



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:50 AM UTC

PDB ID : 1PPG / pdb_00001ppg
Title : The refined 2.3 angstroms crystal structure of human leukocyte elastase in a complex with a valine chloromethyl ketone inhibitor
Authors : Bode, W.; Wei, A-Z.
Deposited on : 1991-10-24
Resolution : 2.30 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

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

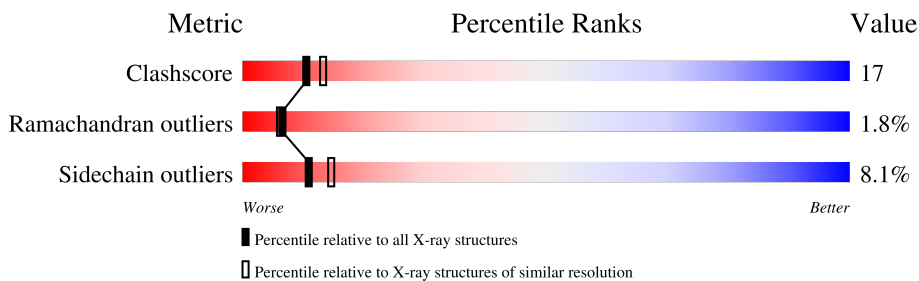
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	E	218	41% 37% 17% 6%
2	I	6	17% 83%
3	A	8	38% 62%
4	B	8	88% 12%

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
3	NAG	A	5	-	-	X	-
4	NDG	B	5	X	-	-	-
4	GLC	B	6	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2053 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.

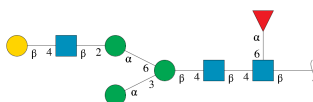
- Molecule 1 is a protein called HUMAN LEUKOCYTE ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	218	Total	C	N	O	S	43	0	0
			1636	1026	316	283	11			

- Molecule 2 is a protein called MEO-SUCCINYL-ALA-ALA-PRO-VAL CHLOROMETHYLKETONE.

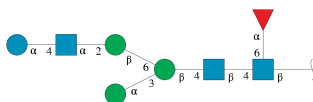
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	1
			33	22	4	7			

- 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
3	A	8	Total	C	N	O	60	0	0
			96	54	3	39			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-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
4	B	8	Total	C	N	O	72	0	0
			96	54	3	39			

- Molecule 5 is water.

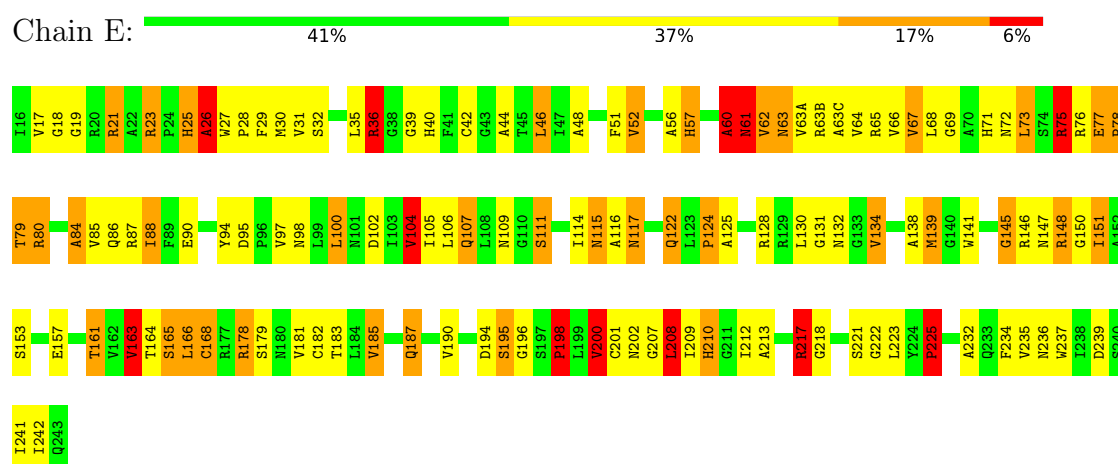
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	189	Total	O	29	0
			189	189		
5	I	3	Total	O	1	0
			3	3		

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



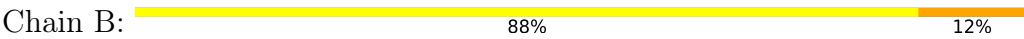
• Molecule 2: MEO-SUCCINYL-ALA-ALA-PRO-VAL CHLOROMETHYLKETONE



• 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



• Molecule 4: alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-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



NA61
NA62
BM43
BM44
ND95
GLC6
MAN7
FO68

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	74.20Å 74.20Å 70.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.145 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2053	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: NAG, OQE, MAN, FUC, GAL, NDG, HMB, VAI, GLC, BMA

