



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:47 PM UTC

PDB ID : 1FC1 / pdb_00001fc1
Title : CRYSTALLOGRAPHIC REFINEMENT AND ATOMIC MODELS OF A HUMAN FC FRAGMENT AND ITS COMPLEX WITH FRAGMENT B OF PROTEIN A FROM STAPHYLOCOCCUS AUREUS AT 2.9-AND 2.8-ANGSTROMS RESOLUTION
Authors : Deisenhofer, J.
Deposited on : 1981-05-21
Resolution : 2.90 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

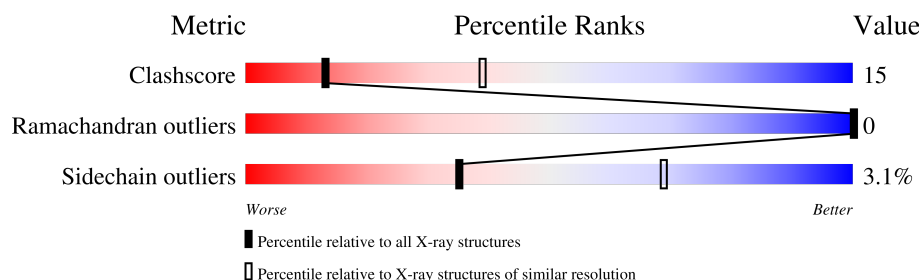
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	
2	C	9	
2	D	9	

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
2	MAN	C	3	X	-	-	-
2	FUC	C	9	X	-	-	-
2	MAN	D	3	X	-	-	-
2	FUC	D	9	X	-	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3532 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.

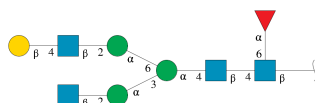
- Molecule 1 is a protein called FC FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	60	0	1
			1656	1054	282	313	7			
1	B	207	Total	C	N	O	S	217	0	1
			1656	1054	282	313	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLN	GLU	conflict	UNP P01857
A	283	GLN	GLU	conflict	UNP P01857
A	294	GLN	GLU	conflict	UNP P01857
A	312	ASN	ASP	conflict	UNP P01857
A	315	ASP	ASN	conflict	UNP P01857
A	356	GLU	ASP	conflict	UNP P01857
A	358	MET	LEU	conflict	UNP P01857
B	272	GLN	GLU	conflict	UNP P01857
B	283	GLN	GLU	conflict	UNP P01857
B	294	GLN	GLU	conflict	UNP P01857
B	312	ASN	ASP	conflict	UNP P01857
B	315	ASP	ASN	conflict	UNP P01857
B	356	GLU	ASP	conflict	UNP P01857
B	358	MET	LEU	conflict	UNP P01857

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



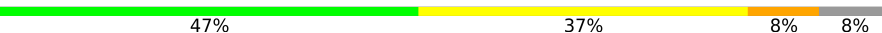
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total 110	C 62	N 4	O 44	18	0	0
2	D	9	Total 110	C 62	N 4	O 44	55	0	0

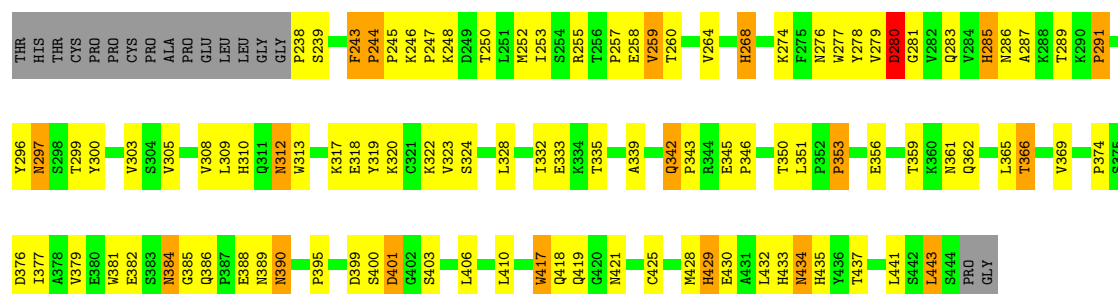
3 Residue-property plots

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.

