Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 09:56 pm GMT

PDB ID	:	1H4H
Title	:	Oligosaccharide-binding to family 11 xylanases: both covalent intermediate and mutant-product complexes display 2,5B conformations at the active-centre
Authors	:	Sabini, E.; Wilson, K.S.; Danielsen, S.; Schulein, M.; Davies, G.J.
Deposited on	:	2001-05-11
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

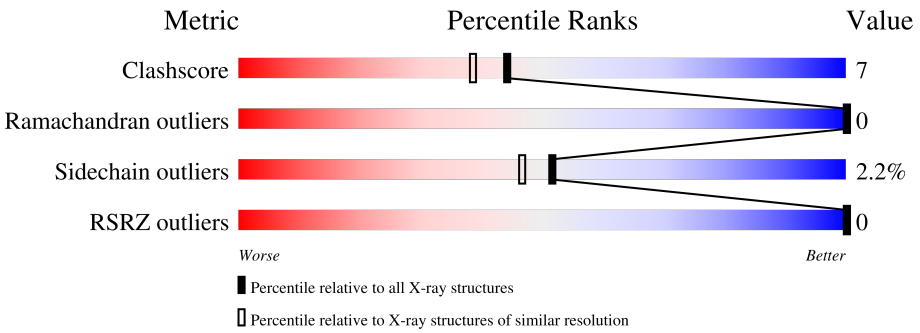
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	209	78% 19% • •
1	B	209	78% 18% •
1	C	209	79% 17% • •
1	D	209	78% 18% •
2	E	3	67% 33%
2	F	3	100%

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Mol	Chain	Length	Quality of chain
2	G	3	100%
2	H	3	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7172 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.

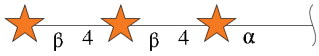
- Molecule 1 is a protein called XYLANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	1640	1032	289	313	6	0	2	0
1	B	209	1652	1040	290	316	6	0	1	0
1	C	207	1636	1030	288	312	6	0	1	0
1	D	208	1643	1034	289	314	6	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLU	modified residue	PDB 1H4H
B	1	PCA	GLU	modified residue	PDB 1H4H
C	1	PCA	GLU	modified residue	PDB 1H4H
D	1	PCA	GLU	modified residue	PDB 1H4H
A	94	ALA	GLU	engineered mutation	PDB 1H4H
B	94	ALA	GLU	engineered mutation	PDB 1H4H
C	94	ALA	GLU	engineered mutation	PDB 1H4H
D	94	ALA	GLU	engineered mutation	PDB 1H4H

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	3	28	15	13	0	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	F	3	28	15	13	0	0	0
2	G	3	28	15	13	0	0	0
2	H	3	28	15	13	0	0	0

- Molecule 3 is water.

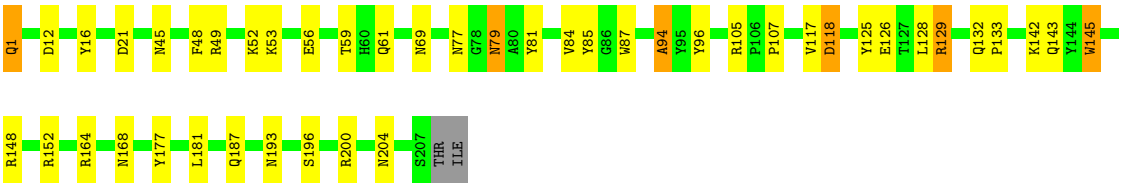
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	131	131	131	0	0
3	B	142	142	142	0	0
3	C	106	106	106	0	0
3	D	110	110	110	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

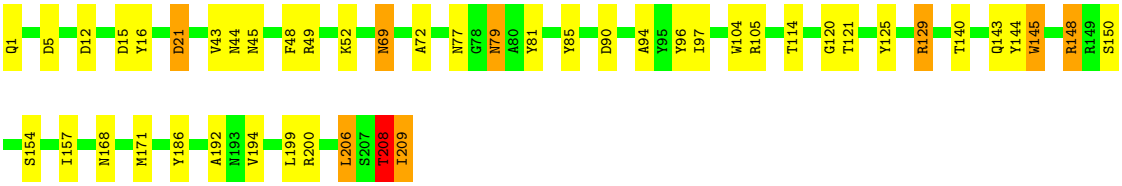
• Molecule 1: XYLANASE

Chain A:



• Molecule 1: XYLANASE

Chain B:

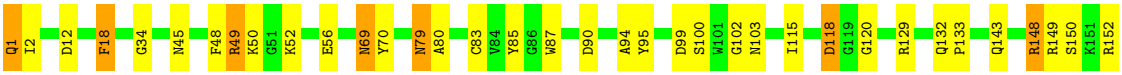


• Molecule 1: XYLANASE

Chain C:

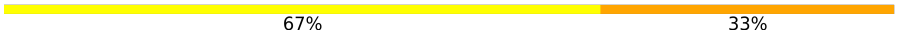
• Molecule 1: XYLANASE

Chain D:



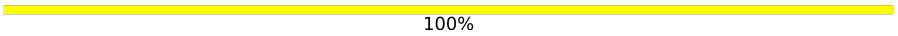
- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose

Chain E:



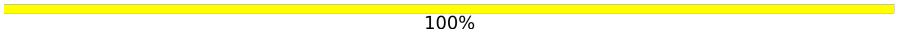
- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose

Chain F:



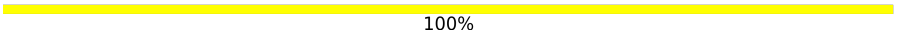
- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose

Chain G:



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-alpha-D-xylopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.34Å 78.89Å 76.27Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 11.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	77.5 (20.00-1.90) 77.5 (11.96-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.241 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.179 for h,-k,-l 0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7172	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PCA, XYP, XYS

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	0.99	3/1687 (0.2%)	1.96	37/2294 (1.6%)
1	B	1.43	4/1694 (0.2%)	1.95	35/2303 (1.5%)
1	C	0.97	2/1678 (0.1%)	1.78	32/2282 (1.4%)
1	D	0.96	3/1685 (0.2%)	1.72	26/2292 (1.1%)
All	All	1.11	12/6744 (0.2%)	1.86	130/9171 (1.4%)

