Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2021 – 08:12 AM GMT

PDB ID	:	6Z9A
Title	:	Fructo-oligosaccharide transporter BT 1762-63
Authors	:	van den Berg, B.
Deposited on	:	2020-06-03
Resolution	:	3.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

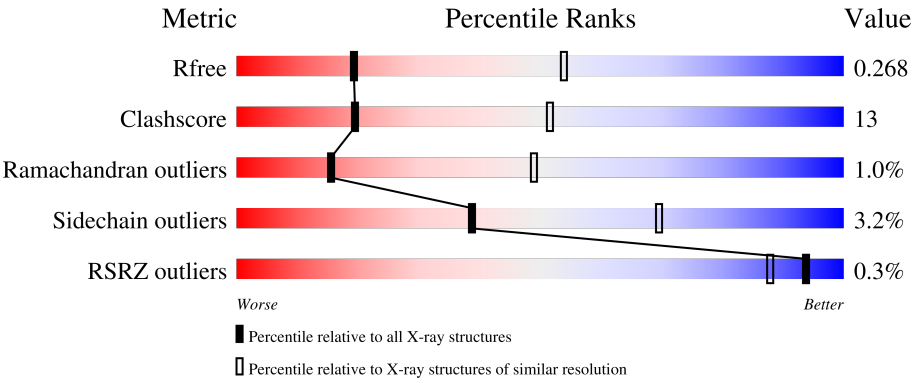
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	580	67% 28% • 5%
2	B	1041	61% 26% • 12%
3	C	7	43% 57%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11765 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4442	2813	737	871	21			

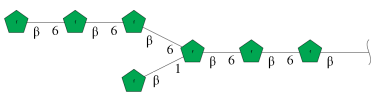
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	ALA	-	expression tag	UNP Q8A6W4
A	554	ALA	-	expression tag	UNP Q8A6W4
A	555	ALA	-	expression tag	UNP Q8A6W4
A	556	ALA	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4
A	559	HIS	-	expression tag	UNP Q8A6W4
A	560	HIS	-	expression tag	UNP Q8A6W4
A	561	HIS	-	expression tag	UNP Q8A6W4
A	562	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	921	Total	C	N	O	S	0	0	0
			7243	4571	1241	1410	21			

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	7	Total C O 78 42 36	0	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

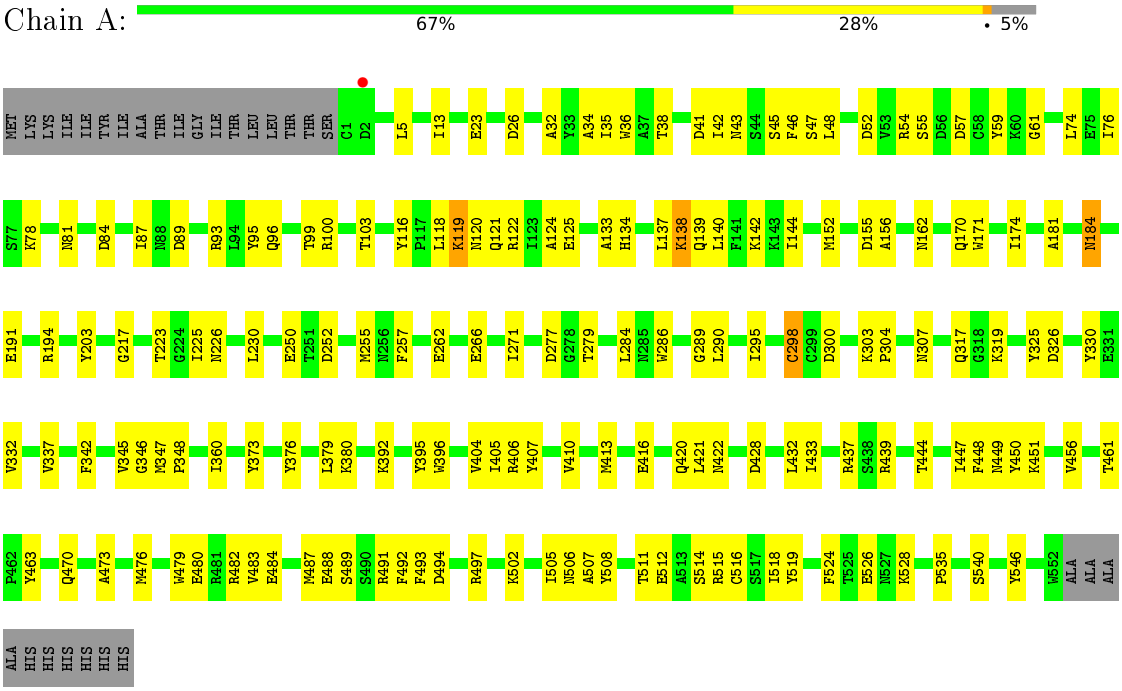
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