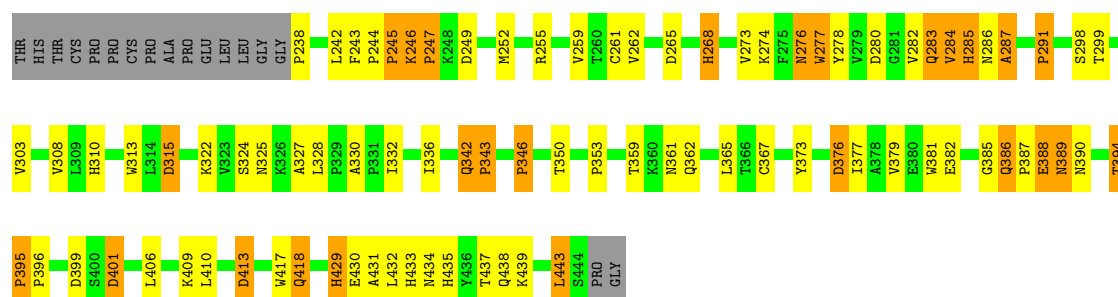
• Molecule 1: FC FRAGMENT

Chain A: 

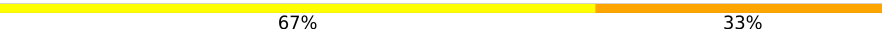


• Molecule 1: FC FRAGMENT

Chain B: 



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



• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyr

anose-(1-3)]alpha-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 D:



MAG1
MAG2
MAN3
MAN4
NAG5
GAL6
MAN7
MAG8
FUC9

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, α , β , γ	80.40Å 146.40Å 50.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3532	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: FUC, GAL, NAG, MAN

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	1.37	17/1702 (1.0%)	1.75	21/2318 (0.9%)
1	B	1.36	16/1702 (0.9%)	1.73	34/2318 (1.5%)
All	All	1.36	33/3404 (1.0%)	1.74	55/4636 (1.2%)

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	A	0	17
1	B	0	22
All	All	0	39

