



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:45 AM UTC

PDB ID : 1LYA / pdb_00001lya
Title : CRYSTAL STRUCTURES OF NATIVE AND INHIBITED FORMS OF HUMAN CATHEPSIN D: IMPLICATIONS FOR LYSOSOMAL TARGETING AND DRUG DESIGN
Authors : Baldwin, E.T.; Bhat, T.N.; Gulnik, S.; Erickson, J.W.
Deposited on : 1993-04-22
Resolution : 2.50 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

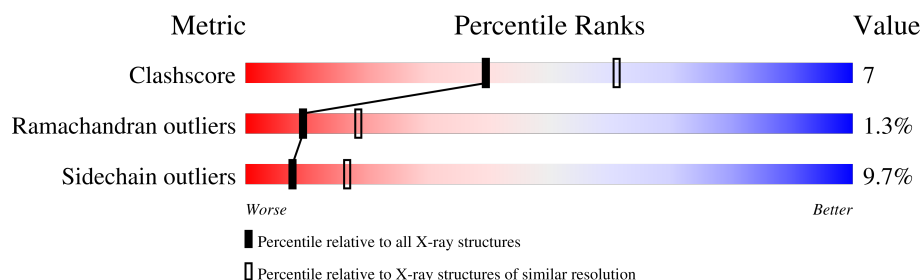
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	97	
1	C	97	
2	B	241	
2	D	241	
3	E	4	
3	F	4	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6662 atoms, of which 1302 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 CATHEPSIN D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	97	Total	C	H	N	O	S	0	0	0
			904	478	156	119	146	5			
1	C	97	Total	C	H	N	O	S	0	0	0
			904	478	156	119	146	5			

- Molecule 2 is a protein called CATHEPSIN D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	241	Total	C	H	N	O	S	0	0	0
			2234	1184	389	302	348	11			
2	D	241	Total	C	H	N	O	S	0	0	0
			2234	1184	389	302	348	11			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	4	Total	C	H	N	O	0	0	0
			96	28	46	2	20			
3	F	4	Total	C	H	N	O	0	0	0
			96	28	46	2	20			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	10	Total	H	O	0	0
			30	20	10		
5	B	12	Total	H	O	0	0
			36	24	12		
5	C	8	Total	H	O	0	0
			24	16	8		
5	D	16	Total	H	O	0	0
			48	32	16		

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: CATHEPSIN D

Chain A: 



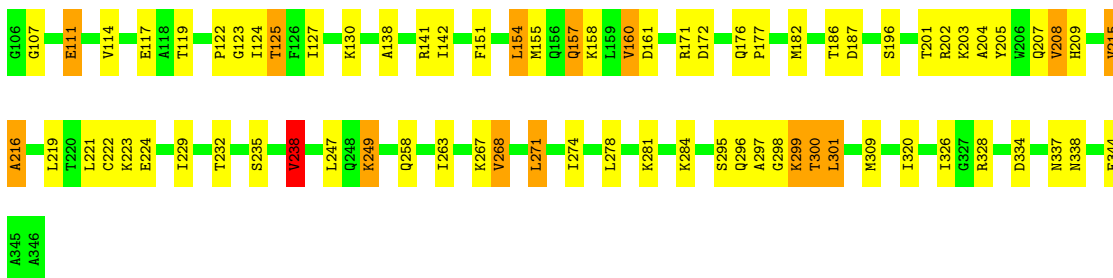
• Molecule 1: CATHEPSIN D

Chain C: 



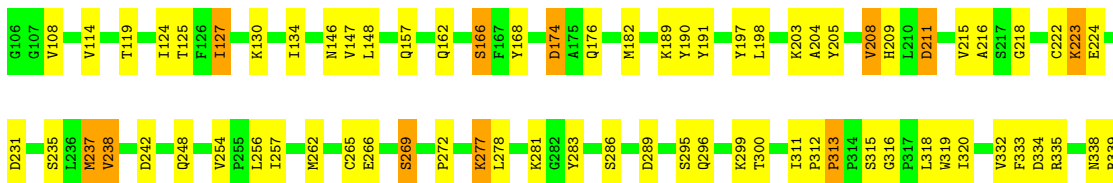
• Molecule 2: CATHEPSIN D

Chain B: 



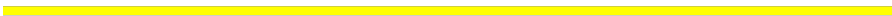
• Molecule 2: CATHEPSIN D

Chain D: 