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.

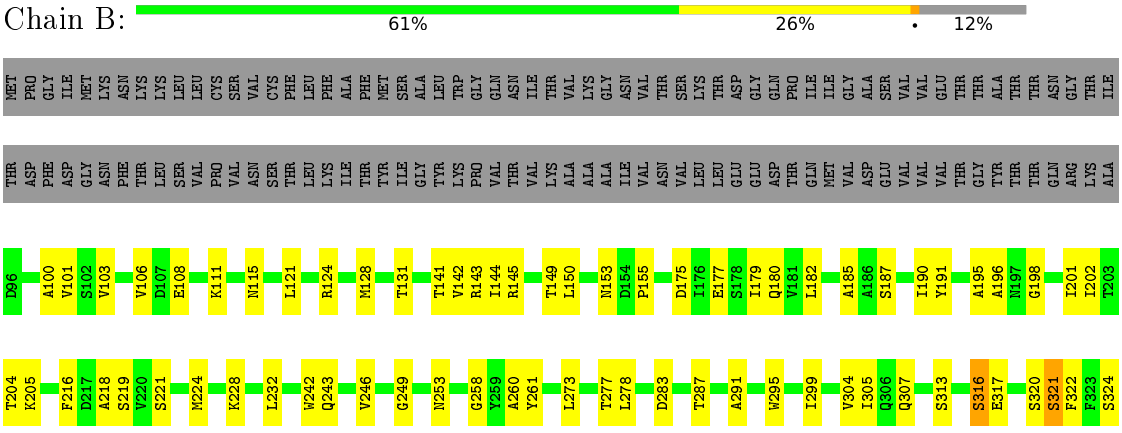
- Molecule 1: SusD homolog

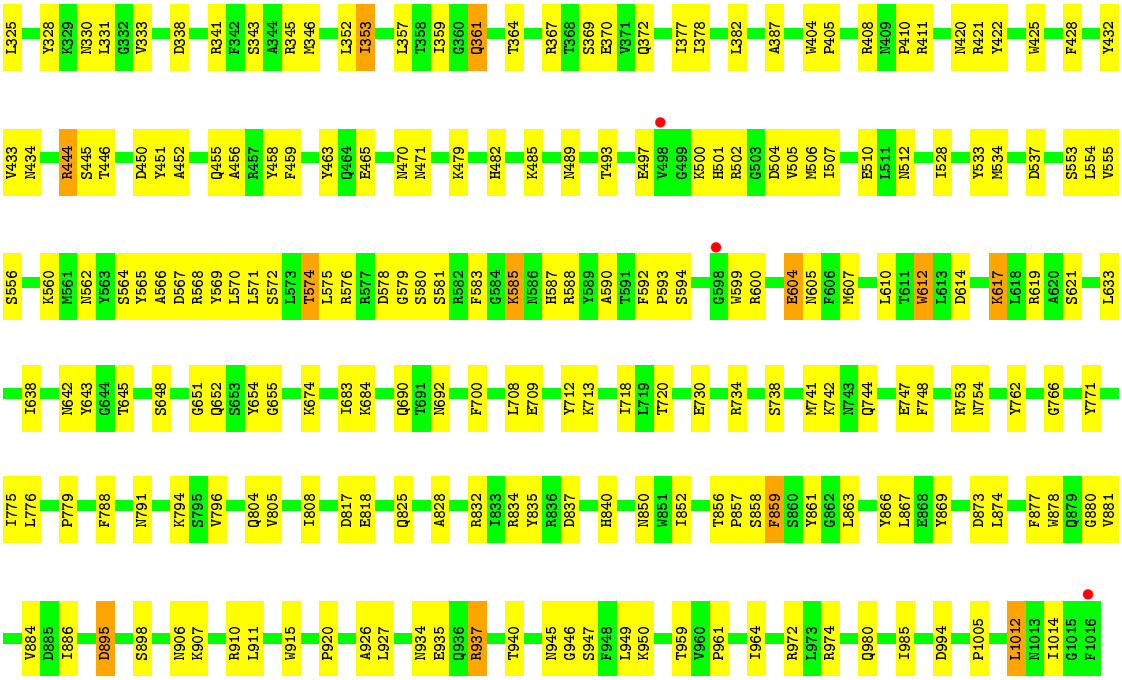
Chain A:



- Molecule 2: SusC homolog

Chain B:





• Molecule 3: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-[beta-D-fructofuranose-(2-1)]beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.72Å 234.62Å 169.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.64 – 3.10 117.31 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (106.64-3.10) 99.9 (117.31-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.206 , 0.268 0.206 , 0.268	Depositor DCC
R_{free} test set	2414 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	1.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.4	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	0.92	EDS
Total number of atoms	11765	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FRU, CL

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	0.49	1/4548 (0.0%)	0.68	1/6171 (0.0%)
2	B	0.47	0/7416	0.70	1/10053 (0.0%)
All	All	0.48	1/11964 (0.0%)	0.69	2/16224 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	GLU	CG-CD	5.21	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	570	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	184	ASN	C-N-CA	-5.44	108.10	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	470	ASN	Peptide

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	4442	0	4211	123	0
2	B	7243	0	6929	180	0
3	C	78	0	72	4	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	11765	0	11212	293	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 13.

All (293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:886:ILE:HG13	2:B:946:GLY:HA3	1.48	0.94
2:B:607:MET:HE3	2:B:610:LEU:HD13	1.53	0.89
2:B:832:ARG:NH2	2:B:926:ALA:O	2.08	0.85
1:A:96:GLN:HA	1:A:99:THR:HG22	1.58	0.85
1:A:99:THR:HG21	2:B:730:GLU:H	1.42	0.85
2:B:346:MET:O	2:B:361:GLN:NE2	2.16	0.77
2:B:304:VAL:HG22	2:B:331:LEU:HD12	1.69	0.73
2:B:504:ASP:HB2	2:B:562:ASN:HD22	1.53	0.73
1:A:277:ASP:OD1	1:A:279:THR:OG1	2.07	0.72
2:B:243:GLN:HB3	2:B:927:LEU:HD12	1.70	0.72
1:A:96:GLN:NE2	2:B:654:TYR:CE1	2.58	0.71
2:B:512:ASN:HB2	2:B:554:LEU:HB2	1.72	0.71
1:A:99:THR:O	1:A:103:THR:HG23	1.89	0.71
2:B:574:THR:HG23	2:B:594:SER:HB2	1.71	0.71
2:B:585:LYS:H	2:B:585:LYS:HD2	1.55	0.71
2:B:434:ASN:HB2	2:B:444:ARG:HD3	1.74	0.68
2:B:377:ILE:HD12	2:B:378:ILE:HG12	1.76	0.68
2:B:420:ASN:HB3	2:B:458:TYR:HD1	1.58	0.67