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	1
1	B	0	2
1	D	0	2
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148[A]	ARG	NE-CZ	30.61	1.72	1.33
1	B	148[B]	ARG	NE-CZ	30.61	1.72	1.33
1	A	87	TRP	NE1-CE2	8.76	1.49	1.37
1	D	87	TRP	NE1-CE2	8.73	1.49	1.37
1	C	87	TRP	NE1-CE2	8.71	1.48	1.37
1	B	145	TRP	NE1-CE2	8.69	1.48	1.37
1	A	145	TRP	NE1-CE2	8.66	1.48	1.37
1	C	145	TRP	NE1-CE2	6.73	1.46	1.37
1	B	43	VAL	C-N	-5.98	1.20	1.34
1	A	16	TYR	CB-CG	5.35	1.59	1.51
1	D	158	SER	CA-CB	5.12	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	GLY	C-O	5.03	1.31	1.23

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148[A]	ARG	CD-NE-CZ	20.96	152.95	123.60
1	A	148[B]	ARG	CD-NE-CZ	20.96	152.95	123.60
1	A	148[A]	ARG	NE-CZ-NH1	20.02	130.31	120.30
1	A	148[B]	ARG	NE-CZ-NH1	20.02	130.31	120.30
1	B	148[A]	ARG	NE-CZ-NH2	-19.79	110.41	120.30
1	B	148[B]	ARG	NE-CZ-NH2	-19.79	110.41	120.30
1	B	148[A]	ARG	NE-CZ-NH1	18.53	129.57	120.30
1	B	148[B]	ARG	NE-CZ-NH1	18.53	129.57	120.30
1	A	148[A]	ARG	NE-CZ-NH2	-13.59	113.50	120.30
1	A	148[B]	ARG	NE-CZ-NH2	-13.59	113.50	120.30
1	C	200	ARG	NE-CZ-NH1	13.43	127.01	120.30
1	B	49	ARG	CG-CD-NE	13.26	139.64	111.80
1	B	148[A]	ARG	CD-NE-CZ	13.20	142.08	123.60
1	B	148[B]	ARG	CD-NE-CZ	13.20	142.08	123.60
1	B	96	TYR	CB-CG-CD2	-13.06	113.17	121.00
1	D	118	ASP	CB-CG-OD1	13.05	130.04	118.30
1	A	96	TYR	CB-CG-CD2	-12.85	113.29	121.00
1	B	96	TYR	CB-CG-CD1	12.32	128.39	121.00
1	D	1	PCA	O-C-N	-11.35	104.54	122.70
1	A	96	TYR	CB-CG-CD1	11.11	127.67	121.00
1	A	118	ASP	CB-CG-OD2	11.11	128.30	118.30
1	C	149	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	177	TYR	CB-CG-CD2	10.28	127.17	121.00
1	B	49	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	A	56	GLU	OE1-CD-OE2	-10.17	111.09	123.30
1	B	105	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	C	16	TYR	CB-CG-CD1	-10.00	115.00	121.00
1	B	49	ARG	CD-NE-CZ	9.79	137.31	123.60
1	A	164	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	A	177	TYR	CB-CG-CD1	-9.49	115.31	121.00
1	C	21	ASP	CB-CG-OD1	9.27	126.64	118.30
1	B	16	TYR	CB-CG-CD1	-9.19	115.49	121.00
1	A	164	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	C	184	GLU	OE1-CD-OE2	-9.06	112.42	123.30
1	A	1	PCA	O-C-N	-8.91	108.44	122.70
1	B	69	ASN	O-C-N	-8.88	108.50	122.70
1	B	16	TYR	CB-CG-CD2	8.65	126.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	85	TYR	CB-CG-CD2	8.62	126.17	121.00
1	C	96	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	D	149	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	C	101	TRP	CG-CD2-CE3	-8.44	126.30	133.90
1	C	1	PCA	O-C-N	-8.35	109.34	122.70
1	B	200	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	69	ASN	O-C-N	-8.09	109.75	122.70
1	D	177	TYR	CB-CG-CD2	-8.01	116.19	121.00
1	C	81	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	D	69	ASN	O-C-N	-7.92	110.02	122.70
1	C	164	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	C	69	ASN	N-CA-CB	-7.87	96.44	110.60
1	B	208	THR	C-N-CA	7.82	141.25	121.70
1	D	148[A]	ARG	CD-NE-CZ	7.75	134.45	123.60
1	D	148[B]	ARG	CD-NE-CZ	7.75	134.45	123.60
1	A	200	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	D	56	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	D	49	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	C	152	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	C	200	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	D	2	ILE	CA-CB-CG1	-7.15	97.41	111.00
1	B	21	ASP	CB-CG-OD1	7.12	124.71	118.30
1	C	96	TYR	CB-CG-CD1	6.97	125.18	121.00
1	B	5	ASP	CB-CG-OD1	6.95	124.55	118.30
1	B	129	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	12	ASP	CB-CG-OD1	6.81	124.43	118.30
1	D	152	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	C	18	PHE	O-C-N	-6.68	112.01	122.70
1	D	18	PHE	O-C-N	-6.68	112.01	122.70
1	A	152	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	90	ASP	CB-CA-C	-6.67	97.07	110.40
1	C	39	GLN	N-CA-CB	-6.65	98.63	110.60
1	A	16	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	D	164	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	48	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	C	25	SER	N-CA-CB	-6.43	100.85	110.50
1	B	90	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	48	PHE	CB-CG-CD1	6.31	125.21	120.80
1	B	5	ASP	N-CA-CB	6.29	121.93	110.60
1	D	48	PHE	CB-CG-CD1	6.28	125.20	120.80
1	D	95	TYR	CB-CG-CD2	-6.24	117.25	121.00
1	D	49	ARG	NE-CZ-NH2	-6.22	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	164	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	B	77	ASN	OD1-CG-ND2	6.18	136.12	121.90
1	C	118	ASP	CB-CG-OD2	6.18	123.86	118.30
1	C	94	ALA	N-CA-CB	6.18	118.75	110.10
1	C	95	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	D	80	ALA	CB-CA-C	-6.17	100.84	110.10
1	D	48	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	A	94	ALA	N-CA-CB	6.12	118.67	110.10
1	A	200	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	1	PCA	O-C-N	-5.96	113.17	122.70
1	A	152	ARG	N-CA-CB	5.77	120.99	110.60
1	C	81	TYR	CG-CD2-CE2	-5.75	116.70	121.30
1	C	164	ARG	CD-NE-CZ	5.74	131.64	123.60
1	A	79	ASN	CB-CG-OD1	-5.72	110.16	121.60
1	C	81	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
1	D	100	SER	N-CA-CB	5.67	119.00	110.50
1	A	196	SER	N-CA-CB	-5.66	102.02	110.50
1	A	118	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	B	105	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	D	79	ASN	CB-CG-OD1	-5.58	110.45	121.60
1	B	69	ASN	CA-C-N	5.56	129.44	117.20
1	A	1	PCA	C-N-CA	5.52	135.50	121.70
1	D	152	ARG	N-CA-CB	5.51	120.53	110.60
1	B	121	THR	O-C-N	5.51	131.52	122.70
1	C	16	TYR	CB-CG-CD2	5.45	124.27	121.00
1	C	79	ASN	CA-CB-CG	-5.44	101.43	113.40
1	B	154	SER	N-CA-CB	5.44	118.66	110.50
1	A	129	ARG	CD-NE-CZ	5.43	131.20	123.60
1	A	48	PHE	CB-CG-CD1	5.40	124.58	120.80
