Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 05:05 PM EDT

PDB ID	:	2FUQ
Title	:	Crystal Structure of Heparinase II
Authors	:	Shaya, D.; Cygler, M.
Deposited on	:	2006-01-27
Resolution	:	2.15 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

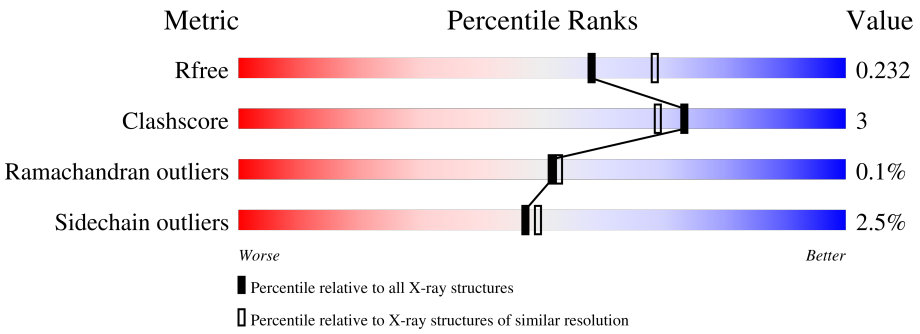
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	747	91% 8% •
1	B	747	89% 10% •
2	C	4	25% 75%
2	D	4	25% 75%

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	XYS	D	3	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12987 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.

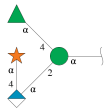
- Molecule 1 is a protein called heparinase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	747	5978	3850	1008	1097	23	0	0	0
1	B	747	5978	3850	1008	1097	23	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	PCA	-	modified residue	GB 924923
A	758	ALA	PRO	engineered mutation	GB 924923
B	26	PCA	-	modified residue	GB 924923
B	758	ALA	PRO	engineered mutation	GB 924923

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	4	41	23	18	0	0	0
2	D	4	41	23	18	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

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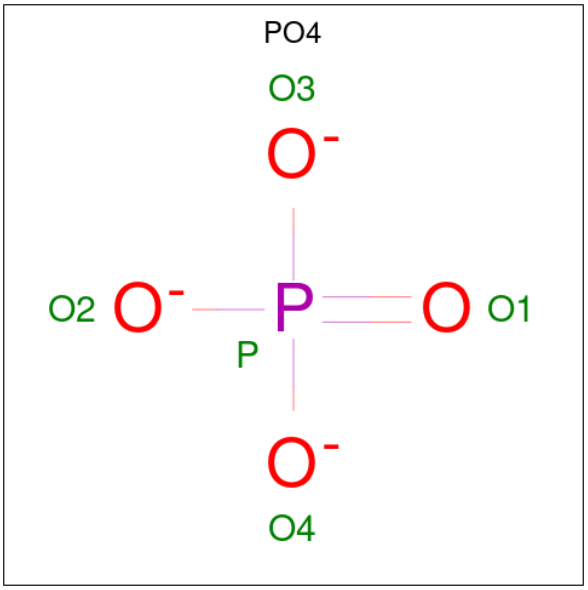
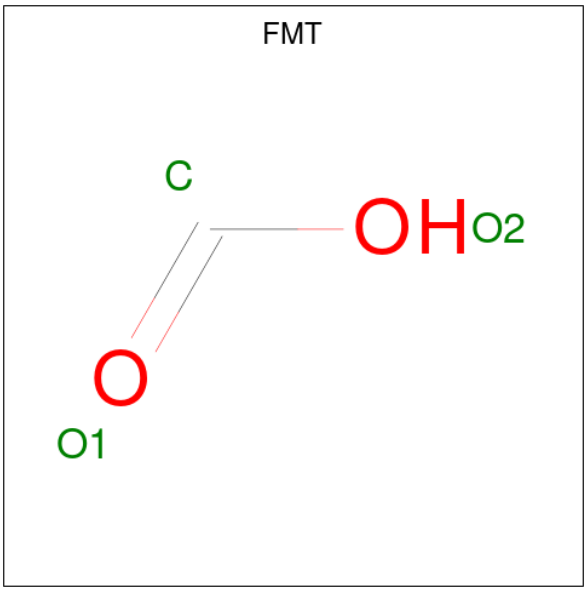
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	5	4	1	0	0
			Total	O	P		
4	B	1	5	4	1	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	3	1	2	0	0
			Total	C	O		
5	A	1	3	1	2	0	0
			Total	C	O		
5	B	1	3	1	2	0	0

- Molecule 6 is water.