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	HIS	CE1-NE2	9.82	1.42	1.32
1	A	268	HIS	ND1-CE1	9.46	1.42	1.32
1	A	433	HIS	CE1-NE2	9.39	1.42	1.32
1	B	381	TRP	NE1-CE2	-9.36	1.27	1.37
1	A	277	TRP	NE1-CE2	-9.29	1.27	1.37
1	A	433	HIS	ND1-CE1	9.21	1.41	1.32
1	B	277	TRP	NE1-CE2	-9.07	1.27	1.37
1	B	268	HIS	CE1-NE2	9.02	1.41	1.32
1	B	313	TRP	NE1-CE2	-9.02	1.27	1.37
1	A	268	HIS	CE1-NE2	9.00	1.41	1.32
1	A	417	TRP	NE1-CE2	-8.92	1.27	1.37
1	B	285	HIS	ND1-CE1	8.91	1.41	1.32
1	A	435	HIS	CE1-NE2	8.89	1.41	1.32
1	B	433	HIS	CE1-NE2	8.87	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	TRP	NE1-CE2	-8.86	1.27	1.37
1	A	285	HIS	ND1-CE1	8.85	1.41	1.32
1	B	285	HIS	CE1-NE2	8.84	1.41	1.32
1	B	433	HIS	ND1-CE1	8.84	1.41	1.32
1	B	417	TRP	NE1-CE2	-8.81	1.27	1.37
1	B	268	HIS	ND1-CE1	8.76	1.41	1.32
1	B	429	HIS	CE1-NE2	8.76	1.41	1.32
1	A	435	HIS	ND1-CE1	8.60	1.41	1.32
1	B	310	HIS	CE1-NE2	8.59	1.41	1.32
1	A	381	TRP	NE1-CE2	-8.54	1.28	1.37
1	B	435	HIS	CE1-NE2	8.38	1.41	1.32
1	A	310	HIS	CE1-NE2	8.34	1.40	1.32
1	B	429	HIS	ND1-CE1	8.30	1.40	1.32
1	B	435	HIS	ND1-CE1	8.22	1.40	1.32
1	A	310	HIS	ND1-CE1	7.77	1.40	1.32
1	A	429	HIS	ND1-CE1	7.76	1.40	1.32
1	B	310	HIS	ND1-CE1	7.58	1.40	1.32
1	A	429	HIS	CE1-NE2	6.62	1.39	1.32
1	A	443	LEU	C-N	-5.05	1.26	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	HIS	CA-CB-CG	-9.41	104.39	113.80
1	B	395	PRO	N-CA-CB	7.51	107.13	103.22
1	B	396	PRO	N-CA-CB	6.75	108.70	103.30
1	A	366	THR	CA-C-N	-6.70	113.55	122.99
1	A	366	THR	C-N-CA	-6.70	113.55	122.99
1	A	280	ASP	CA-CB-CG	-6.69	105.91	112.60
1	B	343	PRO	N-CA-CB	6.68	108.93	103.32
1	A	342	GLN	CA-C-N	6.66	126.69	119.90
1	A	342	GLN	C-N-CA	6.66	126.69	119.90
1	A	243	PHE	CA-C-N	6.51	127.08	120.38
1	A	243	PHE	C-N-CA	6.51	127.08	120.38
1	B	315	ASP	CA-CB-CG	-6.41	106.19	112.60
1	A	244	PRO	CB-CA-C	-6.29	103.24	110.92
1	B	328	LEU	CA-C-N	6.02	125.23	118.97
1	B	328	LEU	C-N-CA	6.02	125.23	118.97
1	B	394	THR	CA-C-N	5.98	123.97	119.66
1	B	394	THR	C-N-CA	5.98	123.97	119.66
1	B	353	PRO	N-CA-CB	5.97	108.54	103.35
1	B	346	PRO	CB-CA-C	-5.87	104.36	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASN	N-CA-CB	-5.81	100.66	110.49
1	B	291	PRO	CA-C-N	5.63	132.29	121.54
1	B	291	PRO	C-N-CA	5.63	132.29	121.54
1	A	343	PRO	N-CA-CB	5.53	108.12	103.25
1	B	244	PRO	CA-C-N	5.48	125.43	119.78
1	B	244	PRO	C-N-CA	5.48	125.43	119.78
1	B	243	PHE	CA-C-N	5.48	126.02	120.38
1	B	243	PHE	C-N-CA	5.48	126.02	120.38
1	A	247	PRO	N-CA-CB	5.46	108.98	103.25
1	A	434	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	388	GLU	N-CA-C	5.40	118.07	110.14
1	A	291	PRO	CA-C-N	5.37	131.79	121.54
1	A	291	PRO	C-N-CA	5.37	131.79	121.54
1	B	286	ASN	CA-CB-CG	-5.36	107.24	112.60
1	A	297	ASN	CA-C-N	5.32	131.70	121.54
1	A	297	ASN	C-N-CA	5.32	131.70	121.54
1	B	386	GLN	O-C-N	5.32	126.66	121.66
1	A	238	PRO	N-CA-CB	5.30	108.83	103.00
1	B	332	ILE	N-CA-C	5.30	115.98	107.98
1	B	245	PRO	N-CA-CB	5.29	107.95	103.35
1	B	376	ASP	CB-CA-C	-5.23	102.04	110.77
1	B	413	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	286	ASN	CA-CB-CG	-5.16	107.44	112.60
1	B	330	ALA	CA-C-N	5.14	125.38	119.83
1	B	330	ALA	C-N-CA	5.14	125.38	119.83
1	B	401	ASP	CB-CA-C	-5.13	98.98	110.21
1	B	386	GLN	CA-C-N	5.13	125.11	120.03
1	B	386	GLN	C-N-CA	5.13	125.11	120.03
1	B	282	VAL	N-CA-C	5.12	115.68	108.36
1	B	395	PRO	CB-CA-C	-5.09	106.39	111.17
1	B	247	PRO	N-CA-CB	5.07	108.57	103.25
1	A	353	PRO	N-CA-CB	5.06	107.75	103.35
1	A	388	GLU	N-CA-C	5.06	117.95	110.46
1	B	385	GLY	N-CA-C	-5.05	107.78	115.66
1	B	327	ALA	O-C-N	5.04	127.26	122.07
1	B	342	GLN	CB-CG-CD	-5.03	104.05	112.60