1	C	170	GLY	CA-C-O	-5.37	110.93	120.60
1	D	99	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	147	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	D	129	ARG	CD-NE-CZ	5.28	130.98	123.60
1	A	84	VAL	N-CA-CB	5.26	123.07	111.50
1	A	48	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	D	90	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	96	TYR	CB-CA-C	-5.22	99.97	110.40
1	C	101	TRP	CE2-CD2-CE3	5.21	124.95	118.70
1	A	85	TYR	CB-CG-CD1	5.19	124.11	121.00
1	C	21	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	15	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	114	THR	O-C-N	5.13	130.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	81	TYR	CG-CD1-CE1	5.12	125.39	121.30
1	A	16	TYR	CB-CG-CD1	5.09	124.06	121.00
1	D	129	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	85	TYR	C-N-CA	-5.08	111.64	122.30
1	A	12	ASP	OD1-CG-OD2	-5.06	113.69	123.30
1	D	102	GLY	N-CA-C	-5.06	100.46	113.10
1	C	181	LEU	CB-CG-CD1	5.02	119.53	111.00
1	B	206	LEU	CA-CB-CG	-5.00	103.80	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PCA	Mainchain
1	B	208	THR	Peptide
1	B	97	ILE	Mainchain
1	D	1	PCA	Mainchain
1	D	120	GLY	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1640	0	1552	19	0
1	B	1652	0	1566	32	0
1	C	1636	0	1548	19	0
1	D	1643	0	1555	17	0
2	E	28	0	9	2	0
2	F	28	0	9	0	0
2	G	28	0	9	0	0
2	H	28	0	9	0	0
3	A	131	0	0	5	0
3	B	142	0	0	8	0
3	C	106	0	0	8	0
3	D	110	0	0	6	0
All	All	7172	0	6257	86	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 (86) 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:148[A]:ARG:CZ	1:B:148[A]:ARG:NE	1.72	1.52
1:B:81:TYR:OH	3:B:2065:HOH:O	1.84	0.94
1:B:12:ASP:OD1	1:B:209:ILE:HA	1.72	0.89
1:A:181:LEU:HD21	3:A:2052:HOH:O	1.79	0.83
1:B:148[A]:ARG:HD3	1:B:150:SER:O	1.79	0.81
1:B:208:THR:HG22	1:B:209:ILE:HB	1.64	0.80
1:A:126:GLU:OE2	1:A:142:LYS:HE2	1.83	0.79
1:C:39:GLN:OE1	3:C:2028:HOH:O	2.03	0.76
1:A:143[B]:GLN:OE1	3:A:2091:HOH:O	2.04	0.75
1:C:148[A]:ARG:HD3	1:C:150:SER:O	1.87	0.74
1:B:12:ASP:OD1	1:B:208:THR:HG23	1.87	0.74
1:B:206:LEU:HD22	3:B:2044:HOH:O	1.91	0.70
1:B:199:LEU:O	1:B:206:LEU:HD12	1.92	0.70
1:C:194:VAL:HG13	3:C:2043:HOH:O	1.92	0.69
1:B:72:ALA:HB1	3:B:2060:HOH:O	1.91	0.69
1:B:194:VAL:HG13	3:B:2128:HOH:O	1.92	0.68
1:B:157:ILE:HD11	3:B:2072:HOH:O	1.93	0.67
1:B:208:THR:CG2	1:B:209:ILE:HD12	2.28	0.63
1:A:52:LYS:HD2	1:A:53:LYS:O	2.01	0.60
1:B:199:LEU:HB3	1:B:206:LEU:HD13	1.84	0.60
1:C:28:MET:HB2	1:C:48:PHE:CD2	2.38	0.59
1:C:192:ALA:CB	3:C:2097:HOH:O	2.51	0.58
1:D:148[A]:ARG:HD3	1:D:150:SER:O	2.03	0.58
1:B:192:ALA:HB1	3:B:2060:HOH:O	2.05	0.57
1:D:12:ASP:O	1:D:208:THR:HG22	2.05	0.56
1:B:208:THR:HG22	1:B:209:ILE:CB	2.34	0.56
1:C:28:MET:HB2	1:C:48:PHE:HD2	1.71	0.56
1:D:70:TYR:HD2	3:D:2043:HOH:O	1.88	0.56
1:D:157:ILE:HD11	3:D:2054:HOH:O	2.05	0.55
1:D:118:ASP:OD2	3:D:2064:HOH:O	2.18	0.54
1:D:34:GLY:HA2	1:D:50:LYS:HD3	1.89	0.54
1:B:209:ILE:HG22	3:B:2139:HOH:O	2.07	0.54
1:C:165:ALA:HB3	3:C:2079:HOH:O	2.08	0.53
1:A:49:ARG:HD3	3:A:2043:HOH:O	2.09	0.53
1:A:187:GLN:NE2	3:A:2114:HOH:O	2.41	0.52
1:B:12:ASP:OD1	1:B:209:ILE:CA	2.52	0.52
1:A:128:LEU:HD13	1:A:142:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:HG2	1:B:104:TRP:CE2	2.44	0.51
1:A:187:GLN:NE2	1:B:79:ASN:OD1	2.44	0.51
1:B:208:THR:CG2	1:B:209:ILE:N	2.74	0.50
1:C:115:ILE:HD12	1:C:165:ALA:HB2	1.93	0.50
1:D:132:GLN:HB3	1:D:133:PRO:HD2	1.93	0.50
1:C:43:VAL:O	1:C:187:GLN:HA	2.12	0.49
1:D:157:ILE:CD1	3:D:2054:HOH:O	2.60	0.49
1:A:125:TYR:HB2	1:A:145:TRP:HB2	1.95	0.49
1:D:201:ILE:O	1:D:202:ASN:HB2	2.12	0.49
1:B:209:ILE:HG23	1:B:209:ILE:O	2.12	0.49
1:B:79:ASN:HB3	1:B:186:TYR:O	2.13	0.48
1:C:21:ASP:OD1	1:C:44:ASN:HB3	2.14	0.48
1:A:193:ASN:ND2	3:A:2120:HOH:O	2.46	0.48
1:D:85:TYR:HD2	3:D:2033:HOH:O	1.96	0.48
1:C:194:VAL:HG23	3:C:2097:HOH:O	2.12	0.47
1:B:208:THR:CG2	1:B:209:ILE:CD1	2.92	0.47
1:C:192:ALA:HB3	3:C:2097:HOH:O	2.12	0.47
1:D:115:ILE:HD12	1:D:165:ALA:HB2	1.96	0.47
1:A:204:ASN:ND2	1:A:204:ASN:N	2.63	0.46
1:C:14:TYR:HB3	1:C:50:LYS:HG2	1.97	0.46
1:C:94:ALA:O	1:C:143:GLN:HA	2.16	0.46
1:B:94:ALA:O	1:B:143:GLN:HA	2.16	0.45
1:A:132:GLN:HB3	1:A:133:PRO:CD	2.48	0.44
1:A:117:VAL:HG22	1:A:118:ASP:N	2.32	0.44
1:B:120:GLY:HA3	1:B:148[A]:ARG:CZ	2.47	0.44
1:C:193:ASN:ND2	3:C:2098:HOH:O	2.50	0.44
1:A:105:ARG:HH11	1:A:105:ARG:HD3	1.61	0.43
1:A:132:GLN:HB3	1:A:133:PRO:HD2	2.00	0.43
1:B:52:LYS:HD3	1:B:206:LEU:HD21	2.00	0.42
1:B:144:TYR:CZ	1:B:171:MET:HB3	2.53	0.42
1:D:49:ARG:HH11	1:D:49:ARG:HD3	1.73	0.42
1:C:39:GLN:HG3	3:C:2096:HOH:O	2.19	0.42
1:A:129:ARG:HH21	2:E:1:XYS:H2	1.84	0.42
1:C:18:PHE:C	1:C:18:PHE:CD1	2.91	0.42
1:D:79:ASN:ND2	3:D:2049:HOH:O	2.51	0.42
1:D:18:PHE:C	1:D:18:PHE:CD1	2.93	0.42
1:C:118:ASP:OD1	1:C:158:SER:OG	2.35	0.42
1:B:21:ASP:OD1	1:B:44:ASN:HB2	2.19	0.42
2:E:1:XYS:H2	2:E:1:XYS:H51	1.56	0.42
1:B:79:ASN:ND2	3:B:2065:HOH:O	2.49	0.41
1:D:52:LYS:HD3	1:D:206:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:THR:HB	1:A:61:GLN:OE1	2.20	0.41
1:D:94:ALA:O	1:D:143:GLN:HA	2.21	0.41
1:B:129:ARG:O	1:B:140:THR:HA	2.20	0.41
1:C:34:GLY:HA2	1:C:50:LYS:HD3	2.03	0.41
1:B:125:TYR:HB2	1:B:145:TRP:HB2	2.02	0.40
1:B:206:LEU:HD12	1:B:206:LEU:H	1.86	0.40
1:D:83:CYS:O	1:D:181:LEU:HD22	2.21	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	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
1	B	208/209 (100%)	199 (96%)	9 (4%)	0	100	100
1	C	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
1	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
All	All	828/836 (99%)	794 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/175 (100%)	170 (97%)	5 (3%)	42	35
1	B	176/175 (101%)	171 (97%)	5 (3%)	43	36
1	C	174/175 (99%)	173 (99%)	1 (1%)	86	87
1	D	175/175 (100%)	171 (98%)	4 (2%)	50	45
All	All	700/700 (100%)	685 (98%)	15 (2%)	52	48

