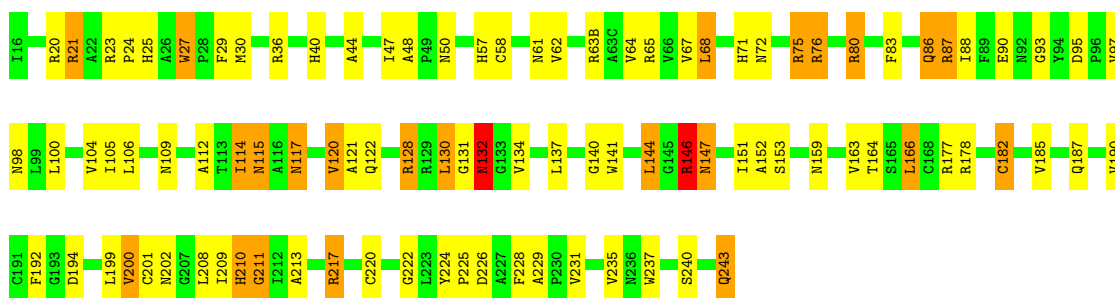
### 3 Residue-property plots

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.

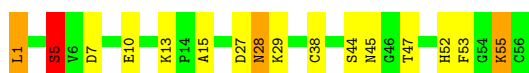
- Molecule 1: HUMAN LEUKOCYTE ELASTASE

Chain E: 

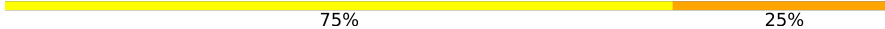


- Molecule 2: TURKEY OVOMUCOID INHIBITOR (OMTKY3)

Chain I: 



- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 



- Molecule 4: alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 

MAG1
MAG2
BMA3
MAN4
MAG5
GLC6
MAN7
FUC8

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.05Å 72.55Å 52.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	EREF	Depositor
R, $R_{free}$	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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: BMA, MAN, NAG, GLC, FUC, GAL

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	E	1.84	28/1666 (1.7%)	2.12	50/2263 (2.2%)
2	I	1.40	3/426 (0.7%)	2.05	11/576 (1.9%)
All	All	1.76	31/2092 (1.5%)	2.11	61/2839 (2.1%)

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
1	E	1	12
2	I	0	4
All	All	1	16

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	25	HIS	ND1-CE1	14.65	1.47	1.32
1	E	57	HIS	CE1-NE2	13.99	1.46	1.32
1	E	40	HIS	ND1-CE1	11.48	1.44	1.32
1	E	27	TRP	NE1-CE2	-9.49	1.27	1.37
1	E	71	HIS	CE1-NE2	8.98	1.41	1.32
1	E	25	HIS	CE1-NE2	8.76	1.41	1.32
1	E	57	HIS	ND1-CE1	8.69	1.41	1.32
1	E	209	ILE	N-CA	8.51	1.56	1.46
1	E	210	HIS	ND1-CE1	8.34	1.40	1.32
1	E	141	TRP	NE1-CE2	-7.98	1.28	1.37
1	E	87	ARG	NE-CZ	7.25	1.41	1.33
1	E	210	HIS	CE1-NE2	7.19	1.39	1.32
1	E	68	LEU	N-CA	7.13	1.54	1.45
2	I	52	HIS	ND1-CE1	7.12	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	ILE	C-N	-7.06	1.26	1.33
1	E	146	ARG	NE-CZ	6.38	1.40	1.33
1	E	237	TRP	NE1-CE2	-6.38	1.30	1.37
1	E	146	ARG	CZ-NH1	6.13	1.41	1.32
1	E	20	ARG	CZ-NH2	6.10	1.41	1.33
2	I	52	HIS	CE1-NE2	6.07	1.38	1.32
1	E	76	ARG	C-N	-5.80	1.25	1.33
1	E	112	ALA	C-N	-5.67	1.25	1.33
1	E	182	CYS	C-N	-5.58	1.26	1.33
2	I	13	LYS	N-CA	5.56	1.54	1.45
1	E	75	ARG	NE-CZ	5.39	1.39	1.33
1	E	75	ARG	CD-NE	5.32	1.53	1.46
1	E	61	ASN	C-N	5.30	1.41	1.33
1	E	27	TRP	CA-CB	5.18	1.59	1.53
1	E	44	ALA	N-CA	5.12	1.52	1.46
1	E	50	ASN	N-CA	-5.08	1.40	1.46
1	E	121	ALA	N-CA	5.04	1.52	1.45