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	1.88	31/1666 (1.9%)	2.34	96/2263 (4.2%)
2	I	1.50	0/17	1.28	0/23
All	All	1.88	31/1683 (1.8%)	2.33	96/2286 (4.2%)

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	0	24
2	I	1	0
All	All	1	24

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	40	HIS	CE1-NE2	13.37	1.46	1.32
1	E	57	HIS	CE1-NE2	13.05	1.45	1.32
1	E	71	HIS	CE1-NE2	11.11	1.43	1.32
1	E	210	HIS	CE1-NE2	10.57	1.43	1.32
1	E	57	HIS	ND1-CE1	10.30	1.42	1.32
1	E	25	HIS	CE1-NE2	10.19	1.42	1.32
1	E	40	HIS	ND1-CE1	9.94	1.42	1.32
1	E	141	TRP	NE1-CE2	-9.15	1.27	1.37
1	E	237	TRP	NE1-CE2	-8.01	1.28	1.37
1	E	25	HIS	ND1-CE1	7.72	1.40	1.32
1	E	75	ARG	NE-CZ	7.39	1.41	1.33
1	E	27	TRP	NE1-CE2	-6.90	1.29	1.37
1	E	71	HIS	ND1-CE1	6.84	1.39	1.32
1	E	178	ARG	C-N	-6.82	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	157	GLU	N-CA	6.31	1.53	1.46
1	E	65	ARG	NE-CZ	5.89	1.39	1.33
1	E	194	ASP	N-CA	-5.80	1.38	1.46
1	E	76	ARG	CZ-NH1	5.74	1.40	1.32
1	E	107	GLN	N-CA	-5.68	1.38	1.46
1	E	210	HIS	ND1-CE1	5.56	1.38	1.32
1	E	111	SER	N-CA	-5.55	1.39	1.46
1	E	94	TYR	C-N	-5.44	1.26	1.33
1	E	242	ILE	N-CA	5.44	1.53	1.46
1	E	86	GLN	C-N	-5.43	1.26	1.33
1	E	236	ASN	C-N	5.39	1.40	1.33
1	E	163	VAL	N-CA	-5.37	1.40	1.46
1	E	80	ARG	N-CA	5.34	1.52	1.45
1	E	139	MET	N-CA	5.19	1.52	1.46
1	E	25	HIS	CG-ND1	5.14	1.44	1.38
1	E	151	ILE	C-N	5.08	1.40	1.33
1	E	35	LEU	N-CA	5.02	1.51	1.45