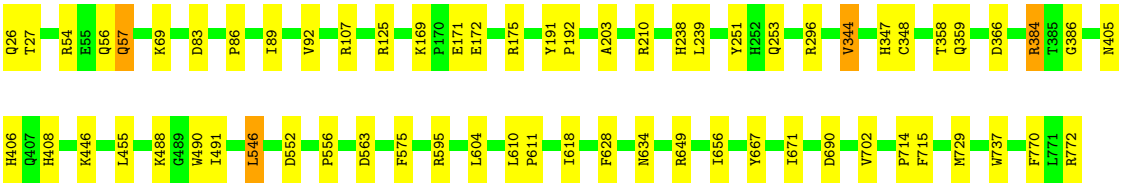
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	461	461	461	0	0
			Total	O		
6	B	467	467	467	0	0

3 Residue-property plots (i)

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.

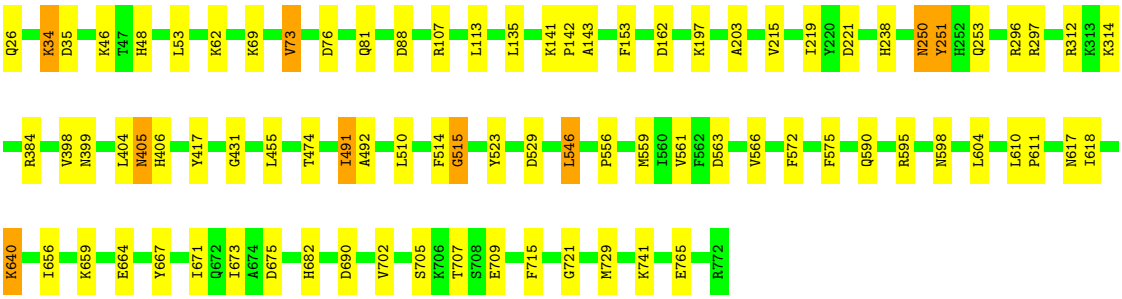
• Molecule 1: heparinase II protein

Chain A:



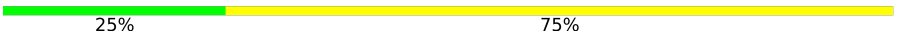
• Molecule 1: heparinase II protein

Chain B:



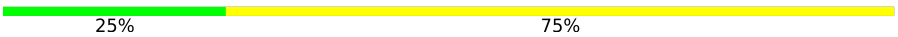
• Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-mannopyranose

Chain C:



• Molecule 2: alpha-D-xylopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-2)-[alpha-L-rhamnopyranose-(1-4)]alpha-D-mannopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.05Å 119.34Å 200.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.60 – 2.15 46.25 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (102.60-2.15) 97.3 (46.25-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.53 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.235 0.194 , 0.232	Depositor DCC
R_{free} test set	6824 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	1.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6404e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ZN, MAN, RAM, PCA, XYS, GCU, FMT, PO4

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	0.58	7/6133 (0.1%)	0.57	3/8303 (0.0%)
1	B	0.44	1/6133 (0.0%)	0.55	0/8303
All	All	0.51	8/12266 (0.1%)	0.56	3/16606 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	ARG	CZ-NH1	21.95	1.61	1.33
1	A	172	GLU	CD-OE2	13.82	1.40	1.25
1	A	175	ARG	CZ-NH1	8.96	1.44	1.33
1	A	125	ARG	NE-CZ	6.90	1.42	1.33
1	B	572	PHE	CG-CD2	5.92	1.47	1.38
1	A	175	ARG	CZ-NH2	5.61	1.40	1.33
1	A	169	LYS	CE-NZ	5.03	1.61	1.49
1	A	172	GLU	CD-OE1	5.01	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	125	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	384	ARG	NE-CZ-NH2	-5.66	117.47	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	5978	0	5889	29	0
1	B	5978	0	5889	50	0
2	C	41	0	30	0	0
2	D	41	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	6	0	3	0	0
5	B	3	0	1	0	0
6	A	461	0	0	0	0
6	B	467	0	0	4	0
All	All	12987	0	11842	79	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 3.