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

Chain E:  100%



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

Chain F:  100%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	125.90Å 125.90Å 104.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6662	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: MAN, NAG, 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	A	1.04	4/771 (0.5%)	1.69	11/1051 (1.0%)
1	C	1.08	6/771 (0.8%)	1.66	10/1051 (1.0%)
2	B	0.88	2/1884 (0.1%)	1.70	21/2551 (0.8%)
2	D	0.85	1/1884 (0.1%)	1.67	34/2551 (1.3%)
All	All	0.92	13/5310 (0.2%)	1.68	76/7204 (1.1%)

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
2	D	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	56	HIS	CD2-NE2	-6.61	1.30	1.37
1	C	57	HIS	CD2-NE2	-6.45	1.30	1.37
1	C	45	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	45	HIS	CD2-NE2	-6.25	1.30	1.37
1	C	56	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	77	HIS	CD2-NE2	-6.05	1.31	1.37
2	D	209	HIS	CD2-NE2	-6.00	1.31	1.37
1	C	77	HIS	CD2-NE2	-5.82	1.31	1.37
2	B	238	VAL	CA-CB	5.38	1.64	1.55
2	B	209	HIS	CD2-NE2	-5.34	1.31	1.37
1	C	45	HIS	CG-ND1	-5.24	1.32	1.38
1	C	57	HIS	CG-ND1	-5.03	1.32	1.38

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	297	ALA	N-CA-C	-10.39	90.41	110.56
2	D	204	ALA	N-CA-C	-9.04	97.88	111.34
2	B	157	GLN	OE1-CD-NE2	-7.39	115.21	122.60
2	B	258	GLN	N-CA-C	7.10	121.19	111.39
2	B	172	ASP	CA-CB-CG	7.09	119.69	112.60
2	D	174	ASP	CA-CB-CG	7.09	119.69	112.60
2	D	319	TRP	N-CA-C	-7.06	100.07	110.52
2	D	211	ASP	CA-CB-CG	6.98	119.58	112.60
2	D	242	ASP	CA-CB-CG	6.95	119.55	112.60
2	B	208	VAL	N-CA-CB	-6.79	101.03	112.44
2	B	223	LYS	N-CA-C	-6.60	100.07	109.96
2	D	338	ASN	OD1-CG-ND2	-6.59	116.01	122.60
2	B	205	TYR	N-CA-C	-6.47	100.33	110.36
2	D	208	VAL	N-CA-CB	-6.45	100.43	112.36
2	D	231	ASP	CA-CB-CG	6.41	119.01	112.60
2	D	215	VAL	N-CA-C	-6.41	98.42	108.23
2	D	296	GLN	N-CA-C	-6.24	98.25	108.41
2	D	254	VAL	CA-C-N	6.22	126.17	119.76
2	D	254	VAL	C-N-CA	6.22	126.17	119.76
1	C	33	ASP	CA-CB-CG	6.22	118.82	112.60
2	D	182	MET	CA-CB-CG	-6.21	101.68	114.10
2	D	127	ILE	N-CA-C	-6.12	104.33	111.00
1	C	41	VAL	O-C-N	-6.10	117.45	121.72
2	D	248	GLN	OE1-CD-NE2	-6.05	116.55	122.60
2	B	216	ALA	N-CA-C	6.01	120.15	112.34