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	194	ASP	CA-CB-CG	-11.74	100.86	112.60
1	E	63	ASN	CA-CB-CG	-11.08	101.52	112.60
1	E	210	HIS	CA-C-N	-11.08	109.73	121.48
1	E	210	HIS	C-N-CA	-11.08	109.73	121.48
1	E	207	GLY	N-CA-C	-8.84	103.72	115.21
1	E	208	LEU	N-CA-CB	-8.72	96.17	111.08
1	E	18	GLY	CA-C-N	8.71	130.89	122.27
1	E	18	GLY	C-N-CA	8.71	130.89	122.27
1	E	185	VAL	CA-C-N	-8.14	109.78	121.42
1	E	185	VAL	C-N-CA	-8.14	109.78	121.42
1	E	242	ILE	CA-C-N	7.85	135.82	121.70
1	E	242	ILE	C-N-CA	7.85	135.82	121.70
1	E	78	PRO	CA-C-N	7.72	131.65	120.38
1	E	78	PRO	C-N-CA	7.72	131.65	120.38
1	E	19	GLY	O-C-N	-7.54	115.72	122.88
1	E	71	HIS	CA-CB-CG	-7.52	106.28	113.80
1	E	117	ASN	N-CA-C	-7.51	102.34	113.61
1	E	196	GLY	N-CA-C	-7.48	106.18	115.08
1	E	178	ARG	CA-C-N	-7.45	110.80	122.49
1	E	178	ARG	C-N-CA	-7.45	110.80	122.49
1	E	26	ALA	N-CA-C	-7.18	103.78	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	138	ALA	N-CA-C	-7.06	98.72	109.95
1	E	217	ARG	NH1-CZ-NH2	-7.04	110.15	119.30
1	E	239	ASP	CA-CB-CG	-6.98	105.62	112.60
1	E	198	PRO	N-CA-CB	-6.86	96.95	103.33
1	E	241	ILE	CB-CA-C	-6.80	104.77	111.30
1	E	90	GLU	N-CA-CB	-6.70	100.53	110.85
1	E	130	LEU	CA-C-N	-6.67	114.00	120.34
1	E	130	LEU	C-N-CA	-6.67	114.00	120.34
1	E	29	PHE	O-C-N	6.52	130.13	122.24
1	E	109	ASN	CA-CB-CG	-6.48	106.12	112.60
1	E	207	GLY	CA-C-N	-6.47	112.65	122.81
1	E	207	GLY	C-N-CA	-6.47	112.65	122.81
1	E	23	ARG	NE-CZ-NH1	-6.37	115.14	121.50
1	E	65	ARG	CA-CB-CG	-6.36	101.38	114.10
1	E	153	SER	N-CA-C	-6.34	104.25	112.68
1	E	36	ARG	CD-NE-CZ	-6.28	115.61	124.40
1	E	145	GLY	CA-C-O	-6.25	115.58	121.96
1	E	125	ALA	O-C-N	6.25	130.09	123.03
1	E	187	GLN	CB-CG-CD	-6.14	102.16	112.60
1	E	79	THR	O-C-N	6.13	129.19	122.20
1	E	100	LEU	CA-C-O	-6.13	114.23	121.16
1	E	190	VAL	CA-CB-CG2	6.09	120.76	110.40
1	E	161	THR	CA-C-O	-6.07	114.14	120.70
1	E	181	VAL	CA-C-O	-6.07	114.05	120.48
1	E	44	ALA	O-C-N	5.96	129.37	122.99
1	E	117	ASN	CA-CB-CG	-5.89	106.71	112.60
1	E	73	LEU	CA-C-N	-5.85	110.17	121.58
1	E	73	LEU	C-N-CA	-5.85	110.17	121.58
1	E	161	THR	CA-C-N	5.81	128.88	120.98
1	E	161	THR	C-N-CA	5.81	128.88	120.98
1	E	40	HIS	ND1-CG-CD2	5.80	111.90	106.10
1	E	88	ILE	CA-C-O	5.77	127.13	120.67
1	E	241	ILE	CA-C-O	-5.68	114.96	120.30
1	E	179	SER	N-CA-C	-5.64	105.08	112.41
1	E	225	PRO	O-C-N	-5.61	116.12	122.91
1	E	85	VAL	N-CA-C	-5.59	100.53	108.58
1	E	42	CYS	CA-C-N	5.57	128.51	122.16
1	E	42	CYS	C-N-CA	5.57	128.51	122.16
1	E	61	ASN	N-CA-C	5.51	121.50	113.40
1	E	195	SER	CA-C-O	-5.51	115.71	121.55
1	E	42	CYS	O-C-N	5.49	129.29	123.42
1	E	221	SER	CA-C-N	-5.47	114.13	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	SER	C-N-CA	-5.47	114.13	122.28
1	E	148	ARG	CA-CB-CG	-5.42	103.26	114.10
1	E	107	GLN	O-C-N	-5.38	117.08	123.22
1	E	178	ARG	O-C-N	-5.37	114.44	122.39
1	E	107	GLN	CA-CB-CG	-5.37	103.36	114.10
1	E	77	GLU	O-C-N	5.35	127.68	121.10
1	E	62	VAL	N-CA-C	5.28	116.91	108.89
1	E	23	ARG	CA-C-O	-5.26	114.86	120.23
1	E	25	HIS	CA-C-N	5.25	129.49	120.72
1	E	25	HIS	C-N-CA	5.25	129.49	120.72
1	E	181	VAL	CA-CB-CG1	5.24	119.31	110.40
1	E	212	ILE	N-CA-CB	-5.22	104.72	111.82
1	E	21	ARG	CA-CB-CG	-5.19	103.72	114.10
1	E	202	ASN	OD1-CG-ND2	5.19	127.79	122.60
1	E	222	GLY	N-CA-C	-5.15	108.88	115.42
1	E	104	VAL	CA-CB-CG1	5.13	119.13	110.40
1	E	87	ARG	N-CA-CB	-5.13	103.61	111.56
1	E	77	GLU	CA-C-N	5.12	125.42	119.47
1	E	77	GLU	C-N-CA	5.12	125.42	119.47
1	E	168	CYS	CA-C-O	-5.11	115.46	121.44
1	E	200	VAL	O-C-N	5.10	129.56	122.88
1	E	165	SER	CA-C-O	-5.09	115.97	121.87
1	E	61	ASN	CA-CB-CG	-5.07	107.53	112.60
1	E	209	ILE	O-C-N	5.07	127.87	122.45
1	E	102	ASP	CA-C-N	5.06	129.98	122.94
1	E	102	ASP	C-N-CA	5.06	129.98	122.94
1	E	198	PRO	N-CD-CG	-5.05	95.62	103.20
1	E	67	VAL	CA-C-O	-5.03	115.11	120.59
1	E	148	ARG	N-CA-C	5.03	119.39	113.16
1	E	190	VAL	CA-CB-CG1	5.02	118.93	110.40
1	E	60	ALA	N-CA-CB	-5.00	101.94	109.94
1	E	134	VAL	CA-C-N	5.00	128.97	121.72
1	E	134	VAL	C-N-CA	5.00	128.97	121.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	1	HMB	CG