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	217	ARG	CD-NE-CZ	11.68	140.75	124.40
2	I	28	ASN	OD1-CG-ND2	11.38	133.98	122.60
1	E	243	GLN	N-CA-CB	10.54	128.42	110.50
1	E	217	ARG	NE-CZ-NH1	9.39	130.89	121.50
2	I	47	THR	CA-C-N	-8.82	111.04	122.77
2	I	47	THR	C-N-CA	-8.82	111.04	122.77
1	E	192	PHE	CA-CB-CG	-8.55	105.25	113.80
2	I	28	ASN	CB-CA-C	-8.41	98.36	111.39
1	E	217	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	E	132	ASN	CA-CB-CG	-7.91	104.69	112.60
1	E	90	GLU	N-CA-CB	-7.83	99.30	111.05
1	E	65	ARG	CA-CB-CG	-7.52	99.06	114.10
2	I	28	ASN	CA-CB-CG	-7.21	105.39	112.60
1	E	130	LEU	CA-C-N	-7.04	115.05	122.30
1	E	130	LEU	C-N-CA	-7.04	115.05	122.30
1	E	48	ALA	N-CA-CB	-6.93	104.15	111.29
1	E	235	VAL	N-CA-C	6.86	117.62	110.62
2	I	10	GLU	N-CA-C	-6.84	105.26	112.93
1	E	202	ASN	CA-CB-CG	-6.81	105.79	112.60
2	I	7	ASP	CA-CB-CG	-6.81	105.79	112.60
1	E	146	ARG	NE-CZ-NH2	-6.75	113.12	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	146	ARG	CD-NE-CZ	6.73	133.82	124.40
1	E	21	ARG	N-CA-CB	6.67	119.89	109.69
1	E	80	ARG	O-C-N	6.40	130.19	122.96
1	E	147	ASN	CA-CB-CG	-6.27	106.33	112.60
1	E	128	ARG	NE-CZ-NH1	6.21	127.71	121.50
2	I	5	SER	CB-CA-C	-6.20	97.40	109.68
1	E	199	LEU	CA-C-N	-5.80	116.00	123.19
1	E	199	LEU	C-N-CA	-5.80	116.00	123.19
1	E	231	VAL	N-CA-CB	-5.80	103.22	110.47
1	E	120	VAL	CA-CB-CG1	5.79	120.25	110.40
1	E	202	ASN	CA-C-O	-5.76	115.16	121.84
1	E	146	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	E	210	HIS	CA-C-N	-5.65	115.49	121.48
1	E	210	HIS	C-N-CA	-5.65	115.49	121.48
1	E	163	VAL	CA-CB-CG2	5.65	120.00	110.40
1	E	159	ASN	CA-CB-CG	-5.52	107.08	112.60
1	E	117	ASN	CA-CB-CG	-5.52	107.08	112.60
1	E	57	HIS	CG-CD2-NE2	5.50	112.70	107.20
2	I	55	LYS	CB-CA-C	-5.45	98.51	109.68
1	E	24	PRO	CA-C-O	-5.42	115.41	121.32
1	E	211	GLY	O-C-N	5.41	128.63	123.65
1	E	98	ASN	CA-CB-CG	-5.40	107.20	112.60
1	E	114	ILE	N-CA-C	5.36	116.47	108.54
1	E	30	MET	CA-C-O	-5.31	114.64	120.69
1	E	201	CYS	CA-CB-SG	5.26	126.50	114.40
1	E	213	ALA	O-C-N	5.23	129.43	122.95
2	I	5	SER	CA-C-O	-5.23	114.11	120.54
1	E	147	ASN	N-CA-C	5.15	118.35	111.24
1	E	201	CYS	CA-C-N	5.15	129.67	122.36
1	E	201	CYS	C-N-CA	5.15	129.67	122.36
2	I	38	CYS	N-CA-C	5.12	117.52	111.33
1	E	209	ILE	N-CA-CB	5.11	117.60	111.31
1	E	222	GLY	N-CA-C	-5.11	108.57	115.36
1	E	144	LEU	CA-C-N	-5.08	113.12	122.27
1	E	144	LEU	C-N-CA	-5.08	113.12	122.27
1	E	182	CYS	N-CA-CB	5.06	119.72	111.08
1	E	62	VAL	N-CA-CB	5.05	120.96	112.47
1	E	122	GLN	N-CA-CB	-5.05	102.20	110.43
1	E	177	ARG	CG-CD-NE	-5.03	100.93	112.00
1	E	86	GLN	N-CA-CB	-5.01	102.80	110.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	243	GLN	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	132	ASN	Mainchain
1	E	137	LEU	Mainchain
1	E	146	ARG	Mainchain
1	E	185	VAL	Mainchain
1	E	217	ARG	Mainchain
1	E	220	CYS	Mainchain
1	E	224	TYR	Mainchain
1	E	228	PHE	Mainchain
1	E	240	SER	Mainchain
1	E	58	CYS	Mainchain
1	E	64	VAL	Mainchain
1	E	93	GLY	Mainchain
2	I	15	ALA	Mainchain
2	I	5	SER	Mainchain
2	I	53	PHE	Mainchain
2	I	55	LYS	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	E	1636	0	1650	32	9
2	I	418	0	396	3	8
3	A	96	0	82	2	1
4	B	96	0	82	1	10
5	E	210	0	0	5	13
5	I	62	0	0	1	6
All	All	2518	0	2210	35	24