2	D	162	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	A	26	GLN	N-CA-C	-5.96	99.52	109.24
2	B	122	PRO	N-CA-C	5.96	120.44	111.14
2	B	338	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	45	HIS	N-CA-C	-5.93	105.86	112.57
2	D	289	ASP	CA-CB-CG	5.87	118.47	112.60
2	D	208	VAL	O-C-N	-5.78	116.49	123.02
2	B	337	ASN	OD1-CG-ND2	-5.70	116.90	122.60
2	B	338	ASN	CB-CG-ND2	5.69	124.94	116.40
1	C	66	THR	N-CA-C	5.68	119.83	113.02
1	A	11	MET	N-CA-C	5.67	119.38	111.90
1	A	38	ASN	CB-CG-ND2	5.66	124.89	116.40
2	B	157	GLN	CG-CD-NE2	5.65	124.88	116.40
2	B	334	ASP	CA-CB-CG	5.64	118.24	112.60
2	B	176	GLN	OE1-CD-NE2	-5.64	116.96	122.60
2	D	265	CYS	N-CA-C	5.62	118.13	111.33
2	D	146	ASN	OD1-CG-ND2	-5.60	117.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	TRP	CG-CD2-CE3	5.54	139.44	133.90
2	D	209	HIS	CB-CG-CD2	-5.53	124.01	131.20
2	B	201	THR	O-C-N	-5.51	115.26	122.59
2	D	176	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	C	83	LEU	CA-CB-CG	5.43	135.32	116.30
1	C	57	HIS	CB-CG-CD2	-5.40	124.17	131.20
1	A	40	TRP	CB-CG-CD1	-5.40	118.81	126.90
1	C	29	THR	N-CA-C	-5.35	100.98	109.59
2	B	158	LYS	CA-CB-CG	-5.35	103.41	114.10
1	C	55	ILE	O-C-N	-5.34	116.44	122.05
2	B	125	THR	N-CA-C	5.33	118.57	111.75
1	A	77	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	45	HIS	CB-CG-CD2	-5.31	124.30	131.20
2	D	157	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	C	50	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	268	VAL	N-CA-C	5.26	115.98	110.62
2	D	237	MET	CG-SD-CE	-5.25	89.34	100.90
2	D	208	VAL	CB-CA-C	5.24	119.16	110.30
2	D	237	MET	O-C-N	-5.21	117.12	123.16
2	D	334	ASP	CA-CB-CG	5.19	117.79	112.60
2	D	269	SER	N-CA-C	5.18	117.59	111.33
2	B	196	SER	N-CA-C	-5.13	100.53	108.90
1	A	40	TRP	CE2-CD2-CG	-5.13	101.04	107.20
2	D	168	TYR	N-CA-C	-5.11	100.84	109.07
1	C	56	HIS	CA-CB-CG	-5.10	108.70	113.80
2	D	148	LEU	CA-C-N	5.10	125.38	119.92
2	D	148	LEU	C-N-CA	5.10	125.38	119.92
1	A	96	CYS	CA-C-N	5.08	130.85	121.70
1	A	96	CYS	C-N-CA	5.08	130.85	121.70
2	D	190	TYR	N-CA-C	5.08	119.57	113.17
2	B	161	ASP	N-CA-C	5.04	116.47	111.07
1	C	26	GLN	N-CA-C	-5.04	101.02	109.24
2	D	286	SER	CA-C-N	5.01	125.03	119.32
2	D	286	SER	C-N-CA	5.01	125.03	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	313	PRO	Peptide