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	104	VAL	Mainchain
1	E	107	GLN	Mainchain
1	E	111	SER	Mainchain
1	E	122	GLN	Mainchain
1	E	163	VAL	Mainchain
1	E	165	SER	Mainchain
1	E	168	CYS	Mainchain
1	E	178	ARG	Mainchain
1	E	185	VAL	Mainchain
1	E	198	PRO	Mainchain
1	E	217	ARG	Sidechain
1	E	225	PRO	Mainchain
1	E	234	PHE	Mainchain
1	E	26	ALA	Mainchain
1	E	28	PRO	Mainchain
1	E	46	LEU	Mainchain
1	E	52	VAL	Mainchain
1	E	60	ALA	Mainchain
1	E	61	ASN	Mainchain
1	E	63	ASN	Mainchain
1	E	63(B)	ARG	Mainchain
1	E	63(C)	ALA	Mainchain
1	E	69	GLY	Mainchain
1	E	84	ALA	Mainchain

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	E	1636	0	1650	55	26
2	I	33	0	33	8	0
3	A	96	0	82	0	30
4	B	96	0	81	1	0
5	E	189	0	0	3	9
5	I	3	0	0	0	0
All	All	2053	0	1846	56	34

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 17.

All (56) 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:195:SER:OG	2:I:6:0QE:C1	1.78	1.28
1:E:218:GLY:H	2:I:1:HMB:HB1	1.36	0.90
1:E:88:ILE:HG22	1:E:106:LEU:HD22	1.56	0.87
1:E:195:SER:CB	2:I:6:0QE:C1	2.55	0.85
1:E:105:ILE:HG13	5:E:1239:HOH:O	1.85	0.77
1:E:57:HIS:CE1	1:E:195:SER:OG	2.40	0.74
1:E:23:ARG:HB3	1:E:26:ALA:HB2	1.71	0.72
1:E:124:PRO:HG2	1:E:232:ALA:HB2	1.73	0.71
1:E:195:SER:CB	2:I:5:VAI:C	2.69	0.71
1:E:63(A):VAL:HA	1:E:64:VAL:HG23	1.74	0.68
1:E:201:CYS:HB2	1:E:210:HIS:HD2	1.59	0.68
1:E:115:ASN:HD22	1:E:117:ASN:H	1.44	0.65
1:E:201:CYS:HB2	1:E:210:HIS:CD2	2.33	0.64
1:E:21:ARG:HD2	5:E:740:HOH:O	2.01	0.61
1:E:39:GLY:HA2	5:E:972:HOH:O	2.00	0.60
1:E:57:HIS:HE1	1:E:195:SER:OG	1.84	0.60
1:E:72:ASN:ND2	1:E:75:ARG:NH1	2.50	0.59
1:E:166:LEU:HB3	1:E:225:PRO:HD2	1.85	0.58
1:E:182:CYS:HB3	1:E:225:PRO:HB2	1.85	0.57
1:E:218:GLY:N	2:I:1:HMB:HB1	2.14	0.56
1:E:84:ALA:HB2	4:B:8:FUC:H5	1.89	0.54
1:E:131:GLY:O	1:E:134:VAL:HG23	2.07	0.54
1:E:31:VAL:HG21	1:E:52:VAL:HG11	1.90	0.54
1:E:105:ILE:O	1:E:106:LEU:HD23	2.07	0.53
1:E:31:VAL:HG11	1:E:66:VAL:HG13	1.91	0.53
1:E:195:SER:HB2	2:I:6:0QE:C1	2.41	0.51
1:E:115:ASN:HD22	1:E:115:ASN:C	2.19	0.51
1:E:88:ILE:HG22	1:E:106:LEU:CD2	2.35	0.50
1:E:122:GLN:HB2	1:E:208:LEU:HD12	1.94	0.49
1:E:95:ASP:HB3	1:E:100:LEU:HB2	1.94	0.49
1:E:63(A):VAL:HA	1:E:64:VAL:CG2	2.41	0.49
1:E:163:VAL:HG21	1:E:225:PRO:HB3	1.95	0.48
1:E:17:VAL:HG22	1:E:145:GLY:HA2	1.95	0.48
1:E:73:LEU:HA	1:E:80:ARG:NH2	2.28	0.48
1:E:166:LEU:HB3	1:E:225:PRO:CD	2.44	0.47
1:E:56:ALA:HA	1:E:104:VAL:HG22	1.96	0.47
1:E:217:ARG:HA	2:I:1:HMB:O	2.15	0.46
1:E:161:THR:O	1:E:183:THR:HA	2.15	0.46
1:E:31:VAL:HG22	1:E:68:LEU:HD22	1.99	0.45
1:E:115:ASN:ND2	1:E:117:ASN:H	2.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:HIS:CE1	1:E:79:THR:HG21	2.52	0.44
1:E:48:ALA:HB3	1:E:51:PHE:HB2	1.99	0.44
1:E:139:MET:HE3	1:E:200:VAL:HG13	1.99	0.44
1:E:132:ASN:ND2	1:E:164:THR:H	2.17	0.43
1:E:31:VAL:HG21	1:E:52:VAL:CG1	2.49	0.43
1:E:31:VAL:CG1	1:E:66:VAL:HG13	2.49	0.43
1:E:77:GLU:O	1:E:80:ARG:HG3	2.19	0.43
1:E:30:MET:SD	1:E:198:PRO:HD2	2.59	0.42
1:E:77:GLU:HA	1:E:78:PRO:HD2	1.72	0.42
1:E:32:SER:HB3	1:E:67:VAL:HB	2.01	0.42
1:E:132:ASN:HD22	1:E:164:THR:H	1.68	0.41
1:E:95:ASP:CG	1:E:98:ASN:HD22	2.28	0.41
2:I:3:ALA:HA	2:I:4:PRO:HD2	1.87	0.41
1:E:166:LEU:HD12	1:E:166:LEU:HA	1.79	0.40
1:E:46:LEU:HA	1:E:46:LEU:HD12	1.92	0.40
1:E:60:ALA:O	1:E:61:ASN:HB2	2.22	0.40