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 8.

All (35) 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:E:80:ARG:HD2	5:E:955:HOH:O	1.90	0.70
1:E:200:VAL:HG22	3:A:8:FUC:H62	1.76	0.65
1:E:131:GLY:O	1:E:134:VAL:HG23	2.01	0.61
1:E:200:VAL:CG2	3:A:8:FUC:H62	2.31	0.61
1:E:144:LEU:HD21	1:E:152:ALA:HB2	1.83	0.60
1:E:88:ILE:HG22	1:E:106:LEU:HD23	1.83	0.60
1:E:88:ILE:HG22	1:E:106:LEU:CD2	2.33	0.58
1:E:128:ARG:HG2	5:E:762:HOH:O	2.04	0.57
1:E:164:THR:HA	5:E:967:HOH:O	2.04	0.57
1:E:182:CYS:HB3	1:E:225:PRO:HB2	1.87	0.55
1:E:115:ASN:HD22	1:E:117:ASN:H	1.56	0.53
1:E:164:THR:HG22	5:E:967:HOH:O	2.08	0.53
1:E:95:ASP:HB3	1:E:100:LEU:HB2	1.91	0.52
2:I:27:ASP:O	2:I:28:ASN:HB2	2.09	0.52
1:E:115:ASN:ND2	1:E:117:ASN:H	2.08	0.51
1:E:115:ASN:HD22	1:E:115:ASN:C	2.18	0.51
1:E:132:ASN:HD22	1:E:164:THR:H	1.59	0.51
1:E:190:VAL:HG22	1:E:226:ASP:CG	2.39	0.47
1:E:130:LEU:HD11	1:E:210:HIS:CG	2.49	0.47
1:E:47:ILE:HD11	1:E:105:ILE:HD12	1.95	0.47
1:E:140:GLY:HA3	1:E:194:ASP:OD1	2.15	0.46
1:E:115:ASN:HD22	1:E:117:ASN:N	2.13	0.46
1:E:211:GLY:HA2	1:E:229:ALA:O	2.16	0.46
2:I:5:SER:HA	5:I:764:HOH:O	2.16	0.45
1:E:109:ASN:HD22	4:B:1:NAG:H83	1.82	0.45
1:E:132:ASN:ND2	1:E:164:THR:H	2.14	0.45
1:E:23:ARG:HD2	5:E:1168:HOH:O	2.17	0.44
1:E:68:LEU:HD12	1:E:83:PHE:HE2	1.84	0.43
1:E:27:TRP:C	1:E:29:PHE:H	2.25	0.42
1:E:166:LEU:HD12	1:E:166:LEU:HA	1.81	0.42
1:E:47:ILE:C	1:E:120:VAL:HG13	2.44	0.42
1:E:67:VAL:CG1	1:E:80:ARG:HD3	2.49	0.41
2:I:1:LEU:HD13	2:I:1:LEU:HA	1.81	0.41
1:E:72:ASN:HA	1:E:153:SER:O	2.21	0.40
1:E:95:ASP:OD1	1:E:97:VAL:HB	2.21	0.40