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	276	ASN	Sidechain
1	A	280	ASP	Mainchain
1	A	287	ALA	Mainchain
1	A	309	LEU	Mainchain
1	A	312	ASN	Sidechain
1	A	318	GLU	Sidechain
1	A	342	GLN	Sidechain
1	A	361	ASN	Sidechain
1	A	362	GLN	Sidechain
1	A	376	ASP	Sidechain
1	A	382	GLU	Sidechain
1	A	384	ASN	Mainchain
1	A	401	ASP	Mainchain
1	A	417	TRP	Mainchain
1	A	419	GLN	Sidechain
1	A	430	GLU	Sidechain
1	B	246	LYS	Mainchain
1	B	249	ASP	Sidechain
1	B	268	HIS	Mainchain
1	B	276	ASN	Sidechain
1	B	280	ASP	Sidechain
1	B	283	GLN	Sidechain
1	B	287	ALA	Mainchain
1	B	298	SER	Mainchain
1	B	315	ASP	Mainchain,Sidechain
1	B	325	ASN	Sidechain
1	B	342	GLN	Sidechain
1	B	376	ASP	Sidechain
1	B	382	GLU	Sidechain
1	B	388	GLU	Sidechain
1	B	389	ASN	Mainchain
1	B	399	ASP	Sidechain
1	B	401	ASP	Mainchain
1	B	413	ASP	Sidechain
1	B	418	GLN	Sidechain
1	B	438	GLN	Sidechain
1	B	443	LEU	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	A	1656	0	1629	56	4
1	B	1656	0	1629	37	1
2	C	110	0	94	5	0
2	D	110	0	94	1	0
All	All	3532	0	3446	92	4

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 15.