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	77	ASN
1	A	79	ASN
1	A	107	PRO
1	A	168	ASN
1	B	45	ASN
1	B	69	ASN
1	B	79	ASN
1	B	168	ASN
1	B	209	ILE
1	C	28	MET
1	D	45	ASN
1	D	69	ASN
1	D	103	ASN
1	D	206	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	42	ASN
1	A	168	ASN
1	A	187	GLN
1	A	193	ASN
1	A	204	ASN
1	B	39	GLN
1	B	79	ASN
1	B	168	ASN
1	B	187	GLN
1	B	193	ASN
1	C	31	ASN

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Mol	Chain	Res	Type
1	C	41	ASN
1	C	42	ASN
1	C	143	GLN
1	C	193	ASN
1	D	31	ASN
1	D	79	ASN
1	D	103	ASN
1	D	193	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	B	1	1	7,8,9	1.28	1 (14%)	9,10,12	1.70	1 (11%)
1	PCA	A	1	1	7,8,9	1.45	2 (28%)	9,10,12	2.46	3 (33%)
1	PCA	D	1	1	7,8,9	1.54	2 (28%)	9,10,12	2.17	3 (33%)
1	PCA	C	1	1	7,8,9	1.97	2 (28%)	9,10,12	3.67	7 (77%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CG-CD	3.36	1.59	1.50
1	D	1	PCA	O-C	2.89	1.31	1.19
1	C	1	PCA	O-C	2.73	1.30	1.19
1	B	1	PCA	CG-CD	2.59	1.57	1.50
1	A	1	PCA	CG-CD	2.22	1.56	1.50
1	D	1	PCA	CG-CD	2.07	1.56	1.50
1	A	1	PCA	OE-CD	2.02	1.27	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	PCA	OE-CD-CG	-7.14	114.30	126.76
1	A	1	PCA	CB-CA-C	-5.62	104.97	112.70
1	C	1	PCA	CB-CA-C	-5.43	105.24	112.70
1	D	1	PCA	OE-CD-CG	-4.62	118.70	126.76
1	C	1	PCA	O-C-CA	3.88	134.94	124.78
1	B	1	PCA	CB-CA-C	-3.55	107.81	112.70
1	A	1	PCA	CB-CA-N	2.84	111.44	103.30
1	C	1	PCA	CB-CA-N	2.55	110.62	103.30
1	C	1	PCA	CB-CG-CD	-2.52	100.34	104.40
1	D	1	PCA	CB-CG-CD	-2.43	100.48	104.40
1	C	1	PCA	CA-N-CD	-2.27	105.80	113.58
1	A	1	PCA	CA-N-CD	-2.26	105.86	113.58
1	D	1	PCA	CB-CA-C	-2.17	109.71	112.70
1	C	1	PCA	OE-CD-N	-2.04	120.10	124.86

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)