All (24) 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)
2:I:29:LYS:NZ	4:B:7:MAN:O2[3_645]	1.16	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ARG:CG	5:E:956:HOH:O[4_565]	1.20	1.00
1:E:21:ARG:CB	5:E:956:HOH:O[4_565]	1.33	0.87
1:E:187:GLN:CG	5:E:883:HOH:O[3_645]	1.35	0.85
2:I:45:ASN:N	4:B:6:GLC:O2[3_645]	1.41	0.79
2:I:44:SER:C	4:B:6:GLC:O2[3_645]	1.47	0.73
4:B:5:NAG:O7	5:I:894:HOH:O[3_655]	1.66	0.54
2:I:44:SER:O	4:B:6:GLC:O2[3_645]	1.71	0.49
2:I:45:ASN:CA	4:B:6:GLC:O2[3_645]	1.71	0.49
4:B:6:GLC:O6	5:E:1165:HOH:O[3_654]	1.78	0.42
1:E:97:VAL:CG2	3:A:5:NAG:C6[4_465]	1.82	0.38
5:E:988:HOH:O	5:I:634:HOH:O[3_645]	2.02	0.18
1:E:187:GLN:CD	5:E:883:HOH:O[3_645]	2.03	0.17
5:E:937:HOH:O	5:I:767:HOH:O[2_574]	2.04	0.16
2:I:44:SER:CB	4:B:5:NAG:O3[3_645]	2.04	0.16
1:E:87:ARG:CD	5:I:1017:HOH:O[2_574]	2.05	0.15
5:E:620:HOH:O	5:I:1142:HOH:O[3_645]	2.05	0.15
2:I:45:ASN:N	4:B:6:GLC:C2[3_645]	2.07	0.13
2:I:44:SER:CA	4:B:5:NAG:O3[3_645]	2.08	0.12
1:E:63(B):ARG:NH2	5:E:907:HOH:O[2_575]	2.09	0.11
1:E:187:GLN:OE1	5:E:883:HOH:O[3_645]	2.11	0.09
1:E:21:ARG:CD	5:E:956:HOH:O[4_565]	2.16	0.04
5:E:561:HOH:O	5:E:901:HOH:O[2_575]	2.18	0.02
5:E:1090:HOH:O	5:I:1019:HOH:O[2_574]	2.19	0.01