All (92) 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:B:274:LYS:HB3	1:B:324:SER:HB2	1.47	0.96
1:A:297:ASN:HB3	1:A:299:THR:HG22	1.61	0.81
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.64	0.77
1:A:250:THR:HG22	1:A:257:PRO:HB3	1.68	0.76
1:A:296:TYR:HD2	2:C:1:NAG:H62	1.52	0.75
1:A:432:LEU:HD13	1:A:437:THR:HG22	1.71	0.73
1:B:346:PRO:HD3	1:B:429:HIS:HD2	1.53	0.72
1:A:258:GLU:HG3	2:C:6:GAL:H62	1.71	0.71
1:A:418:GLN:HA	1:A:443:LEU:HD22	1.72	0.70
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.75	0.69
1:B:246:LYS:HG3	2:D:6:GAL:H5	1.75	0.69
1:A:296:TYR:CD2	2:C:1:NAG:H62	2.29	0.68
1:B:283:GLN:HG2	1:B:285:HIS:H	1.61	0.65
1:B:238:PRO:HA	1:B:265:ASP:HB2	1.79	0.65
1:B:350:THR:HG22	1:B:367:CYS:HB3	1.77	0.65
1:A:268:HIS:HA	1:A:300:TYR:HE2	1.62	0.65
1:B:278:TYR:HA	1:B:283:GLN:HA	1.79	0.65
1:A:268:HIS:HA	1:A:300:TYR:CE2	2.33	0.63
1:A:351:LEU:HB2	1:A:366:THR:HB	1.82	0.62
1:A:365:LEU:HB2	1:A:410:LEU:HB3	1.83	0.61
1:A:339:ALA:HB3	1:A:374:PRO:HB3	1.83	0.61
1:B:343:PRO:HB2	1:B:431:ALA:HB2	1.83	0.60
1:B:242:LEU:HB3	1:B:336:ILE:HD12	1.85	0.59
1:A:252:MET:HB2	1:A:255:ARG:HD2	1.85	0.58
1:A:369:VAL:HG11	1:A:377:ILE:HD11	1.85	0.58
1:A:259:VAL:HG23	1:A:308:VAL:HG21	1.84	0.58
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:C	1:A:285:HIS:H	2.10	0.58
1:A:283:GLN:HG2	1:A:285:HIS:H	1.70	0.56
1:A:395:PRO:HG2	1:B:395:PRO:HG2	1.89	0.55
1:A:297:ASN:CB	1:A:299:THR:HG22	2.34	0.55
1:A:345:GLU:HG3	1:A:432:LEU:HD23	1.89	0.55
1:B:379:VAL:HG21	1:B:406:LEU:HD11	1.89	0.54
1:A:246:LYS:HE2	2:C:6:GAL:C1	2.38	0.54
1:A:379:VAL:HG21	1:A:406:LEU:HD11	1.89	0.54
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.89	0.53
1:B:284:VAL:HB	1:B:287:ALA:HB2	1.90	0.53
1:A:248:LYS:HG3	1:A:428:MET:HE1	1.91	0.52
1:B:418:GLN:HA	1:B:443:LEU:HD22	1.92	0.52
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.39	0.52
1:A:260:THR:HG23	1:A:305:VAL:HG22	1.91	0.51
1:A:401:ASP:HB2	1:A:403:SER:H	1.75	0.51
1:A:350:THR:HB	1:A:441:LEU:HG	1.93	0.50
1:B:377:ILE:HG13	1:B:429:HIS:HB2	1.93	0.50
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.92	0.50
1:B:418:GLN:HA	1:B:443:LEU:CD2	2.42	0.50
1:A:384:ASN:C	1:A:386:GLN:H	2.21	0.49
1:A:278:TYR:HD1	1:A:320:LYS:HD2	1.77	0.49
1:A:278:TYR:CD1	1:A:320:LYS:HD2	2.48	0.48
1:A:245:PRO:HA	2:C:6:GAL:H61	1.95	0.48
1:A:346:PRO:HG2	1:A:432:LEU:HD11	1.96	0.48
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.95	0.48
1:B:365:LEU:CD1	1:B:410:LEU:HD23	2.43	0.48
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.49	0.48
1:B:361:ASN:ND2	1:B:362:GLN:HG3	2.28	0.48
1:B:245:PRO:HD3	1:B:259:VAL:HG22	1.96	0.48
1:A:280:ASP:HB2	1:A:317:LYS:HD2	1.96	0.48
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.96	0.47
1:B:343:PRO:HG3	1:B:430:GLU:OE2	2.15	0.47
1:A:274:LYS:HE2	1:A:324:SER:HB2	1.97	0.47
1:A:418:GLN:HA	1:A:443:LEU:CD2	2.41	0.47
1:A:289:THR:HA	1:A:305:VAL:O	2.15	0.46
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.83	0.46
1:A:421:ASN:N	1:A:421:ASN:HD22	2.15	0.45
1:A:390:ASN:HD22	1:A:390:ASN:C	2.24	0.45
1:A:312:ASN:HB3	1:A:317:LYS:HG3	1.98	0.45
1:B:261:CYS:HB2	1:B:277:TRP:HZ2	1.81	0.44
1:A:384:ASN:CG	1:A:385:GLY:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:SER:HB2	1:A:264:VAL:CG2	2.48	0.44
1:A:399:ASP:CG	1:A:400:SER:H	2.26	0.44
1:A:322:LYS:HD2	1:A:333:GLU:OE1	2.17	0.44
1:B:432:LEU:HD13	1:B:437:THR:HG22	2.00	0.43
1:A:279:VAL:C	1:A:281:GLY:H	2.27	0.43
1:A:291:PRO:HA	1:A:303:VAL:O	2.19	0.43
1:A:374:PRO:O	1:A:429:HIS:HE1	2.02	0.43
1:B:242:LEU:HD13	1:B:336:ILE:HG22	2.01	0.43
1:A:319:TYR:O	1:A:335:THR:HA	2.19	0.42
1:A:320:LYS:HD3	1:A:333:GLU:HB3	2.01	0.42
1:B:262:VAL:HG22	1:B:303:VAL:HG13	2.00	0.42
1:B:246:LYS:HA	1:B:247:PRO:HD3	1.89	0.42
1:A:283:GLN:C	1:A:285:HIS:N	2.78	0.42
1:B:252:MET:SD	1:B:255:ARG:HD2	2.60	0.42
1:A:356:GLU:O	1:A:359:THR:HB	2.19	0.41
1:A:243:PHE:HA	1:A:244:PRO:HD3	1.88	0.41
1:B:242:LEU:HD23	1:B:242:LEU:HA	1.92	0.41
1:B:346:PRO:HG2	1:B:432:LEU:HD11	2.01	0.41
1:A:253:ILE:H	1:A:253:ILE:HG13	1.58	0.41
1:B:291:PRO:HA	1:B:303:VAL:O	2.21	0.41
1:B:273:VAL:HA	1:B:324:SER:O	2.21	0.40
1:B:283:GLN:C	1:B:285:HIS:H	2.29	0.40
1:B:343:PRO:HA	1:B:373:TYR:O	2.21	0.40
1:A:320:LYS:HB2	1:A:335:THR:HG22	2.04	0.40

All (4) 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:A:389:ASN:OD1	1:B:389:ASN:ND2[4_566]	1.69	0.51
1:A:268:HIS:CG	1:A:285:HIS:NE2[2_674]	1.81	0.39
1:A:268:HIS:ND1	1:A:285:HIS:NE2[2_674]	2.01	0.19
1:A:268:HIS:CB	1:A:285:HIS:NE2[2_674]	2.16	0.04

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	B	58/224 (26%)	54 (93%)	4 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	193/207 (93%)	189 (98%)	4 (2%)	47	77
1	B	193/207 (93%)	185 (96%)	8 (4%)	27	61
All	All	386/414 (93%)	374 (97%)	12 (3%)	35	69