All (34) 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)
1:E:97:VAL:CB	3:A:5:NAG:C5[4_564]	0.32	1.88
1:E:97:VAL:CA	3:A:5:NAG:C6[4_564]	0.62	1.58
3:A:4:MAN:C3	5:E:1234:HOH:O[4_565]	0.74	1.46
1:E:97:VAL:CG1	3:A:5:NAG:O5[4_564]	0.86	1.34
1:E:97:VAL:CG2	3:A:5:NAG:C4[4_564]	0.89	1.31
1:E:97:VAL:CG2	3:A:5:NAG:C5[4_564]	1.23	0.97
1:E:97:VAL:CB	3:A:5:NAG:C6[4_564]	1.33	0.87
3:A:4:MAN:C2	5:E:1234:HOH:O[4_565]	1.34	0.86
1:E:147:ASN:O	1:E:187:GLN:NE2[2_665]	1.35	0.85
1:E:98:ASN:N	3:A:5:NAG:O6[4_564]	1.39	0.81
1:E:97:VAL:CB	3:A:5:NAG:O5[4_564]	1.41	0.79
1:E:97:VAL:N	3:A:5:NAG:C6[4_564]	1.50	0.70
5:E:708:HOH:O	5:E:838:HOH:O[4_565]	1.55	0.65
1:E:97:VAL:C	3:A:5:NAG:C6[4_564]	1.56	0.64
1:E:116:ALA:O	3:A:7:MAN:O4[3_455]	1.57	0.63
1:E:97:VAL:CG1	3:A:5:NAG:C5[4_564]	1.58	0.62
1:E:97:VAL:CG2	3:A:5:NAG:C3[4_564]	1.59	0.61
1:E:97:VAL:CG2	3:A:5:NAG:O4[4_564]	1.60	0.60
1:E:97:VAL:C	3:A:5:NAG:O6[4_564]	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:VAL:CA	3:A:5:NAG:C5[4_564]	1.74	0.46
1:E:97:VAL:CB	3:A:5:NAG:C4[4_564]	1.83	0.37
1:E:97:VAL:O	3:A:6:GAL:C1[4_564]	1.84	0.36
1:E:25:HIS:O	3:A:7:MAN:O3[3_455]	1.88	0.32
3:A:4:MAN:C4	5:E:1234:HOH:O[4_565]	1.90	0.30
3:A:4:MAN:C1	5:E:1234:HOH:O[4_565]	1.94	0.26
1:E:97:VAL:CA	3:A:5:NAG:O6[4_564]	1.95	0.25
1:E:150:GLY:CA	5:E:592:HOH:O[2_665]	2.03	0.17
3:A:4:MAN:O3	5:E:1234:HOH:O[4_565]	2.05	0.15
3:A:3:BMA:O6	5:E:1234:HOH:O[4_565]	2.06	0.14
1:E:36:ARG:NH2	1:E:164:THR:OG1[2_665]	2.09	0.11
1:E:97:VAL:CG1	3:A:5:NAG:C6[4_564]	2.09	0.11
1:E:97:VAL:CG1	3:A:5:NAG:C1[4_564]	2.11	0.09
1:E:97:VAL:CG1	3:A:5:NAG:O6[4_564]	2.15	0.05
3:A:6:GAL:O2	5:E:1129:HOH:O[4_565]	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%)	201 (93%)	11 (5%)	4 (2%)	6	5
2	I	3/6 (50%)	3 (100%)	0	0	100	100
All	All	219/224 (98%)	204 (93%)	11 (5%)	4 (2%)	6	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	36	ARG
1	E	146	ARG
1	E	213	ALA
1	E	124	PRO