## 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	E	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
2	I	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
All	All	270/274 (98%)	259 (96%)	11 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	E	172/172 (100%)	157 (91%)	15 (9%)	<b>9</b> <b>3</b>
2	I	48/48 (100%)	47 (98%)	1 (2%)	47 36
All	All	220/220 (100%)	204 (93%)	16 (7%)	<b>13</b> <b>4</b>

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	36	ARG
1	E	75	ARG
1	E	76	ARG
1	E	86	GLN
1	E	104	VAL
1	E	114	ILE
1	E	115	ASN
1	E	146	ARG
1	E	147	ASN
1	E	151	ILE
1	E	166	LEU
1	E	178	ARG
1	E	200	VAL
1	E	208	LEU
1	E	243	GLN
2	I	1	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	61	ASN
1	E	92	ASN
1	E	115	ASN
1	E	119	GLN
1	E	132	ASN
1	E	135	GLN

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Mol	Chain	Res	Type
1	E	156	GLN
1	E	210	HIS
2	I	36	ASN

### 5.3.3 RNA [i](#)

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](#)

16 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
3	NAG	A	1	3,1	14,14,15	1.08	0	17,19,21	1.84	6 (35%)
3	NAG	A	2	3	14,14,15	1.44	2 (14%)	17,19,21	2.12	5 (29%)
3	BMA	A	3	3	11,11,12	2.85	7 (63%)	15,15,17	2.07	4 (26%)
3	MAN	A	4	3	11,11,12	0.47	0	15,15,17	1.71	1 (6%)
3	NAG	A	5	3	14,14,15	0.67	0	17,19,21	1.42	1 (5%)
3	GAL	A	6	3	11,11,12	0.57	0	15,15,17	1.41	1 (6%)
3	MAN	A	7	3	11,11,12	0.59	0	15,15,17	2.01	1 (6%)
3	FUC	A	8	3	10,10,11	1.01	1 (10%)	14,14,16	1.35	1 (7%)
4	NAG	B	1	4,1	14,14,15	1.29	2 (14%)	17,19,21	1.76	5 (29%)
4	NAG	B	2	4	14,14,15	1.25	1 (7%)	17,19,21	2.45	5 (29%)
4	BMA	B	3	4	11,11,12	1.67	2 (18%)	15,15,17	1.66	4 (26%)
4	MAN	B	4	4	11,11,12	0.72	0	15,15,17	1.92	2 (13%)
4	NAG	B	5	4	14,14,15	0.71	0	17,19,21	1.69	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GLC	B	6	4	11,11,12	0.61	0	15,15,17	1.47	1 (6%)
4	MAN	B	7	4	11,11,12	0.57	0	15,15,17	1.45	1 (6%)
4	FUC	B	8	4	10,10,11	1.13	1 (10%)	14,14,16	1.62	3 (21%)