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	VAL
1	A	390	ASN
1	A	425	CYS
1	A	434	ASN
1	B	284	VAL
1	B	299	THR
1	B	359	THR
1	B	390	ASN
1	B	394	THR
1	B	409	LYS
1	B	434	ASN
1	B	439	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	347	GLN
1	A	361	ASN
1	A	390	ASN
1	A	418	GLN
1	A	419	GLN
1	A	421	ASN
1	A	429	HIS
1	A	438	GLN
1	B	283	GLN
1	B	342	GLN
1	B	347	GLN
1	B	361	ASN
1	B	390	ASN
1	B	418	GLN
1	B	419	GLN
1	B	429	HIS
1	B	438	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 ⓘ

18 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	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.72	0	17,19,21	1.77	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	2	2	14,14,15	1.02	0	17,19,21	1.58	2 (11%)
2	MAN	C	3	2	11,11,12	0.50	0	15,15,17	1.44	2 (13%)
2	MAN	C	4	2	11,11,12	0.55	0	15,15,17	1.23	1 (6%)
2	NAG	C	5	2	14,14,15	0.96	0	17,19,21	1.68	1 (5%)
2	GAL	C	6	2	11,11,12	0.54	0	15,15,17	1.47	1 (6%)
2	MAN	C	7	2	11,11,12	0.75	0	15,15,17	1.48	1 (6%)
2	NAG	C	8	2	14,14,15	0.81	0	17,19,21	1.84	1 (5%)
2	FUC	C	9	2	10,10,11	0.77	0	14,14,16	1.14	1 (7%)
2	NAG	D	1	2,1	14,14,15	0.78	0	17,19,21	1.53	2 (11%)
2	NAG	D	2	2	14,14,15	0.95	1 (7%)	17,19,21	1.37	1 (5%)
2	MAN	D	3	2	11,11,12	0.58	0	15,15,17	1.77	2 (13%)
2	MAN	D	4	2	11,11,12	0.61	0	15,15,17	1.52	1 (6%)
2	NAG	D	5	2	14,14,15	0.84	0	17,19,21	1.70	1 (5%)
2	GAL	D	6	2	11,11,12	0.59	0	15,15,17	1.24	1 (6%)
2	MAN	D	7	2	11,11,12	0.81	1 (9%)	15,15,17	1.55	1 (6%)
2	NAG	D	8	2	14,14,15	0.97	1 (7%)	17,19,21	1.67	1 (5%)
2	FUC	D	9	2	10,10,11	0.73	0	14,14,16	1.11	1 (7%)

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	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	MAN	C	3	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	0/6/23/26	0/1/1/1
2	GAL	C	6	2	-	1/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	NAG	C	8	2	-	0/6/23/26	0/1/1/1
2	FUC	C	9	2	2/2/4/5	-	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	MAN	D	3	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	NAG	D	5	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	D	6	2	-	1/2/19/22	0/1/1/1
2	MAN	D	7	2	-	0/2/19/22	0/1/1/1
2	NAG	D	8	2	-	0/6/23/26	0/1/1/1
2	FUC	D	9	2	2/2/4/5	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	NAG	C1-C2	2.60	1.55	1.52
2	D	7	MAN	C2-C3	2.17	1.55	1.52
2	D	2	NAG	C1-C2	2.12	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	NAG	C1-O5-C5	7.21	121.84	112.19
2	D	8	NAG	C1-O5-C5	5.98	120.20	112.19
2	D	5	NAG	C1-O5-C5	5.76	119.91	112.19
2	D	3	MAN	C1-O5-C5	5.73	119.86	112.19
2	C	5	NAG	C1-O5-C5	5.48	119.54	112.19
2	D	1	NAG	C1-O5-C5	5.41	119.43	112.19
2	C	7	MAN	C1-O5-C5	5.31	119.31	112.19
2	C	1	NAG	C1-O5-C5	5.22	119.18	112.19
2	D	7	MAN	C1-O5-C5	5.20	119.16	112.19
2	D	4	MAN	C1-O5-C5	5.11	119.03	112.19
2	C	2	NAG	C1-O5-C5	4.72	118.51	112.19
2	D	2	NAG	C1-O5-C5	4.16	117.76	112.19
2	C	6	GAL	C1-O5-C5	3.98	117.53	112.19
2	C	3	MAN	C1-O5-C5	3.98	117.51	112.19
2	D	6	GAL	C1-O5-C5	3.97	117.50	112.19
2	C	4	MAN	C1-O5-C5	3.85	117.34	112.19
2	C	9	FUC	C1-O5-C5	3.29	120.72	112.97
2	C	1	NAG	O5-C1-C2	-3.22	106.31	111.29
2	D	9	FUC	C1-O5-C5	3.16	120.42	112.97
2	C	2	NAG	C2-N2-C7	2.47	126.21	122.90
2	D	1	NAG	O5-C1-C2	-2.29	107.75	111.29
2	C	3	MAN	O3-C3-C4	-2.28	105.00	110.38
2	D	3	MAN	O3-C3-C4	-2.25	105.08	110.38
2	C	1	NAG	C4-C3-C2	-2.04	108.02	111.02