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	E	172/172 (100%)	158 (92%)	14 (8%)	11	14
2	I	1/1 (100%)	1 (100%)	0	100	100
All	All	173/173 (100%)	159 (92%)	14 (8%)	11	14

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	36	ARG
1	E	62	VAL
1	E	75	ARG
1	E	104	VAL
1	E	114	ILE
1	E	115	ASN
1	E	128	ARG
1	E	148	ARG
1	E	151	ILE
1	E	166	LEU
1	E	200	VAL
1	E	208	LEU
1	E	223	LEU
1	E	235	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	92	ASN
1	E	115	ASN
1	E	117	ASN
1	E	119	GLN
1	E	132	ASN
1	E	202	ASN
1	E	210	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	VAI	I	5	2,1	6,6,7	0.68	0	4,7,9	0.52	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
2	VAI	I	5	2,1	-	1/6/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	5	VAI	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	5	VAI	1	0

5.5 Carbohydrates ⓘ

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	1.02	0	17,19,21	2.65	8 (47%)
3	NAG	A	2	3	14,14,15	0.77	0	17,19,21	1.45	2 (11%)
3	BMA	A	3	3	11,11,12	0.81	1 (9%)	15,15,17	1.70	2 (13%)
3	MAN	A	4	3	11,11,12	0.42	0	15,15,17	1.93	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	0.55	0	15,15,17	1.66	1 (6%)
3	FUC	A	8	3	10,10,11	1.22	1 (10%)	14,14,16	1.53	3 (21%)
4	NAG	B	1	1,4	14,14,15	1.60	5 (35%)	17,19,21	2.07	4 (23%)
4	NAG	B	2	4	14,14,15	0.96	0	17,19,21	1.64	3 (17%)
4	BMA	B	3	4	11,11,12	0.78	0	15,15,17	1.70	5 (33%)
4	BMA	B	4	4	11,11,12	0.64	0	15,15,17	1.55	3 (20%)
4	NDG	B	5	4	14,14,15	0.91	1 (7%)	17,19,21	2.90	8 (47%)
4	GLC	B	6	4	11,11,12	0.66	0	15,15,17	1.85	1 (6%)
4	MAN	B	7	4	11,11,12	0.57	0	15,15,17	2.02	2 (13%)
4	FUC	B	8	4	10,10,11	1.30	1 (10%)	14,14,16	1.90	4 (28%)