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
3	NAG	A	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	2/6/23/26	0/1/1/1
3	BMA	A	3	3	-	0/2/19/22	0/1/1/1
3	MAN	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	A	5	3	-	0/6/23/26	0/1/1/1
3	GAL	A	6	3	-	1/2/19/22	0/1/1/1
3	MAN	A	7	3	-	0/2/19/22	0/1/1/1
3	FUC	A	8	3	-	-	0/1/1/1
4	NAG	B	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	4/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	NAG	B	5	4	2/2/5/7	2/6/23/26	0/1/1/1
4	GLC	B	6	4	1/1/4/5	1/2/19/22	0/1/1/1
4	MAN	B	7	4	-	0/2/19/22	0/1/1/1
4	FUC	B	8	4	-	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3	BMA	C2-C3	4.70	1.59	1.52
3	A	3	BMA	O2-C2	4.19	1.52	1.43
3	A	3	BMA	C4-C5	3.57	1.60	1.53
3	A	3	BMA	C1-C2	3.16	1.59	1.52
3	A	2	NAG	O3-C3	3.11	1.50	1.43
3	A	3	BMA	O5-C1	3.07	1.48	1.43
4	B	1	NAG	C1-C2	2.79	1.56	1.52
3	A	3	BMA	C4-C3	2.77	1.59	1.52
3	A	8	FUC	C2-C3	2.74	1.56	1.52
3	A	2	NAG	C3-C2	2.70	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3	BMA	C1-C2	2.56	1.58	1.52
4	B	3	BMA	C4-C5	2.54	1.58	1.53
4	B	1	NAG	C2-N2	2.51	1.50	1.46
3	A	3	BMA	O5-C5	2.33	1.48	1.43
4	B	2	NAG	C3-C2	2.09	1.56	1.52
4	B	8	FUC	C2-C3	2.03	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7	MAN	C1-O5-C5	7.28	121.94	112.19
4	B	2	NAG	C1-O5-C5	6.00	120.23	112.19
3	A	4	MAN	C1-O5-C5	5.73	119.87	112.19
4	B	2	NAG	C1-C2-N2	-5.36	101.99	110.43
4	B	6	GLC	C1-O5-C5	5.21	119.17	112.19
3	A	2	NAG	C1-O5-C5	5.19	119.14	112.19
4	B	7	MAN	C1-O5-C5	5.14	119.07	112.19
3	A	6	GAL	C1-O5-C5	5.10	119.02	112.19
3	A	5	NAG	C1-O5-C5	5.01	118.90	112.19
4	B	4	MAN	C1-O5-C5	4.95	118.83	112.19
4	B	5	NAG	C1-O5-C5	4.91	118.77	112.19
3	A	3	BMA	C3-C4-C5	4.26	117.96	110.23
3	A	2	NAG	C3-C4-C5	4.26	117.96	110.23
3	A	3	BMA	O2-C2-C3	4.20	118.84	110.15
4	B	3	BMA	C1-O5-C5	4.18	117.78	112.19
4	B	4	MAN	O2-C2-C3	4.11	118.66	110.15
3	A	1	NAG	C1-O5-C5	3.92	117.44	112.19
4	B	2	NAG	C4-C3-C2	3.88	116.71	111.02
3	A	3	BMA	C1-O5-C5	3.54	116.93	112.19
4	B	1	NAG	O5-C5-C4	-3.36	102.65	110.83
3	A	8	FUC	C1-O5-C5	3.32	120.81	112.97
3	A	1	NAG	C8-C7-N2	-3.12	110.95	116.12
4	B	8	FUC	O4-C4-C3	-3.03	103.22	110.38
4	B	5	NAG	O5-C1-C2	-3.03	106.60	111.29
4	B	2	NAG	C2-N2-C7	2.98	126.89	122.90
4	B	8	FUC	C1-O5-C5	2.87	119.73	112.97
3	A	2	NAG	O7-C7-N2	2.81	126.94	121.98
3	A	2	NAG	O5-C1-C2	-2.74	107.05	111.29
4	B	2	NAG	O5-C5-C4	-2.74	104.17	110.83
3	A	3	BMA	O3-C3-C2	2.72	115.60	110.05
4	B	1	NAG	O5-C5-C6	2.70	112.91	107.66
3	A	1	NAG	C4-C3-C2	2.58	114.80	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C1-O5-C5	-2.54	108.78	112.19
4	B	3	BMA	C1-C2-C3	2.46	113.22	109.64
3	A	1	NAG	O5-C1-C2	-2.28	107.77	111.29
3	A	2	NAG	C8-C7-N2	-2.24	112.41	116.12
4	B	1	NAG	C8-C7-N2	2.22	119.81	116.12
4	B	8	FUC	C2-C3-C4	-2.21	106.98	110.86
4	B	3	BMA	O3-C3-C2	-2.20	105.56	110.05
4	B	1	NAG	C2-N2-C7	-2.13	120.04	122.90
3	A	1	NAG	O5-C5-C4	-2.05	105.85	110.83
4	B	3	BMA	O5-C5-C6	2.04	111.63	107.66
4	B	5	NAG	C3-C4-C5	2.03	113.91	110.23
3	A	1	NAG	O7-C7-C8	2.01	125.63	122.05