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	748	156	702	19	0
1	C	748	156	702	9	0
2	B	1845	389	1849	31	0
2	D	1845	389	1849	25	0
3	E	50	46	43	0	0
3	F	50	46	43	0	0
4	B	14	14	13	0	0
4	D	14	14	13	0	0
5	A	10	20	0	0	0
5	B	12	24	0	1	0
5	C	8	16	0	1	0
5	D	16	32	0	1	0
All	All	5360	1302	5214	70	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 7.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:VAL:HA	2:B:271:LEU:HD22	1.71	0.72
2:D:114:VAL:HG13	2:D:147:VAL:HG13	1.72	0.71
2:D:316:GLY:HA2	2:D:318:LEU:HG	1.75	0.67
2:B:238:VAL:HG13	2:B:320:ILE:HB	1.81	0.62
2:D:311:ILE:HD11	2:D:320:ILE:HD11	1.83	0.61
2:B:207:GLN:HG3	2:B:229:ILE:HG22	1.82	0.60
1:A:2:PRO:HB2	2:B:182:MET:SD	2.43	0.58
1:A:43:SER:HB2	2:B:117:GLU:HB3	1.85	0.57
2:B:142:ILE:HG23	2:B:204:ALA:HB1	1.87	0.55
1:A:78:TYR:HE2	1:A:83:LEU:HD21	1.72	0.53
1:A:88:SER:O	2:B:114:VAL:HA	2.10	0.52
2:B:222:CYS:SG	2:B:222:CYS:O	2.69	0.51
1:C:81:GLY:HA3	2:D:125:THR:HG21	1.92	0.51
2:D:211:ASP:HB2	2:D:277:LYS:HB3	1.92	0.50
1:A:53:CYS:O	1:A:58:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:TYR:HB3	1:C:14:GLN:HB2	1.95	0.49
1:C:23:THR:O	1:C:64:SER:HA	2.12	0.49
2:B:182:MET:HE2	2:B:187:ASP:HB2	1.94	0.49
2:D:256:LEU:HD22	2:D:262:MET:HE2	1.94	0.49
1:A:46:CYS:HA	2:B:119:THR:HA	1.94	0.49
2:D:222:CYS:SG	2:D:222:CYS:O	2.70	0.48
1:C:53:CYS:SG	1:C:58:LYS:HD3	2.53	0.48
2:D:124:ILE:HA	2:D:127:ILE:HD12	1.94	0.48
2:B:299:LYS:C	2:B:301:LEU:H	2.20	0.48
2:D:238:VAL:HG13	2:D:320:ILE:HB	1.95	0.48
2:D:311:ILE:O	2:D:316:GLY:HA3	2.13	0.48
2:B:295:SER:HA	2:B:298:GLY:HA2	1.96	0.48
1:C:31:VAL:CG1	2:D:134:ILE:HG12	2.44	0.48
2:D:295:SER:HA	2:D:299:LYS:O	2.14	0.47
2:D:191:TYR:HB2	2:D:343:ALA:HB3	1.95	0.47
1:A:81:GLY:HA2	2:B:125:THR:HG21	1.95	0.47
1:A:53:CYS:SG	1:A:58:LYS:HG2	2.55	0.46
2:B:299:LYS:O	2:B:301:LEU:N	2.48	0.46
1:A:85:GLY:HA3	2:B:117:GLU:O	2.16	0.46
2:B:141:ARG:NH1	2:B:202:ARG:HE	2.14	0.46
1:C:46:CYS:HA	2:D:119:THR:HA	1.97	0.46
1:A:23:THR:O	1:A:64:SER:HA	2.16	0.45
2:B:215:VAL:HG13	2:B:219:LEU:HB3	1.98	0.45
2:B:299:LYS:HG2	2:B:300:THR:H	1.82	0.45
2:B:249:LYS:N	2:B:249:LYS:HD2	2.32	0.45
1:A:95:PRO:HD2	2:B:107:GLY:HA2	1.99	0.45
1:C:8:LYS:O	1:C:15:TYR:HA	2.17	0.45
5:C:101:HOH:O	2:D:205:TYR:HB3	2.16	0.45
2:D:114:VAL:HG12	5:D:515:HOH:O	2.17	0.45
2:B:123:GLY:O	2:B:127:ILE:HD13	2.16	0.45
1:A:44:ILE:HA	1:A:58:LYS:HB3	2.00	0.44
1:A:78:TYR:CE2	1:A:83:LEU:HD21	2.51	0.44
2:B:154:LEU:HD23	2:B:160:VAL:HG22	1.99	0.44
1:A:44:ILE:HG12	1:A:60:ASN:HA	2.00	0.44
2:B:111:GLU:H	2:B:157:GLN:HE22	1.66	0.44
1:A:10:TYR:HB3	1:A:14:GLN:HB2	2.00	0.43
1:A:10:TYR:CD1	2:B:130:LYS:HD2	2.53	0.43
2:B:215:VAL:HB	2:B:274:ILE:HG12	2.00	0.43
2:B:151:PHE:O	2:B:155:MET:HG3	2.19	0.43
2:D:312:PRO:HA	2:D:313:PRO:HD2	1.85	0.43
1:A:37:SER:OG	2:B:138:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:335:ARG:HA	2:D:335:ARG:HD2	1.79	0.42
2:D:197:TYR:HB3	2:D:339:ARG:HG2	2.02	0.42
2:D:223:LYS:O	2:D:224:GLU:HB2	2.19	0.42
2:D:166:SER:HB3	2:D:332:VAL:HA	2.01	0.41
2:D:278:LEU:HB2	2:D:283:TYR:CE1	2.55	0.41
2:B:263:ILE:HG12	2:B:271:LEU:HD21	2.02	0.41
2:D:256:LEU:HG	2:D:257:ILE:HG22	2.02	0.41
2:B:207:GLN:HB2	5:B:503:HOH:O	2.21	0.41
1:C:76:ILE:HB	1:C:83:LEU:HD13	2.03	0.40
2:D:216:ALA:HB3	2:D:272:PRO:HB2	2.04	0.40
1:A:19:ILE:HG22	1:A:94:VAL:HG22	2.03	0.40
1:A:37:SER:HG	2:B:138:ALA:HB3	1.87	0.40
1:C:34:THR:HG21	2:D:333:PHE:CZ	2.56	0.40
2:B:232:THR:HG22	2:B:326:ILE:HD13	2.04	0.40