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	MAN	C1
2	C	9	FUC	C5
2	C	9	FUC	C1
2	D	3	MAN	C1
2	D	9	FUC	C5
2	D	9	FUC	C1

All (11) torsion outliers are listed below:

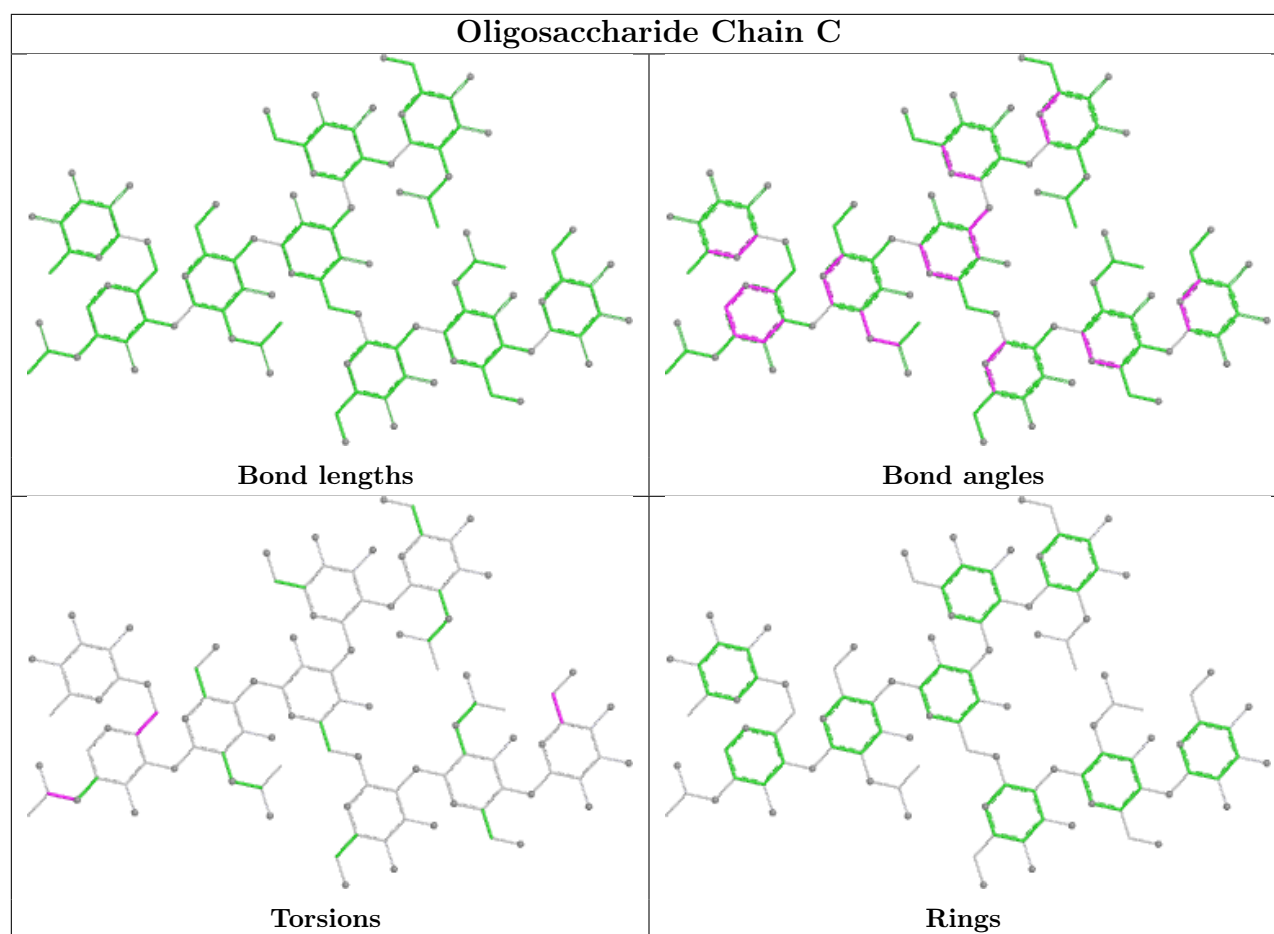
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	6	GAL	O5-C5-C6-O6
2	C	6	GAL	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