All (79) 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:640:LYS:H	1:B:640:LYS:HE3	0.96	1.08
1:B:640:LYS:HE3	1:B:640:LYS:N	1.81	0.95
1:B:640:LYS:H	1:B:640:LYS:CE	1.87	0.83
1:B:62:LYS:HD2	1:B:62:LYS:H	1.44	0.80
1:B:250:ASN:HD22	1:B:251:TYR:H	1.32	0.77
1:A:628:PHE:H	1:A:634:ASN:HD21	1.31	0.77
1:B:707:THR:HG23	1:B:709:GLU:H	1.52	0.74
1:B:431:GLY:HA2	1:B:640:LYS:HE2	1.71	0.72
1:B:491:ILE:HD13	1:B:492:ALA:H	1.54	0.71
1:A:253:GLN:HE22	1:A:406:HIS:H	1.38	0.70
1:B:253:GLN:HE22	1:B:406:HIS:H	1.40	0.70
1:A:210:ARG:HH12	1:A:347:HIS:CD2	2.11	0.69
1:B:515:GLY:HA2	1:B:523:TYR:CE2	2.30	0.67
1:B:253:GLN:HE22	1:B:405:ASN:HB3	1.60	0.67
1:B:62:LYS:HD2	1:B:62:LYS:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ARG:HH12	1:B:598:ASN:HD22	1.47	0.63
1:B:297:ARG:HD3	1:B:417:TYR:CE1	2.36	0.61
1:B:455:LEU:HB2	1:B:575:PHE:HB2	1.82	0.61
1:A:210:ARG:HH12	1:A:347:HIS:HD2	1.49	0.61
1:A:296:ARG:O	1:A:384:ARG:NH2	2.31	0.60
1:B:566:VAL:HG22	1:B:664:GLU:HG3	1.83	0.60
1:B:546:LEU:HD22	1:B:702:VAL:HG21	1.87	0.57
1:A:83:ASP:OD1	1:A:107:ARG:NH2	2.38	0.56
1:A:54:ARG:H	1:A:57:GLN:HE21	1.52	0.56
1:B:48:HIS:HD2	1:B:162:ASP:OD1	1.89	0.56
1:A:455:LEU:HB2	1:A:575:PHE:HB2	1.88	0.55
1:B:69:LYS:HE3	1:B:69:LYS:H	1.73	0.54
1:B:143:ALA:HB1	6:B:1403:HOH:O	2.06	0.54
1:B:296:ARG:O	1:B:384:ARG:NH2	2.40	0.54
1:B:682:HIS:HE1	6:B:994:HOH:O	1.91	0.53
1:B:203:ALA:O	1:B:238:HIS:HE1	1.92	0.53
1:B:690:ASP:O	1:B:715:PHE:HB2	2.10	0.52
1:A:344:VAL:HG13	1:A:348:CYS:HB2	1.93	0.51
1:B:515:GLY:HA2	1:B:523:TYR:CD2	2.46	0.51
1:A:610:LEU:HA	1:A:611:PRO:C	2.33	0.50
1:A:203:ALA:O	1:A:238:HIS:HE1	1.95	0.50
1:B:197:LYS:HE3	1:B:491:ILE:HD12	1.94	0.50
1:B:398:VAL:O	1:B:399:ASN:HB2	2.13	0.49
1:A:618:ILE:HG12	1:A:656:ILE:HG12	1.94	0.49
1:A:253:GLN:HE22	1:A:405:ASN:HB3	1.77	0.49
1:B:610:LEU:HA	1:B:611:PRO:C	2.34	0.48
1:B:604:LEU:HG	1:B:671:ILE:HG23	1.94	0.48