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	5	NAG	C5
4	B	5	NAG	C3
4	B	6	GLC	C3

All (14) torsion outliers are listed below:

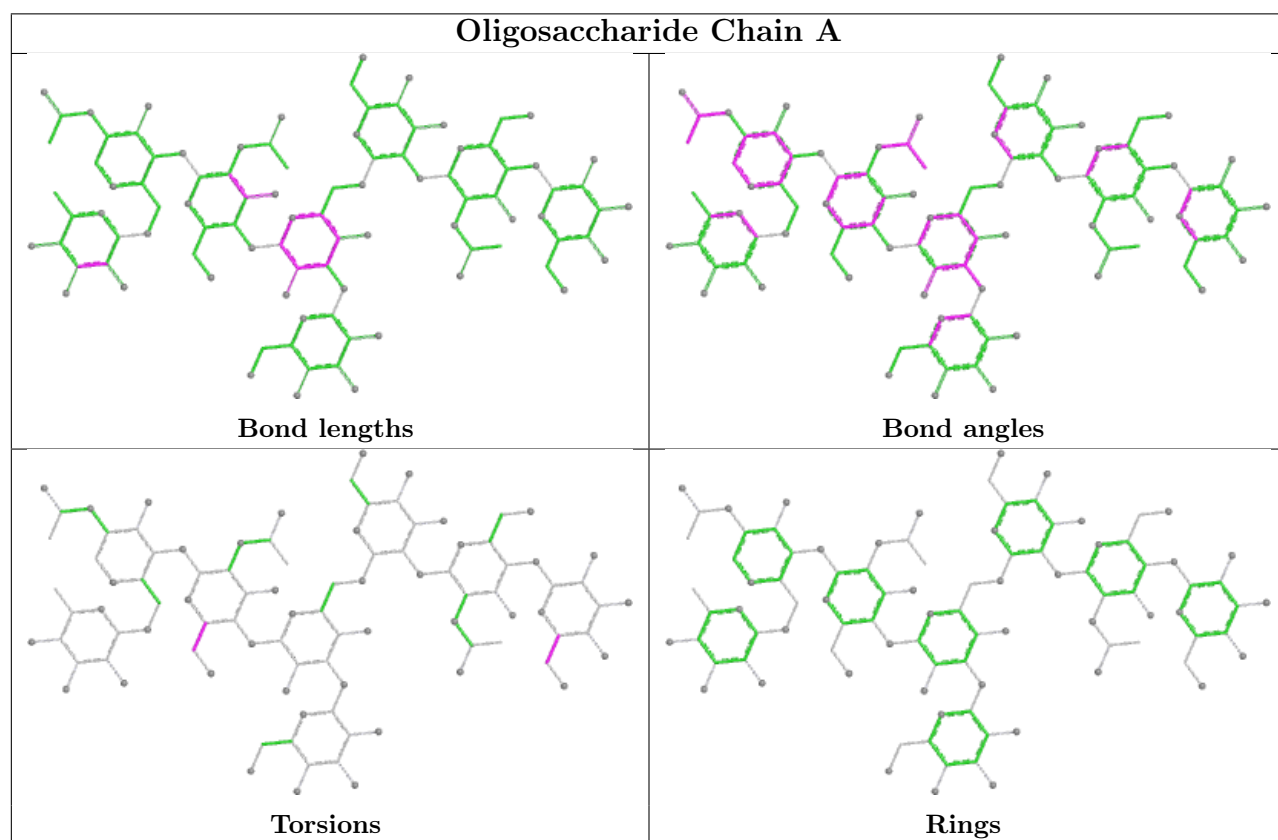
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	B	5	NAG	C8-C7-N2-C2
4	B	5	NAG	O7-C7-N2-C2
4	B	3	BMA	O5-C5-C6-O6
4	B	6	GLC	O5-C5-C6-O6
3	A	6	GAL	O5-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6