12 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	XYS	E	1	2	10,10,10	1.31	1 (10%)	14,14,14	3.80	9 (64%)
2	XYP	E	2	2	9,9,10	1.09	0	10,12,14	2.10	3 (30%)
2	XYP	E	3	2	9,9,10	1.23	1 (11%)	10,12,14	2.81	5 (50%)
2	XYS	F	1	2	10,10,10	1.20	1 (10%)	14,14,14	4.36	10 (71%)
2	XYP	F	2	2	9,9,10	1.49	2 (22%)	10,12,14	2.09	3 (30%)
2	XYP	F	3	2	9,9,10	1.51	1 (11%)	10,12,14	2.16	5 (50%)
2	XYS	G	1	2	10,10,10	1.40	3 (30%)	14,14,14	3.60	10 (71%)
2	XYP	G	2	2	9,9,10	1.07	0	10,12,14	2.09	5 (50%)
2	XYP	G	3	2	9,9,10	1.39	0	10,12,14	2.49	3 (30%)
2	XYS	H	1	2	10,10,10	1.26	1 (10%)	14,14,14	2.98	10 (71%)
2	XYP	H	2	2	9,9,10	1.12	0	10,12,14	2.01	3 (30%)
2	XYP	H	3	2	9,9,10	1.31	0	10,12,14	2.51	5 (50%)

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	XYS	E	1	2	-	-	1/1/1/1
2	XYP	E	2	2	-	-	0/1/1/1
2	XYP	E	3	2	-	-	0/1/1/1
2	XYS	F	1	2	-	-	1/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1
2	XYP	F	3	2	-	-	0/1/1/1
2	XYS	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	XYP	G	3	2	-	-	0/1/1/1
2	XYS	H	1	2	-	-	0/1/1/1
2	XYP	H	2	2	-	-	0/1/1/1
2	XYP	H	3	2	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	XYP	C5-C4	2.63	1.58	1.52
2	G	1	XYS	O4-C4	-2.54	1.38	1.43
2	H	1	XYS	O4-C4	-2.51	1.38	1.43
2	E	1	XYS	C5-C4	2.28	1.57	1.52
2	F	1	XYS	C5-C4	2.26	1.57	1.52
2	E	3	XYP	O5-C1	-2.21	1.38	1.42
2	G	1	XYS	O5-C5	-2.11	1.40	1.43
2	F	2	XYP	O4-C4	-2.07	1.39	1.43
2	F	3	XYP	O5-C5	2.07	1.46	1.42
2	G	1	XYS	O5-C1	-2.05	1.40	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	XYS	O5-C1-C2	-8.50	96.81	109.43
2	E	1	XYS	O5-C1-C2	-7.26	98.64	109.43
2	F	1	XYS	O3-C3-C2	-6.67	94.92	110.35
2	E	3	XYP	C5-O5-C1	6.46	121.45	111.52
2	F	1	XYS	C5-C4-C3	-6.38	101.83	109.67
2	G	1	XYS	O3-C3-C2	-6.20	96.01	110.35
2	G	1	XYS	O3-C3-C4	-6.06	98.39	109.99
2	F	1	XYS	C5-O5-C1	5.99	122.78	112.71
2	E	1	XYS	C5-C4-C3	-5.89	102.42	109.67
2	G	3	XYP	O3-C3-C2	-5.54	99.39	109.99
2	E	1	XYS	O3-C3-C2	-5.35	97.97	110.35
2	H	1	XYS	O3-C3-C2	-5.21	98.30	110.35
2	H	1	XYS	O4-C4-C5	-4.70	99.54	109.15
2	E	1	XYS	O3-C3-C4	-4.63	101.14	109.99
2	G	1	XYS	C5-O5-C1	4.50	120.28	112.71
2	G	3	XYP	C5-O5-C1	4.50	118.44	111.52
2	F	1	XYS	O1-C1-O5	4.22	120.71	109.72
2	F	2	XYP	O3-C3-C4	-4.05	102.25	109.99
2	G	1	XYS	C1-C2-C3	4.01	118.64	110.31
2	F	1	XYS	O4-C4-C3	3.94	118.03	110.14
2	F	3	XYP	C5-C4-C3	-3.91	104.86	109.67
2	F	1	XYS	O5-C5-C4	-3.88	104.79	110.77
2	E	1	XYS	O1-C1-O5	3.87	119.80	109.72
2	H	3	XYP	C4-C3-C2	-3.76	106.46	110.92
2	H	3	XYP	O3-C3-C4	-3.75	102.82	109.99
2	H	1	XYS	O4-C4-C3	3.70	117.54	110.14
2	G	1	XYS	O2-C2-C3	-3.59	102.05	110.35
2	H	3	XYP	O2-C2-C3	-3.58	102.96	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	2	XYP	O2-C2-C3	-3.47	103.18	110.14
2	E	2	XYP	O2-C2-C3	-3.46	103.22	110.14
2	E	1	XYS	C1-C2-C3	-3.43	103.19	110.31
2	G	1	XYS	C4-C3-C2	3.43	116.83	110.89
2	E	3	XYP	C4-C3-C2	-3.40	106.88	110.92
2	G	1	XYS	O4-C4-C3	3.38	116.91	110.14
2	E	2	XYP	C4-C3-C2	-3.37	106.91	110.92
2	E	2	XYP	C5-O5-C1	3.31	116.62	111.52
2	F	3	XYP	C4-C3-C2	-3.24	107.07	110.92
2	H	3	XYP	O3-C3-C2	-3.21	103.86	109.99
2	G	1	XYS	O2-C2-C1	-3.20	101.74	109.16
2	E	1	XYS	O4-C4-C3	3.19	116.53	110.14
2	H	2	XYP	O2-C2-C3	-3.19	103.75	110.14
2	G	1	XYS	O5-C1-C2	3.18	114.15	109.43
2	F	2	XYP	C4-C3-C2	-3.17	107.16	110.92
2	E	1	XYS	O1-C1-C2	-3.16	100.14	109.03
2	H	2	XYP	C4-C3-C2	-3.12	107.21	110.92
2	H	1	XYS	C5-C4-C3	-3.12	105.84	109.67
2	G	2	XYP	C4-C3-C2	-3.11	107.22	110.92
2	H	2	XYP	O3-C3-C4	-3.11	104.05	109.99
2	F	2	XYP	C5-C4-C3	-3.05	105.91	109.67
2	H	1	XYS	O2-C2-C3	-3.04	103.31	110.35
2	H	1	XYS	O3-C3-C4	-3.04	104.17	109.99
2	H	1	XYS	O5-C5-C4	-2.91	106.28	110.77
2	F	1	XYS	C1-C2-C3	-2.91	104.28	110.31
2	H	1	XYS	O1-C1-C2	-2.87	100.95	109.03
2	G	1	XYS	C5-C4-C3	-2.85	106.16	109.67
2	F	3	XYP	C1-C2-C3	-2.82	106.20	109.67
2	E	3	XYP	C5-C4-C3	-2.75	106.28	109.67
2	F	1	XYS	O4-C4-C5	-2.72	103.58	109.15
2	E	3	XYP	C1-C2-C3	-2.66	106.39	109.67
2	E	1	XYS	C4-C3-C2	-2.61	106.38	110.89
2	G	2	XYP	O3-C3-C4	-2.60	105.02	109.99
2	H	3	XYP	C5-O5-C1	2.54	115.43	111.52
2	H	1	XYS	C5-O5-C1	2.45	116.83	112.71
2	F	3	XYP	O2-C2-C1	-2.36	104.33	109.15
2	E	3	XYP	O4-C4-C5	-2.32	104.40	109.15
2	F	1	XYS	O3-C3-C4	-2.27	105.65	109.99
2	F	3	XYP	O3-C3-C4	-2.19	105.80	109.99
2	H	1	XYS	O5-C1-C2	-2.16	106.22	109.43
2	G	2	XYP	C1-C2-C3	-2.08	107.11	109.67
2	G	2	XYP	O4-C4-C5	-2.03	105.01	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	3	XYP	C1-C2-C3	-2.02	107.18	109.67