1:A:690:ASP:O	1:A:715:PHE:HB2	2.14	0.47
1:A:27:THR:HG21	1:A:56:GLN:NE2	2.29	0.47
1:A:54:ARG:H	1:A:57:GLN:NE2	2.12	0.47
1:B:81:GLN:HE21	1:B:107:ARG:HA	1.80	0.47
1:B:510:LEU:HD11	1:B:529:ASP:HB2	1.96	0.46
1:B:253:GLN:NE2	1:B:406:HIS:H	2.10	0.46
1:B:81:GLN:NE2	6:B:1299:HOH:O	2.50	0.45
1:B:618:ILE:HG12	1:B:656:ILE:HG12	1.98	0.45
1:B:491:ILE:HD13	1:B:492:ALA:N	2.26	0.44
1:B:617:ASN:ND2	1:B:659:LYS:HG2	2.32	0.44
1:B:556:PRO:HD2	1:B:673:ILE:O	2.18	0.44
1:B:559:MET:CE	1:B:561:VAL:CG2	2.96	0.44
1:A:563:ASP:HB2	1:A:667:TYR:HB2	1.99	0.44
1:A:191:TYR:HA	1:A:192:PRO:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:PRO:HA	1:A:770:PHE:O	2.18	0.44
1:B:312:ARG:HD3	6:B:1187:HOH:O	2.18	0.44
1:B:721:GLY:O	1:B:765:GLU:HB3	2.17	0.43
1:A:69:LYS:HD2	1:A:358:THR:HB	2.00	0.43
1:A:604:LEU:HG	1:A:671:ILE:HG23	2.00	0.43
1:A:737:TRP:CE2	1:A:772:ARG:HD3	2.53	0.43
1:A:552:ASP:O	1:A:556:PRO:HA	2.18	0.43
1:A:488:LYS:O	1:A:491:ILE:HD12	2.18	0.43
1:A:628:PHE:H	1:A:634:ASN:ND2	2.07	0.43
1:A:546:LEU:HD22	1:A:702:VAL:HG21	1.99	0.42
1:B:135:LEU:HA	1:B:153:PHE:CE2	2.53	0.42
1:B:705:SER:OG	1:B:707:THR:HG22	2.19	0.42
1:A:384:ARG:HD3	1:A:386:GLY:O	2.19	0.42
1:B:563:ASP:HB2	1:B:667:TYR:HB2	2.02	0.42
1:B:48:HIS:HE1	1:B:221:ASP:OD1	2.03	0.42
1:A:408:HIS:CD2	1:A:446:LYS:HG2	2.55	0.41
1:A:86:PRO:HA	1:A:89:ILE:HD12	2.03	0.41
1:B:141:LYS:HA	1:B:142:PRO:HD3	1.92	0.41
1:B:431:GLY:CA	1:B:640:LYS:HE2	2.45	0.41
1:B:73:VAL:O	1:B:76:ASP:HB2	2.20	0.40
1:B:215:VAL:O	1:B:219:ILE:HG12	2.21	0.40
1:B:514:PHE:O	1:B:515:GLY:O	2.39	0.40
1:B:34:LYS:HD2	1:B:35:ASP:N	2.37	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	745/747 (100%)	711 (95%)	34 (5%)	0	100 100
1	B	745/747 (100%)	713 (96%)	30 (4%)	2 (0%)	41 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1490/1494 (100%)	1424 (96%)	64 (4%)	2 (0%)	51 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	515	GLY
1	B	474	THR