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	95/97 (98%)	90 (95%)	3 (3%)	2 (2%)	5	9
1	C	95/97 (98%)	93 (98%)	1 (1%)	1 (1%)	11	22
2	B	239/241 (99%)	223 (93%)	12 (5%)	4 (2%)	7	13
2	D	239/241 (99%)	223 (93%)	14 (6%)	2 (1%)	16	31
All	All	668/676 (99%)	629 (94%)	30 (4%)	9 (1%)	9	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER

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Mol	Chain	Res	Type
1	C	80	SER
2	B	224	GLU
2	B	300	THR
2	B	299	LYS
2	D	174	ASP
2	B	216	ALA
2	D	218	GLY
1	A	95	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	A	85/86 (99%)	77 (91%)	8 (9%)	8	18
1	C	85/86 (99%)	80 (94%)	5 (6%)	18	37
2	B	199/199 (100%)	174 (87%)	25 (13%)	4	9
2	D	199/199 (100%)	182 (92%)	17 (8%)	10	22
All	All	568/570 (100%)	513 (90%)	55 (10%)	8	17

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	8	LYS
1	A	11	MET
1	A	31	VAL
1	A	48	LEU
1	A	49	LEU
1	A	93	SER
1	A	96	CYS
2	B	111	GLU
2	B	124	ILE
2	B	154	LEU
2	B	160	VAL
2	B	171	ARG

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Mol	Chain	Res	Type
2	B	177	PRO
2	B	186	THR
2	B	203	LYS
2	B	208	VAL
2	B	215	VAL
2	B	221	LEU
2	B	235	SER
2	B	238	VAL
2	B	247	LEU
2	B	249	LYS
2	B	267	LYS
2	B	271	LEU
2	B	278	LEU
2	B	281	LYS
2	B	284	LYS
2	B	296	GLN
2	B	301	LEU
2	B	309	MET
2	B	328	ARG
2	B	344	GLU
1	C	44	ILE
1	C	61	SER
1	C	75	ASP
1	C	83	LEU
1	C	93	SER
2	D	108	VAL
2	D	130	LYS
2	D	166	SER
2	D	189	LYS
2	D	198	LEU
2	D	203	LYS
2	D	208	VAL
2	D	223	LYS
2	D	235	SER
2	D	237	MET
2	D	238	VAL
2	D	266	GLU
2	D	269	SER
2	D	277	LYS
2	D	281	LYS
2	D	300	THR
2	D	315	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	89	GLN
2	B	121	GLN
2	B	146	ASN
2	B	338	ASN
1	C	60	ASN
2	D	146	ASN
2	D	162	GLN
2	D	258	GLN
2	D	338	ASN

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 ⓘ

8 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	E	1	3,1	14,14,15	0.77	0	17,19,21	1.92	3 (17%)
3	NAG	E	2	3	14,14,15	0.85	1 (7%)	17,19,21	1.16	1 (5%)
3	BMA	E	3	3	11,11,12	0.91	0	15,15,17	0.95	2 (13%)
3	MAN	E	4	3	11,11,12	0.91	0	15,15,17	1.27	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.77	0	17,19,21	1.60	2 (11%)
3	NAG	F	2	3	14,14,15	0.72	0	17,19,21	2.18	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	F	3	3	11,11,12	0.96	0	15,15,17	2.23	6 (40%)
3	MAN	F	4	3	11,11,12	0.94	0	15,15,17	1.10	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
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C1-C2	2.59	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	5.70	119.82	112.19
3	F	1	NAG	C1-O5-C5	4.54	118.27	112.19
3	F	3	BMA	C1-C2-C3	-4.25	103.45	109.64
3	F	3	BMA	C6-C5-C4	4.14	123.18	113.02
3	F	2	NAG	O4-C4-C3	4.03	119.87	110.38
3	F	2	NAG	C2-N2-C7	3.62	127.75	122.90
3	F	2	NAG	C1-C2-N2	3.57	116.06	110.43
3	E	4	MAN	C1-O5-C5	3.20	116.47	112.19
3	F	3	BMA	O3-C3-C2	3.04	116.26	110.05
3	F	4	MAN	C1-O5-C5	2.74	115.86	112.19
3	F	2	NAG	C4-C3-C2	-2.73	107.01	111.02
3	E	1	NAG	C1-C2-N2	-2.59	106.36	110.43
3	F	3	BMA	C2-C3-C4	-2.58	106.31	110.86
3	F	2	NAG	O5-C5-C4	-2.54	104.64	110.83
3	E	2	NAG	O4-C4-C3	-2.52	104.44	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	C3-C4-C5	-2.43	105.83	110.23
3	E	1	NAG	O5-C1-C2	2.25	114.78	111.29
3	F	3	BMA	O2-C2-C1	2.22	114.31	109.22
3	E	3	BMA	C3-C4-C5	2.18	114.19	110.23
3	F	1	NAG	O5-C5-C6	-2.09	103.60	107.66
3	E	3	BMA	O2-C2-C1	2.07	113.97	109.22
3	F	2	NAG	C3-C4-C5	-2.07	106.48	110.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