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

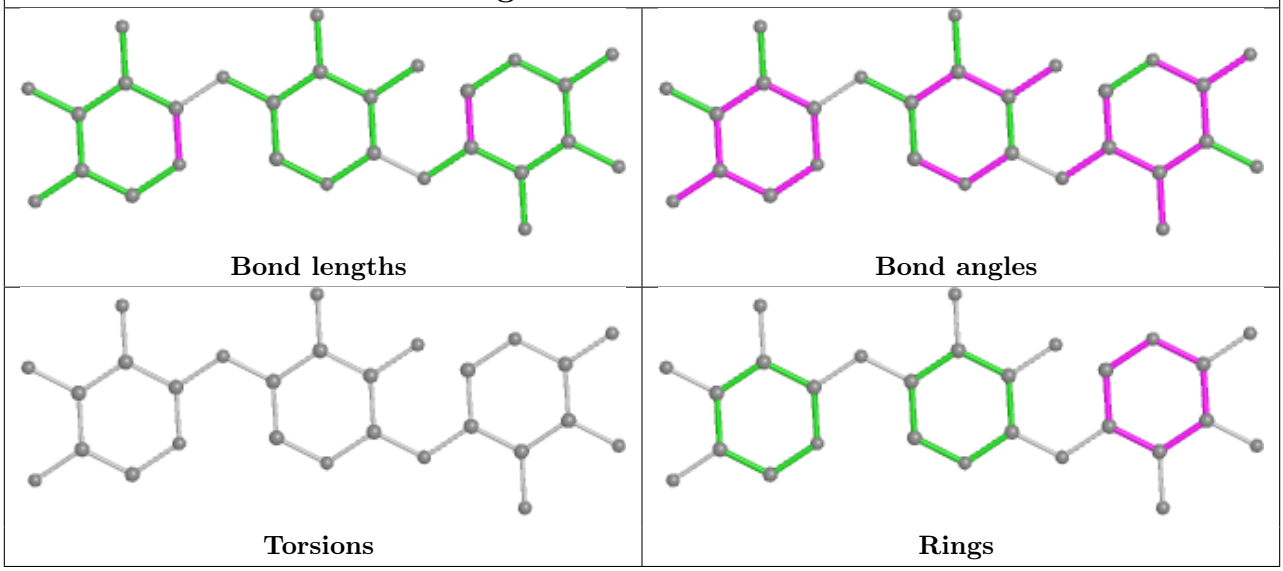
Mol	Chain	Res	Type	Atoms
2	F	1	XYS	C1-C2-C3-C4-C5-O5
2	E	1	XYS	C1-C2-C3-C4-C5-O5

1 monomer is involved in 2 short contacts:

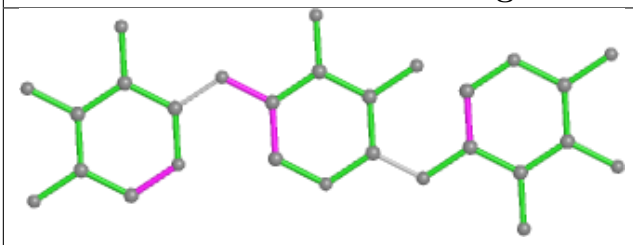
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	XYS	2	0