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	A	632/632 (100%)	619 (98%)	13 (2%)	53 57
1	B	632/632 (100%)	614 (97%)	18 (3%)	43 44
All	All	1264/1264 (100%)	1233 (98%)	31 (2%)	47 49

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	92	VAL
1	A	171	GLU
1	A	239	LEU
1	A	251	TYR
1	A	344	VAL
1	A	359	GLN
1	A	366	ASP
1	A	490	TRP
1	A	546	LEU
1	A	595	ARG
1	A	649	ARG
1	A	729	MET
1	B	34	LYS
1	B	46	LYS
1	B	53	LEU

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Mol	Chain	Res	Type
1	B	73	VAL
1	B	88	ASP
1	B	113	LEU
1	B	250	ASN
1	B	251	TYR
1	B	314	LYS
1	B	404	LEU
1	B	405	ASN
1	B	491	ILE
1	B	546	LEU
1	B	590	GLN
1	B	640	LYS
1	B	675	ASP
1	B	729	MET
1	B	741	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	56	GLN
1	A	57	GLN
1	A	81	GLN
1	A	167	GLN
1	A	238	HIS
1	A	252	HIS
1	A	253	GLN
1	A	347	HIS
1	A	634	ASN
1	A	738	GLN
1	B	48	HIS
1	B	66	ASN
1	B	81	GLN
1	B	167	GLN
1	B	238	HIS
1	B	250	ASN
1	B	253	GLN
1	B	590	GLN
1	B	598	ASN
1	B	682	HIS
1	B	738	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	A	26	1	7,8,9	1.83	1 (14%)	9,10,12	2.15	5 (55%)
1	PCA	B	26	1	7,8,9	1.79	1 (14%)	9,10,12	2.12	5 (55%)

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
1	PCA	A	26	1	-	0/0/11/13	0/1/1/1
1	PCA	B	26	1	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	PCA	CD-N	4.64	1.46	1.34
1	B	26	PCA	CD-N	4.56	1.46	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	PCA	CA-N-CD	-2.98	103.37	113.58
1	B	26	PCA	CA-N-CD	-2.94	103.52	113.58
1	A	26	PCA	CB-CA-C	-2.91	108.70	112.70
1	A	26	PCA	OE-CD-CG	-2.87	121.76	126.76
1	B	26	PCA	OE-CD-CG	-2.81	121.85	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	26	PCA	CB-CA-N	2.80	111.34	103.30
1	A	26	PCA	CB-CA-N	2.61	110.80	103.30
1	B	26	PCA	CB-CA-C	-2.61	109.12	112.70
1	B	26	PCA	CG-CD-N	2.32	114.40	108.39
1	A	26	PCA	CG-CD-N	2.25	114.21	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
2	MAN	C	1	2,1	11,11,12	1.84	2 (18%)	15,15,17	2.47	2 (13%)
2	GCU	C	2	2	9,12,13	1.48	1 (11%)	12,17,19	2.50	3 (25%)
2	XYS	C	3	2	8,8,10	1.26	1 (12%)	8,10,14	1.51	1 (12%)
2	RAM	C	4	2	10,10,11	0.65	0	14,14,16	0.95	0
2	MAN	D	1	2,1	11,11,12	1.82	2 (18%)	15,15,17	2.71	4 (26%)
2	GCU	D	2	2	9,12,13	1.50	1 (11%)	12,17,19	2.15	1 (8%)
2	XYS	D	3	2	8,8,10	1.46	1 (12%)	8,10,14	1.58	1 (12%)
2	RAM	D	4	2	10,10,11	0.57	0	14,14,16	0.72	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	MAN	C	1	2,1	-	0/2/19/22	0/1/1/1
2	GCU	C	2	2	-	0/0/21/24	0/1/1/1
2	XYS	C	3	2	-	-	0/1/1/1
2	RAM	C	4	2	-	-	0/1/1/1
2	MAN	D	1	2,1	-	0/2/19/22	0/1/1/1
2	GCU	D	2	2	-	0/0/21/24	0/1/1/1
2	XYS	D	3	2	1/1/2/4	-	0/1/1/1
2	RAM	D	4	2	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	MAN	O2-C2	-4.24	1.34	1.43
2	D	1	MAN	O2-C2	-4.15	1.34	1.43
2	D	1	MAN	O4-C4	-4.08	1.33	1.43
2	D	2	GCU	O4-C4	-4.06	1.33	1.43
2	C	1	MAN	O4-C4	-4.02	1.33	1.43
2	C	2	GCU	O4-C4	-3.93	1.33	1.43
2	D	3	XYS	O5-C1	-3.58	1.36	1.42
2	C	3	XYS	O5-C1	-3.03	1.37	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	MAN	O2-C2-C3	8.14	126.44	110.14
2	C	1	MAN	O2-C2-C3	7.69	125.54	110.14
2	D	2	GCU	O4-C4-C5	7.04	123.51	110.05
2	C	2	GCU	O4-C4-C5	6.79	123.03	110.05
2	C	2	GCU	O4-C4-C3	4.48	120.70	110.35
2	C	1	MAN	O4-C4-C5	4.46	120.37	109.30
2	D	1	MAN	O4-C4-C3	-4.29	100.43	110.35
2	C	3	XYS	C5-O5-C1	4.20	115.79	109.97
2	D	3	XYS	C4-C3-C2	3.64	114.03	111.12
2	D	1	MAN	O2-C2-C1	-3.53	101.92	109.15
2	D	1	MAN	C1-O5-C5	3.01	116.27	112.19
2	C	2	GCU	C1-C2-C3	2.36	112.57	109.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	3	XYS	C1