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	-	0/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,4	-	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	BMA	B	4	4	-	0/2/19/22	0/1/1/1
4	NDG	B	5	4	1/1/5/7	4/6/23/26	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	1/1/1/1
4	FUC	B	8	4	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	C3-C2	2.55	1.57	1.52
4	B	1	NAG	C1-C2	2.47	1.55	1.52
4	B	1	NAG	C4-C3	2.38	1.58	1.52
4	B	1	NAG	C8-C7	2.28	1.55	1.50
4	B	5	NDG	C1-C2	2.24	1.55	1.52
3	A	3	BMA	C1-C2	2.21	1.57	1.52
4	B	1	NAG	O3-C3	2.21	1.48	1.43
4	B	8	FUC	O3-C3	2.13	1.48	1.43
3	A	8	FUC	O5-C1	-2.04	1.40	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	7	MAN	C1-O5-C5	7.19	121.82	112.19
3	A	4	MAN	C1-O5-C5	6.78	121.27	112.19
4	B	6	GLC	C1-O5-C5	6.41	120.78	112.19
4	B	5	NDG	C1-O5-C5	6.36	120.71	112.19
3	A	7	MAN	C1-O5-C5	6.02	120.26	112.19
4	B	5	NDG	C3-C4-C5	-5.63	100.02	110.23
3	A	3	BMA	C1-O5-C5	5.49	119.54	112.19
4	B	1	NAG	C2-N2-C7	-5.17	115.97	122.90
3	A	6	GAL	C1-O5-C5	5.08	118.99	112.19
3	A	5	NAG	C1-O5-C5	5.00	118.89	112.19
3	A	1	NAG	O7-C7-N2	4.50	129.93	121.98
4	B	8	FUC	C2-C3-C4	-4.27	103.35	110.86
3	A	1	NAG	C1-O5-C5	4.11	117.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	NAG	C2-N2-C7	-4.00	117.54	122.90
4	B	5	NDG	C2-N2-C7	3.84	128.05	122.90
3	A	1	NAG	O4-C4-C3	-3.84	101.33	110.38
3	A	1	NAG	C8-C7-N2	-3.81	109.81	116.12
4	B	2	NAG	O5-C5-C6	-3.80	100.26	107.66
3	A	1	NAG	C1-C2-N2	3.80	116.43	110.43
4	B	3	BMA	O5-C5-C6	3.71	114.89	107.66
4	B	5	NDG	O3-C3-C2	-3.70	101.73	109.40
3	A	1	NAG	O7-C7-C8	-3.50	115.82	122.05
4	B	4	BMA	C3-C4-C5	3.45	116.49	110.23
3	A	1	NAG	C2-N2-C7	-3.41	118.32	122.90
4	B	2	NAG	C1-O5-C5	3.36	116.69	112.19
4	B	5	NDG	O5-C5-C6	3.31	114.11	107.66
4	B	5	NDG	C1-C2-N2	-3.24	105.33	110.43
3	A	8	FUC	C1-C2-C3	3.13	114.20	109.64
4	B	4	BMA	O2-C2-C1	3.11	116.35	109.22
4	B	1	NAG	C4-C3-C2	2.99	115.40	111.02
4	B	1	NAG	C1-C2-N2	-2.98	105.74	110.43
4	B	4	BMA	C1-O5-C5	2.85	116.01	112.19
3	A	2	NAG	O4-C4-C3	-2.80	103.77	110.38
4	B	8	FUC	O2-C2-C3	2.69	115.73	110.15
4	B	1	NAG	O5-C1-C2	-2.63	107.23	111.29
4	B	8	FUC	C1-O5-C5	2.53	118.94	112.97
4	B	5	NDG	C4-C3-C2	2.53	114.72	111.02
4	B	2	NAG	C4-C3-C2	2.47	114.64	111.02
4	B	8	FUC	O2-C2-C1	2.40	114.72	109.22
3	A	3	BMA	O5-C1-C2	-2.33	105.23	110.79
4	B	3	BMA	O6-C6-C5	-2.32	103.43	111.33
3	A	1	NAG	O6-C6-C5	-2.29	103.55	111.33
4	B	3	BMA	C3-C4-C5	-2.27	106.11	110.23
4	B	7	MAN	O5-C5-C6	2.20	111.94	107.66
3	A	8	FUC	C1-O5-C5	2.20	118.15	112.97
3	A	8	FUC	O5-C1-C2	-2.18	105.59	110.79
4	B	5	NDG	O3-C3-C4	-2.14	105.34	110.38
4	B	3	BMA	C1-O5-C5	2.11	115.02	112.19
4	B	3	BMA	C1-C2-C3	2.07	112.65	109.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	5	NDG	C3
4	B	6	GLC	C3

All (14) torsion outliers are listed below:

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

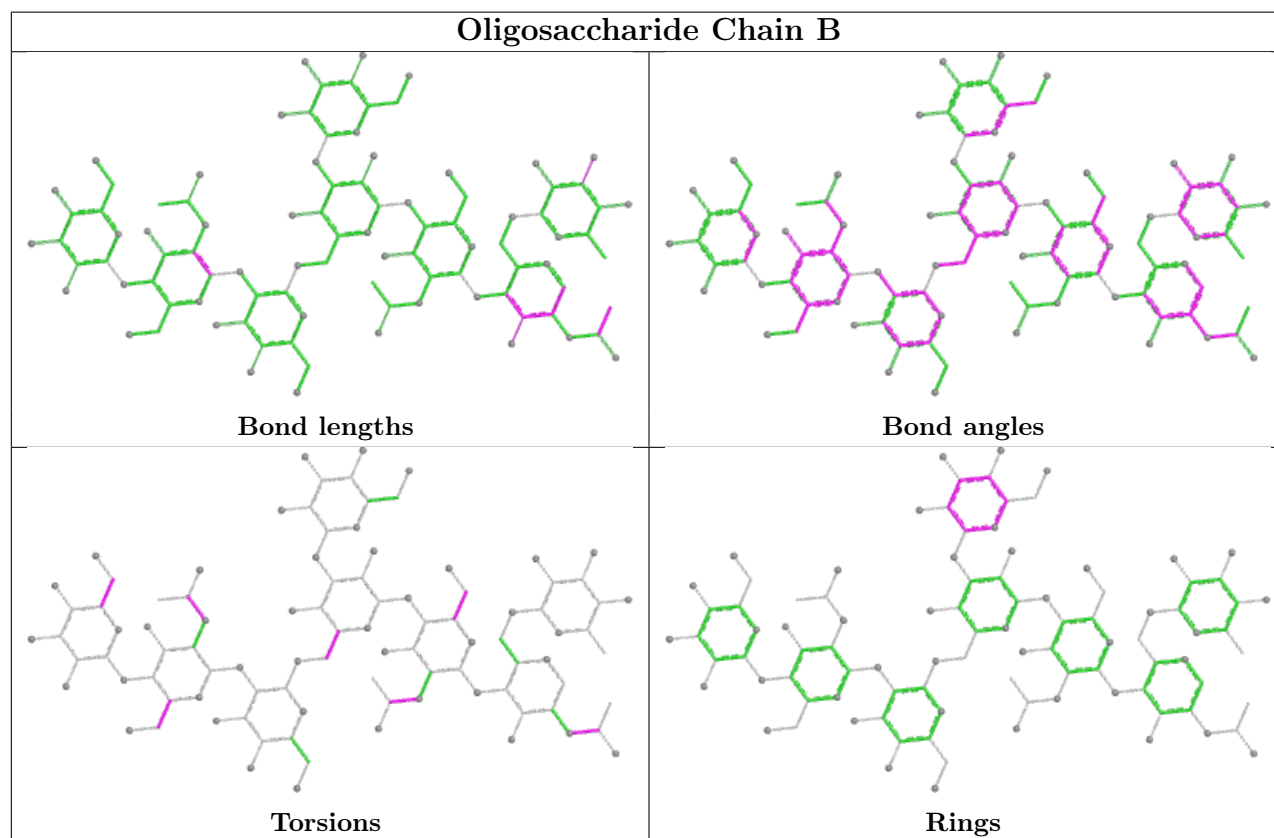
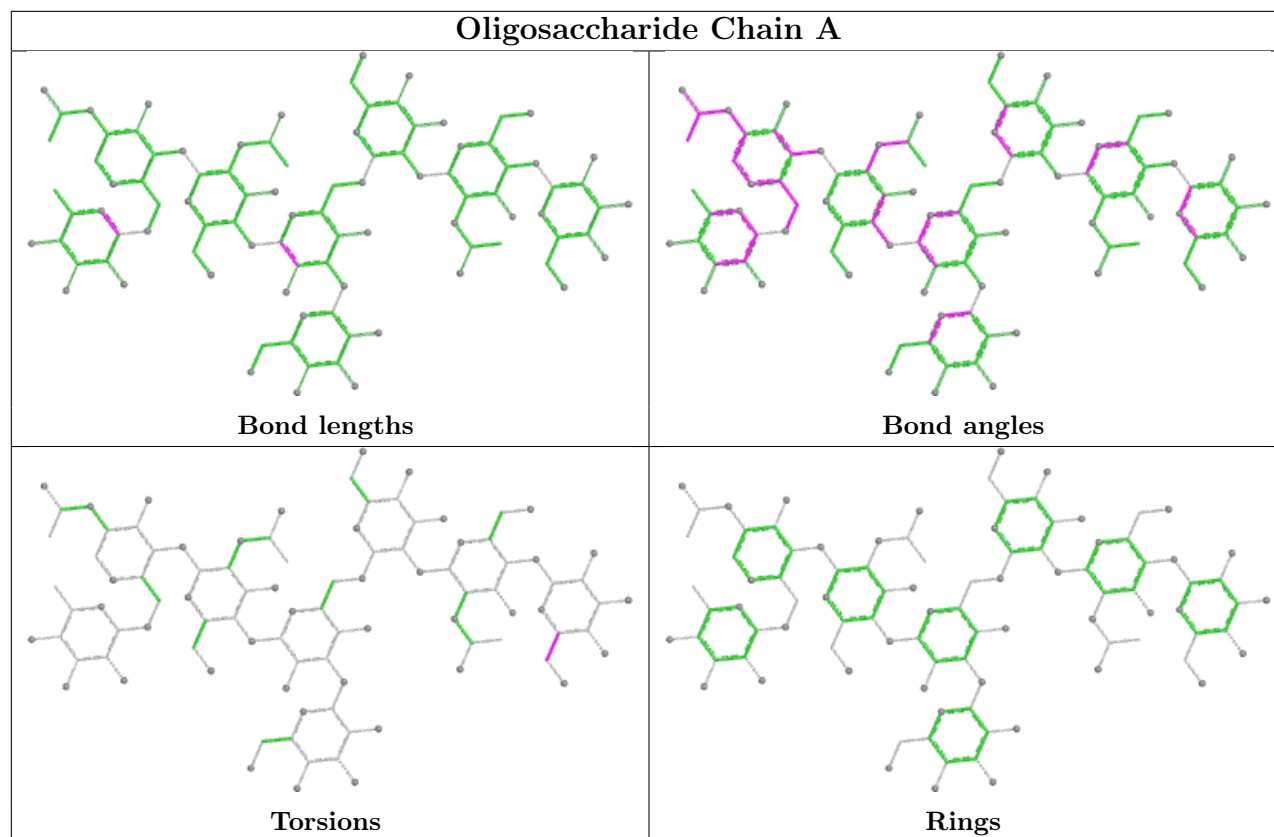
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	7	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7	MAN	0	2
3	A	4	MAN	0	5
3	A	6	GAL	0	2
4	B	8	FUC	1	0
3	A	5	NAG	0	20
3	A	3	BMA	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.