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

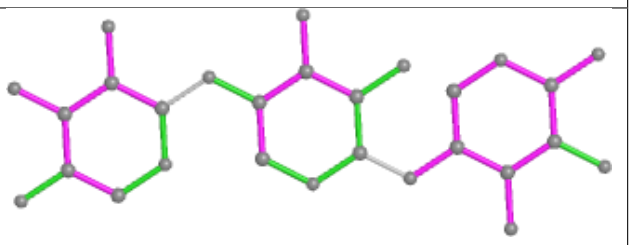
Oligosaccharide Chain E



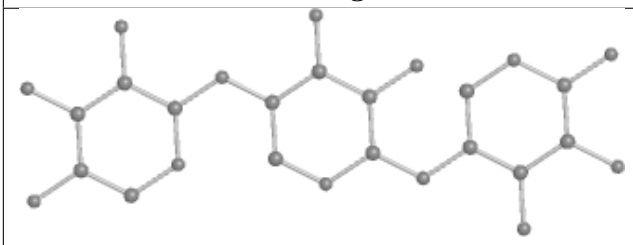
Oligosaccharide Chain F



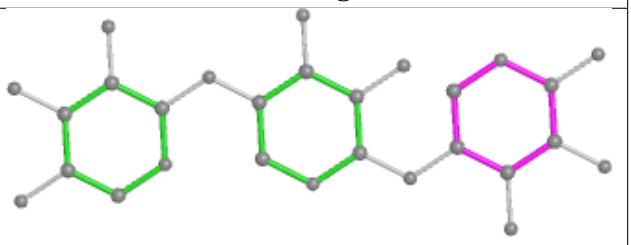
Bond lengths



Bond angles

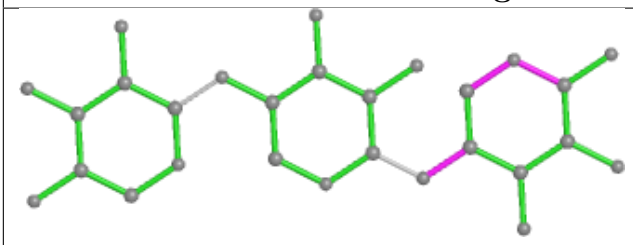


Torsions

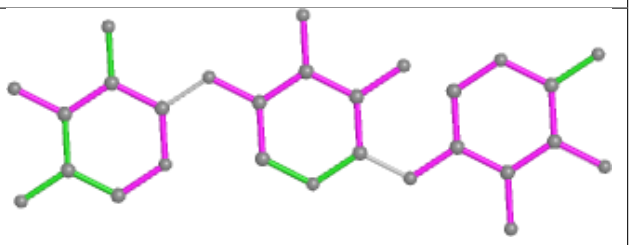


Rings

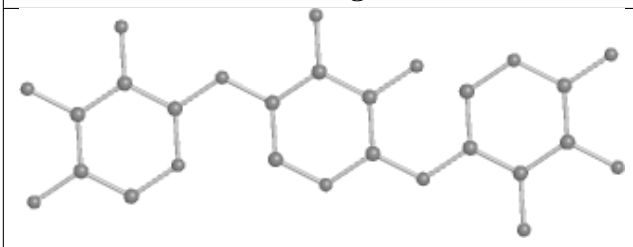
Oligosaccharide Chain G



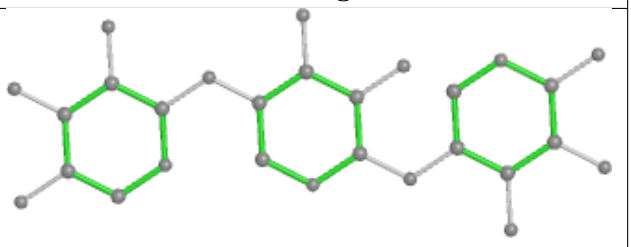
Bond lengths



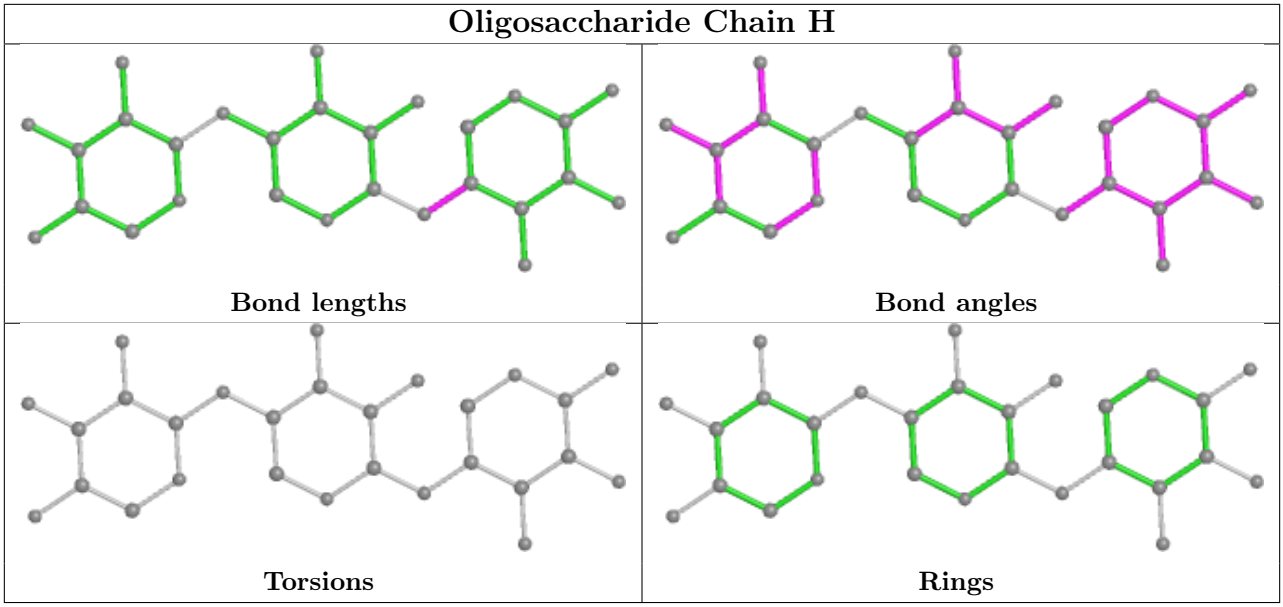
Bond angles



Torsions



Rings



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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	43:VAL	C	44:ASN	N	1.20

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	206/209 (98%)	-0.57	0	100	100	14, 21, 32, 52	0
1	B	208/209 (99%)	-0.55	0	100	100	14, 21, 31, 44	0
1	C	206/209 (98%)	-0.66	0	100	100	16, 23, 32, 51	0
1	D	207/209 (99%)	-0.63	0	100	100	16, 23, 33, 60	0
All	All	827/836 (98%)	-0.60	0	100	100	14, 22, 33, 60	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PCA	C	1	8/9	0.96	0.09	24,26,27,29	0
1	PCA	D	1	8/9	0.96	0.06	26,27,29,30	0
1	PCA	B	1	8/9	0.97	0.06	18,19,21,22	0
1	PCA	A	1	8/9	0.98	0.07	19,21,22,23	0

6.3 Carbohydrates (i)

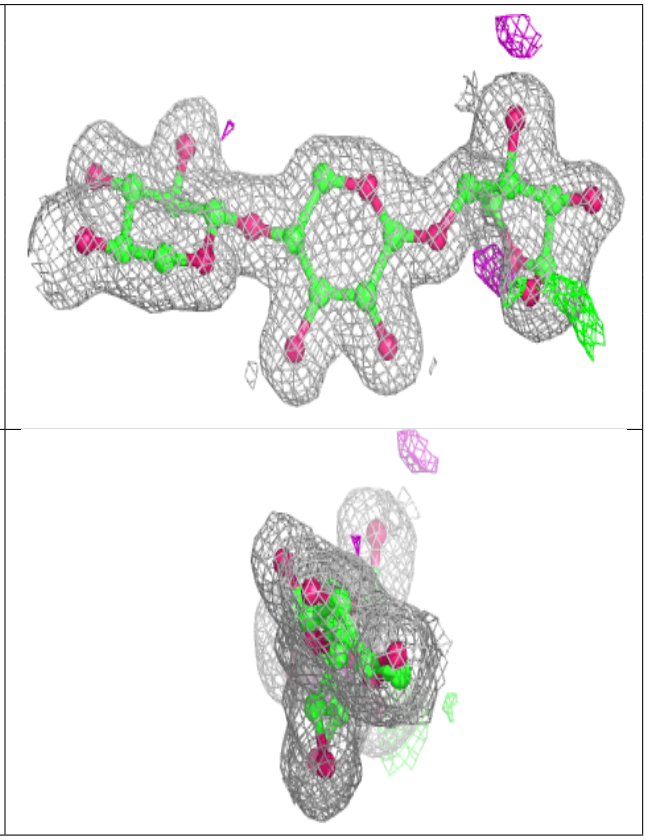
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XYS	F	1	10/10	0.89	0.12	21,29,34,39	0
2	XYS	G	1	10/10	0.89	0.16	26,36,41,42	0
2	XYS	E	1	10/10	0.91	0.10	24,26,33,38	0
2	XYS	H	1	10/10	0.91	0.14	23,33,38,38	0
2	XYP	E	3	9/10	0.92	0.08	27,31,37,40	0
2	XYP	G	3	9/10	0.94	0.07	25,28,29,31	0
2	XYP	F	3	9/10	0.96	0.06	21,28,32,33	0
2	XYP	H	3	9/10	0.96	0.07	27,30,33,34	0
2	XYP	E	2	9/10	0.97	0.06	17,20,23,23	0
2	XYP	H	2	9/10	0.98	0.07	18,21,23,23	0
2	XYP	F	2	9/10	0.98	0.06	16,19,21,22	0
2	XYP	G	2	9/10	0.99	0.06	20,22,23,24	0