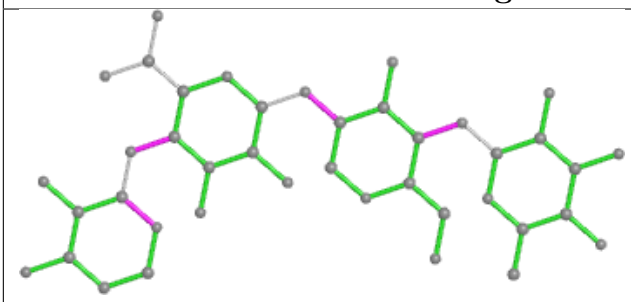
There are no torsion outliers.

There are no ring outliers.

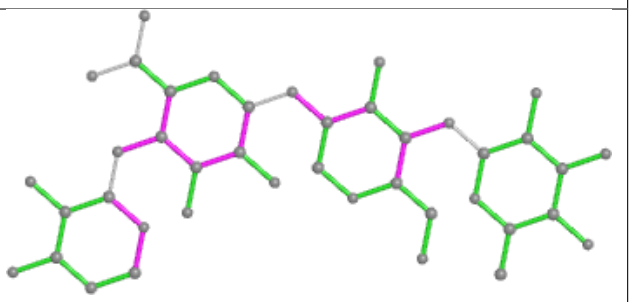
No monomer is involved in short contacts.