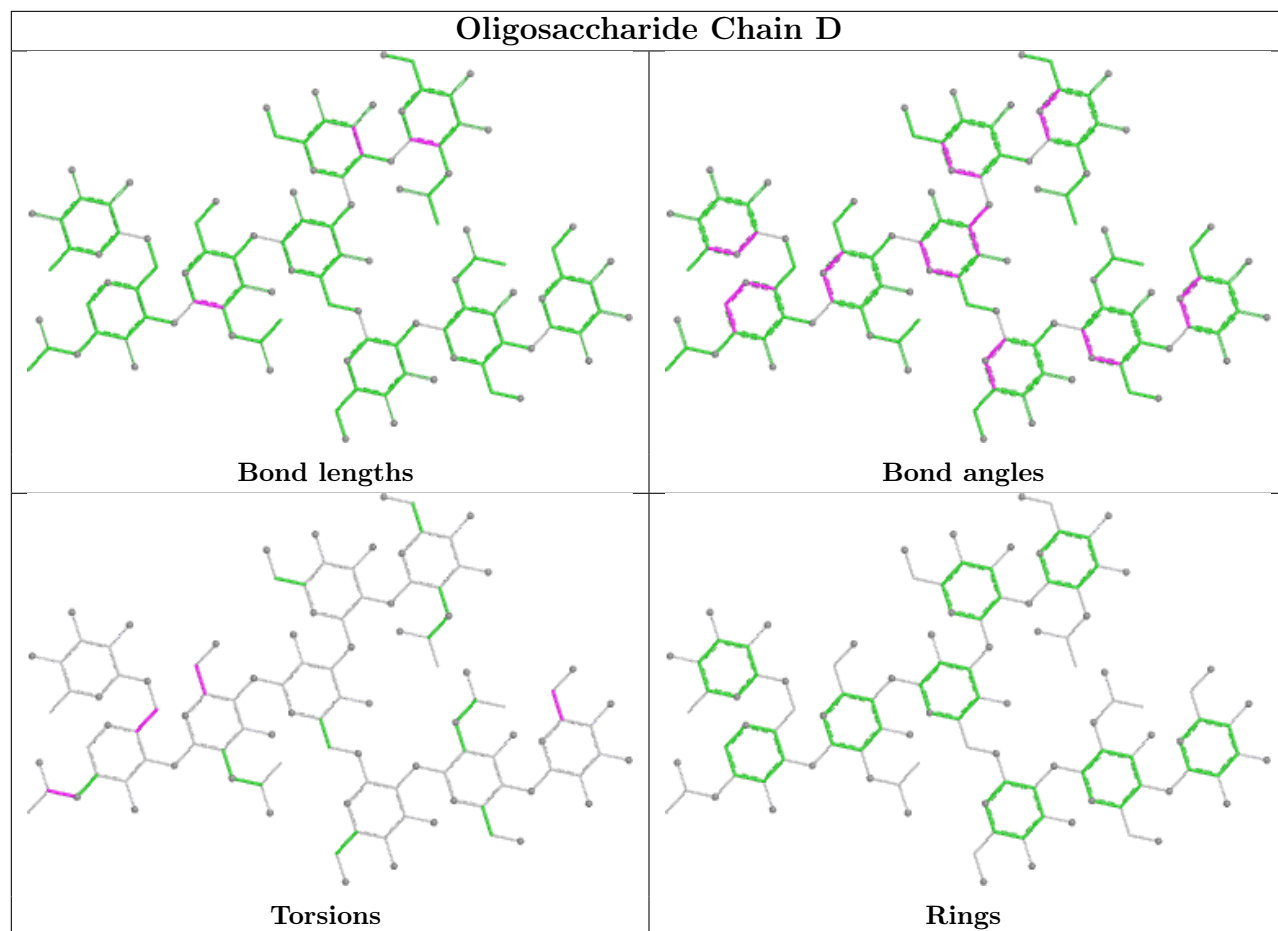
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	GAL	1	0
2	C	1	NAG	2	0
2	C	6	GAL	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](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.