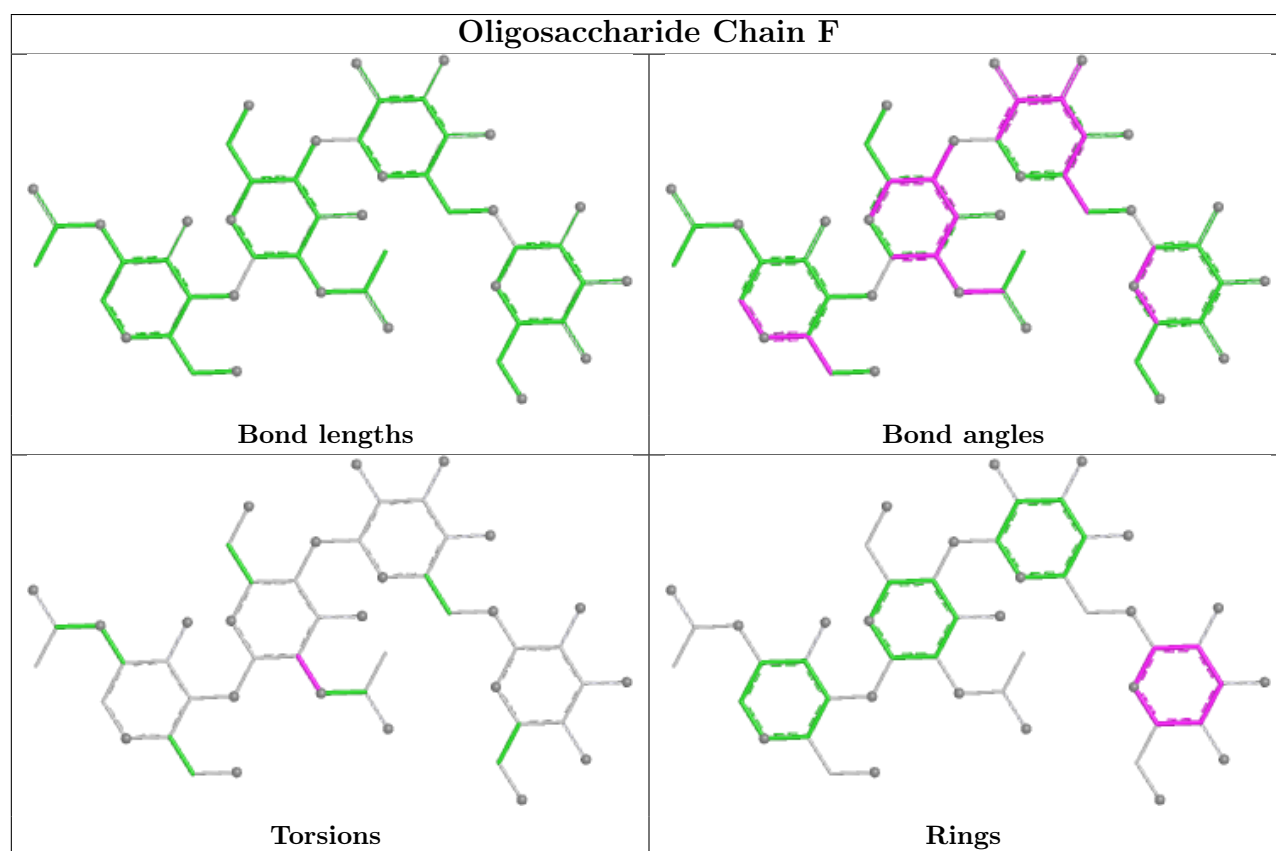
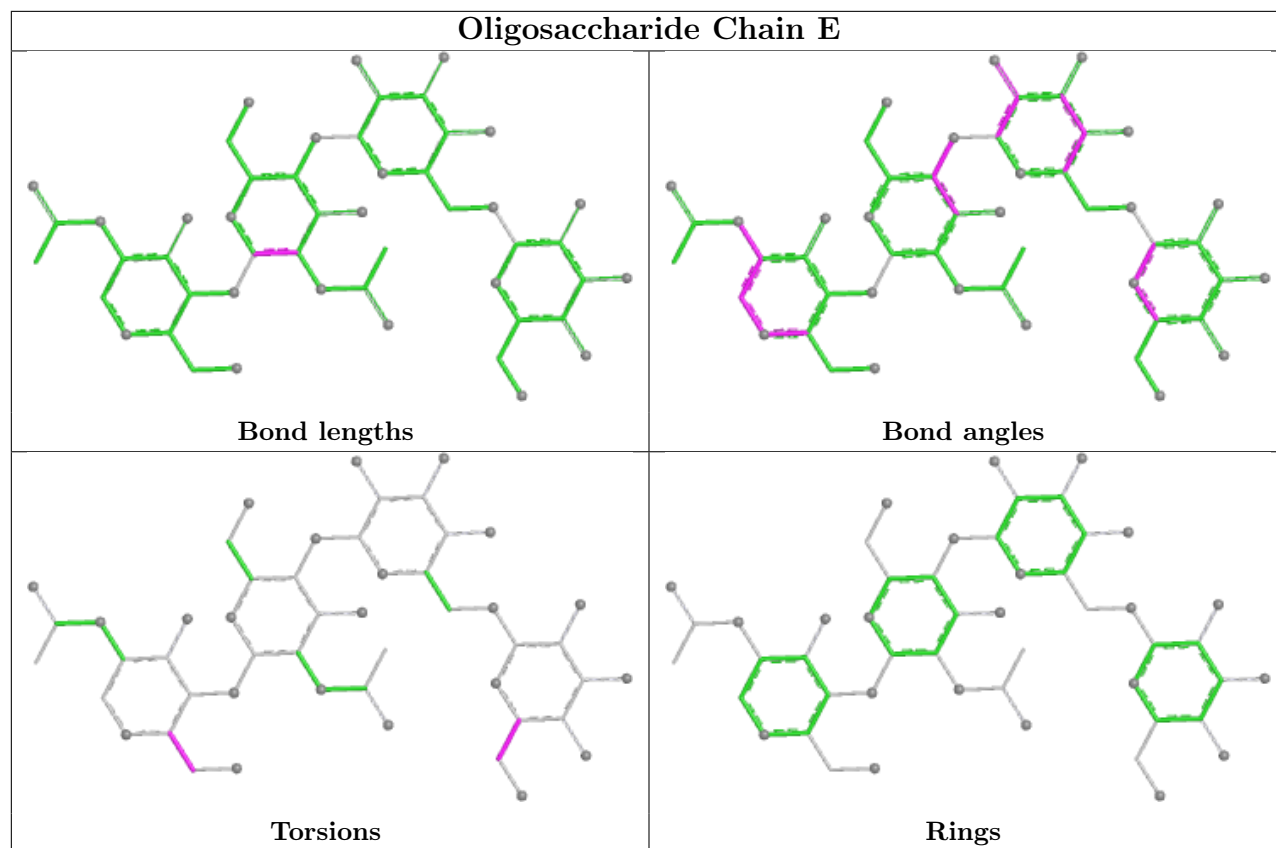
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C1-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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

2 ligands 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	NAG	D	401	2	14,14,15	0.81	0	17,19,21	1.62	3 (17%)
4	NAG	B	401	2	14,14,15	0.98	1 (7%)	17,19,21	1.56	3 (17%)

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	NAG	D	401	2	-	2/6/23/26	0/1/1/1
4	NAG	B	401	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	NAG	C1-C2	3.00	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	NAG	C1-O5-C5	4.46	118.16	112.19
4	B	401	NAG	C3-C4-C5	-3.09	104.63	110.23
4	B	401	NAG	C6-C5-C4	2.80	119.90	113.02
4	B	401	NAG	O4-C4-C5	2.34	115.08	109.32
4	D	401	NAG	C8-C7-N2	2.16	119.70	116.12
4	D	401	NAG	C4-C3-C2	-2.13	107.90	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	401	NAG	C4-C5-C6-O6
4	D	401	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section 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.