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.

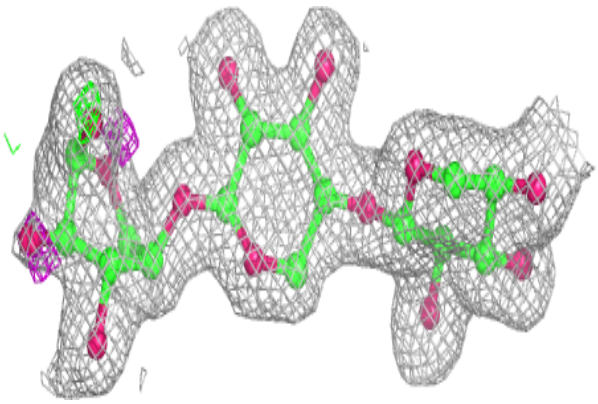
Electron density around Chain E:

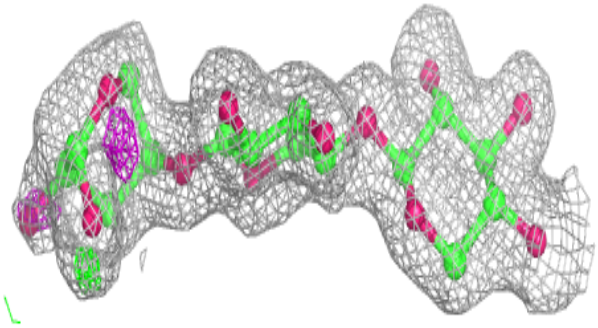
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

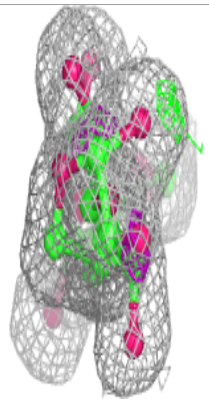


Electron density around Chain F:

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

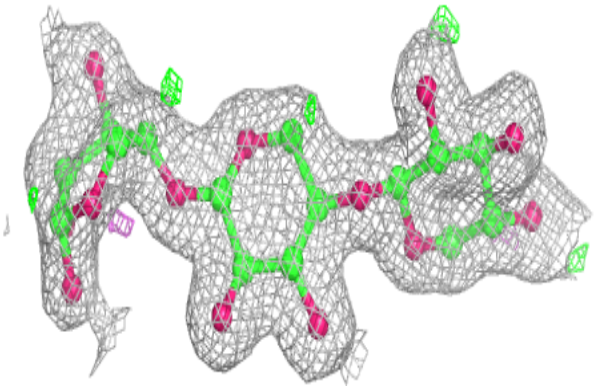


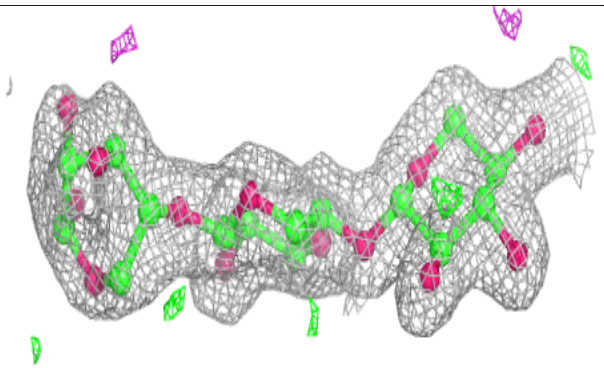


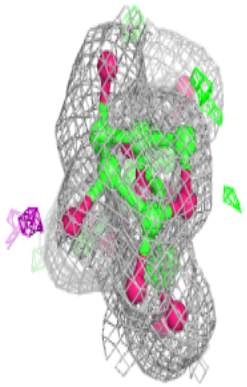


Electron density around Chain G:

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

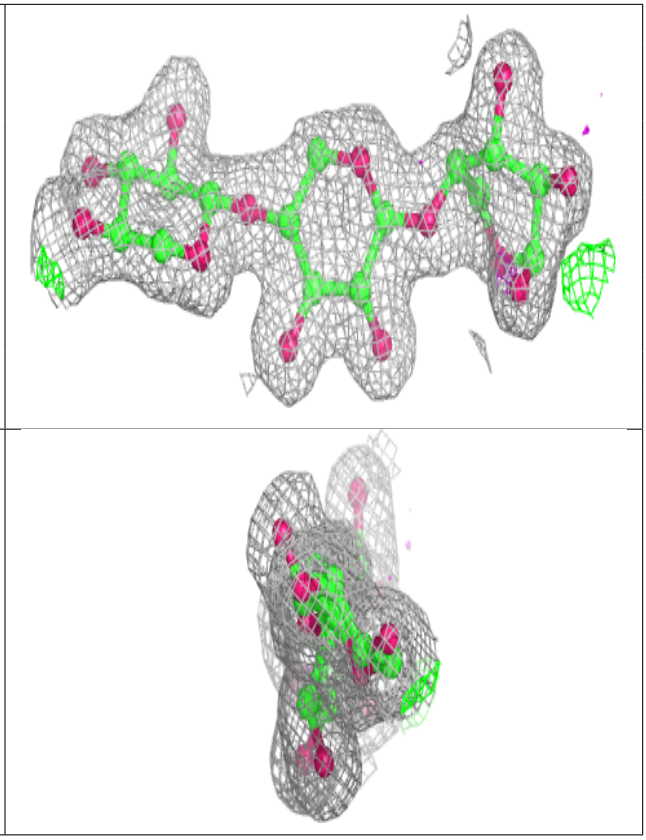






Electron density around Chain H:

$2mF_o$-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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.