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

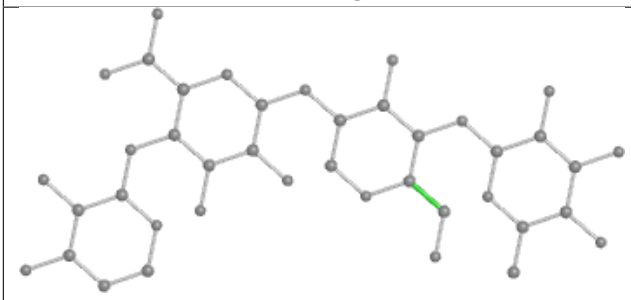
Oligosaccharide Chain C



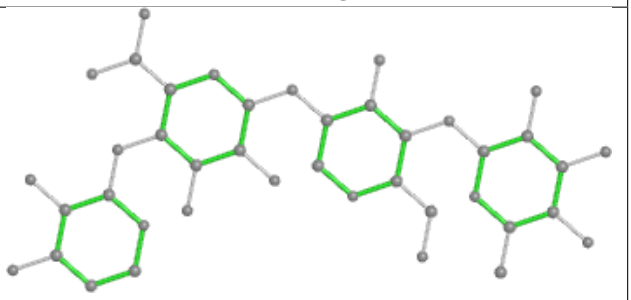
Bond lengths



Bond angles

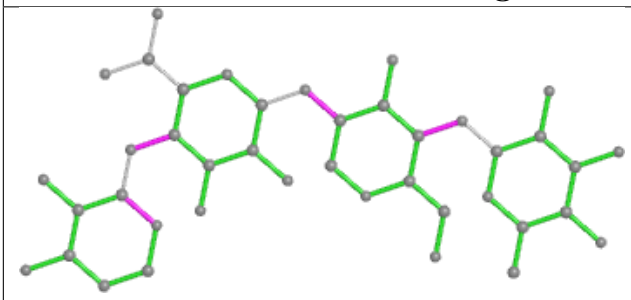


Torsions

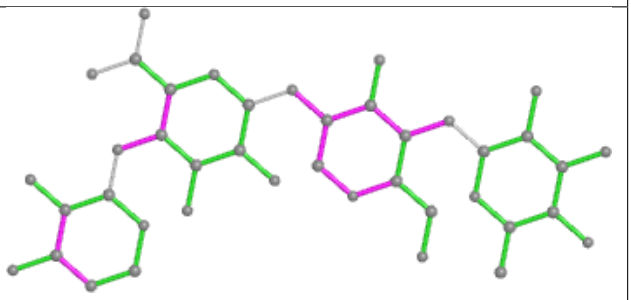


Rings

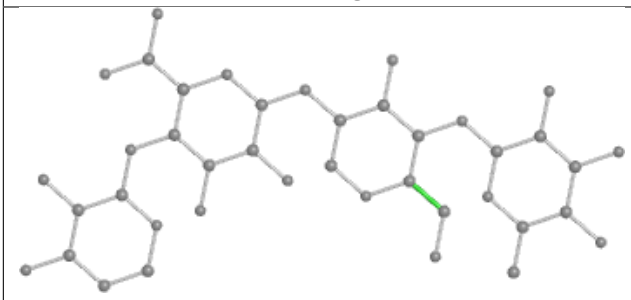
Oligosaccharide Chain D



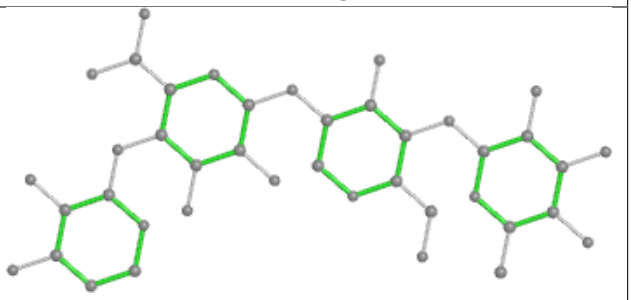
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FMT	A	941	-	0,2,2	-	-	0,1,1	-	-
4	PO4	B	945	-	4,4,4	0.88	0	6,6,6	0.58	0
4	PO4	A	944	-	4,4,4	0.96	0	6,6,6	0.46	0
5	FMT	B	942	-	0,2,2	-	-	0,1,1	-	-
5	FMT	A	943	-	0,2,2	-	-	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