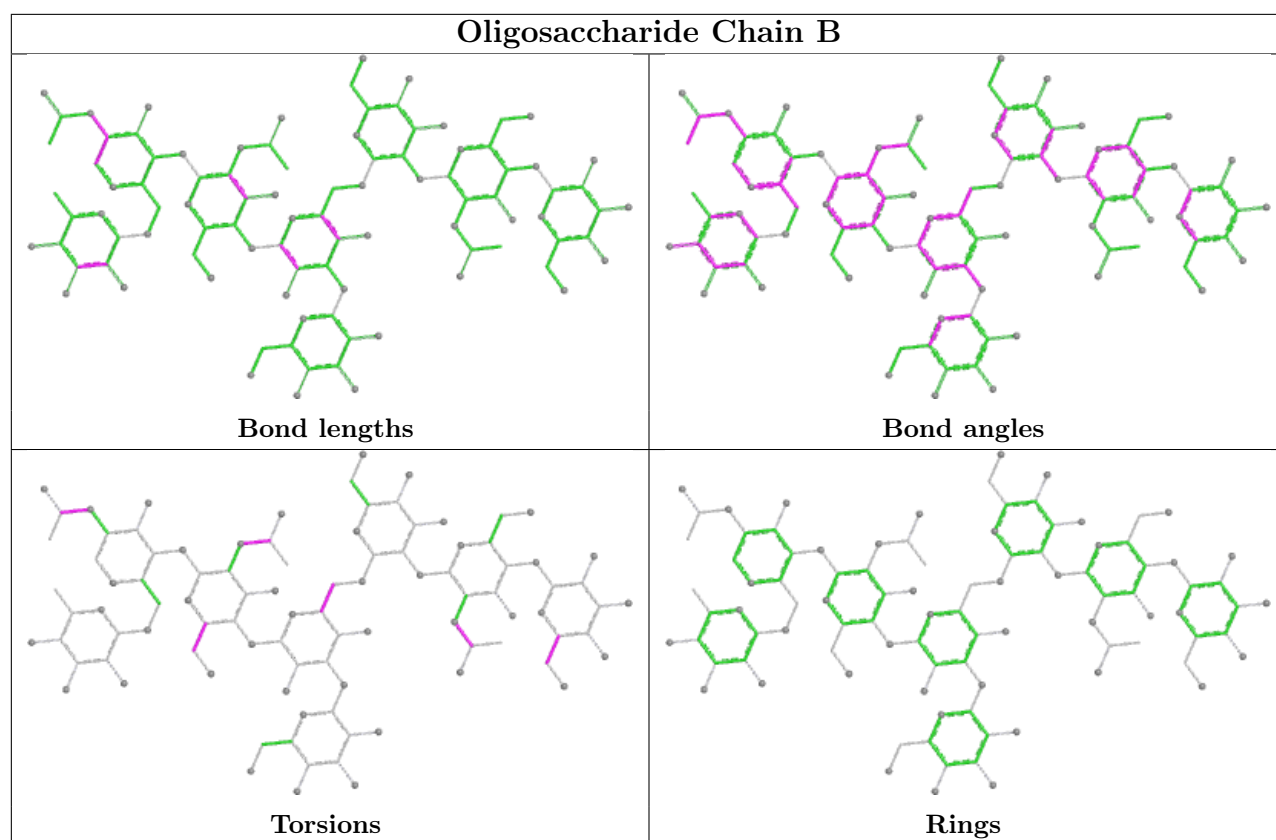
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	8	FUC	2	0
4	B	1	NAG	1	0
4	B	6	GLC	0	6
4	B	5	NAG	0	3
4	B	7	MAN	0	1
3	A	5	NAG	0	1

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](#)

There are no ligands in this entry.

## 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.