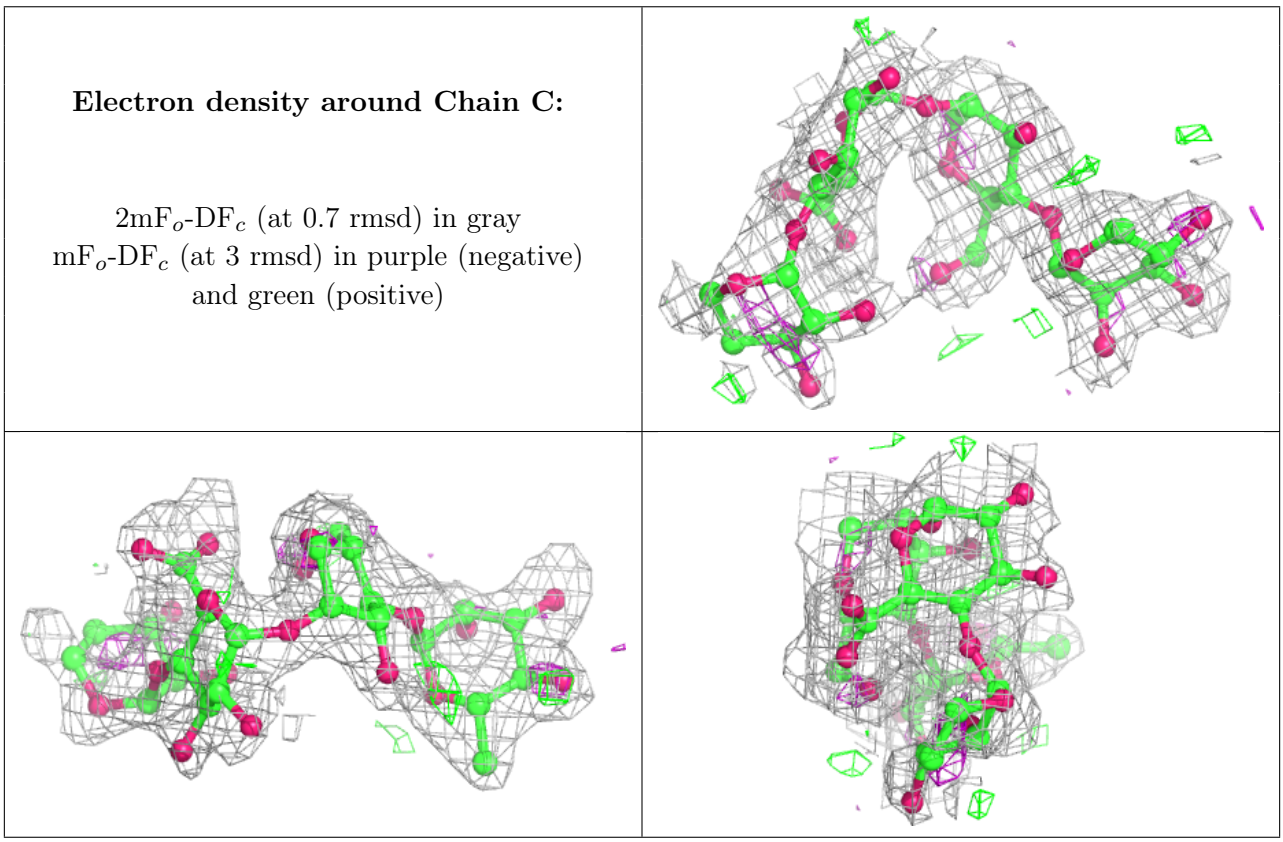
6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

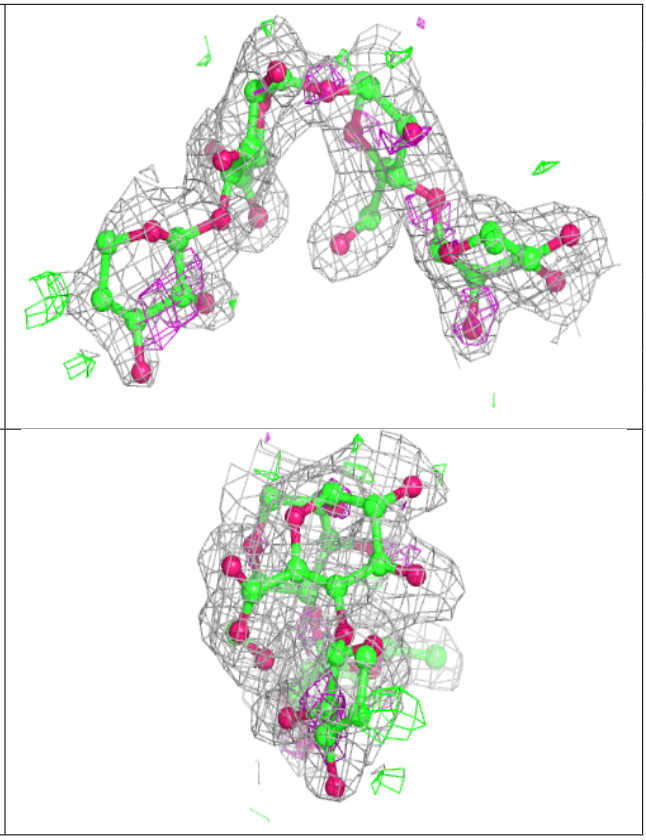
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.