1:A:57:ASP:OD1	1:A:482:ARG:NH1	2.28	0.67
2:B:260:ALA:HB3	2:B:277:THR:HG23	1.77	0.66
1:A:392:LYS:HD2	1:A:396:TRP:CE2	2.32	0.65
2:B:359:ILE:HG12	2:B:433:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:SER:HB3	2:B:576:ARG:HH12	1.61	0.65
2:B:576:ARG:NH1	2:B:578:ASP:OD1	2.29	0.65
2:B:835:TYR:CZ	2:B:937:ARG:HD3	2.32	0.64
2:B:103:VAL:HG13	2:B:180:GLN:HG2	1.78	0.64
2:B:185:ALA:HB2	2:B:690:GLN:HB2	1.77	0.64
2:B:377:ILE:HD12	2:B:378:ILE:N	2.11	0.63
2:B:121:LEU:HD23	2:B:128:MET:HE3	1.79	0.63
2:B:124:ARG:HD3	2:B:877:PHE:CZ	2.33	0.63
1:A:34:ALA:O	1:A:38:THR:HG22	1.98	0.63
2:B:341:ARG:NH1	2:B:343:SER:OG	2.31	0.63
1:A:252:ASP:O	1:A:255:MET:HG3	1.98	0.62
1:A:392:LYS:HD2	1:A:396:TRP:NE1	2.14	0.62
2:B:367:ARG:HD2	2:B:425:TRP:CZ2	2.34	0.62
2:B:432:TYR:HB3	2:B:446:THR:HG22	1.80	0.61
2:B:895:ASP:OD2	2:B:910:ARG:NH1	2.33	0.61
1:A:317:GLN:O	1:A:461:THR:OG1	2.18	0.61
1:A:36:TRP:HB3	1:A:271:ILE:HD12	1.83	0.61
1:A:38:THR:HG21	2:B:655:GLY:O	2.01	0.61
2:B:489:ASN:HB3	2:B:510:GLU:HG3	1.82	0.60
1:A:505:ILE:HD11	1:A:524:PHE:CD2	2.36	0.60
1:A:284:LEU:HD12	1:A:286:TRP:CH2	2.37	0.60
1:A:93:ARG:NH2	2:B:652:GLN:OE1	2.35	0.60
2:B:633:LEU:HB3	2:B:638:ILE:HD11	1.84	0.59
2:B:911:LEU:HB2	2:B:927:LEU:HD21	1.83	0.59
1:A:300:ASP:OD1	1:A:303:LYS:NZ	2.35	0.59
2:B:633:LEU:HD13	2:B:638:ILE:HD12	1.83	0.58
2:B:204:THR:HG21	2:B:345:ARG:CZ	2.34	0.58
2:B:144:ILE:HG22	2:B:145:ARG:HG3	1.85	0.58
2:B:738:SER:HB3	2:B:779:PRO:HG3	1.85	0.58
2:B:574:THR:CG2	2:B:594:SER:HB2	2.34	0.57
2:B:712:TYR:CD1	2:B:744:GLN:HG2	2.40	0.57
1:A:89:ASP:OD1	1:A:93:ARG:NH1	2.37	0.57
1:A:96:GLN:NE2	2:B:654:TYR:HE1	2.00	0.57
2:B:175:ASP:HA	2:B:205:LYS:HD2	1.85	0.57
1:A:502:LYS:O	1:A:506:ASN:HB2	2.05	0.57
2:B:775:ILE:HD12	2:B:796:VAL:HG22	1.87	0.57
1:A:138:LYS:HB2	1:A:144:ILE:HD13	1.88	0.56
1:A:416:GLU:OE2	1:A:497:ARG:NH1	2.38	0.56
2:B:445:SER:HB2	2:B:489:ASN:O	2.06	0.56
1:A:507:ALA:O	1:A:511:THR:HG23	2.05	0.56
1:A:230:LEU:HD22	1:A:420:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:742:LYS:HD3	2:B:776:LEU:HD21	1.88	0.56
2:B:575:LEU:HD12	2:B:593:PRO:HB3	1.86	0.56
1:A:32:ALA:HA	1:A:100:ARG:HB3	1.88	0.56
1:A:13:ILE:HD13	2:B:638:ILE:HD13	1.88	0.56
1:A:138:LYS:HD3	1:A:171:TRP:CE2	2.40	0.56
1:A:138:LYS:HG2	1:A:171:TRP:CZ2	2.41	0.55
1:A:505:ILE:HA	1:A:508:TYR:HB3	1.87	0.55
2:B:708:LEU:HD12	2:B:748:PHE:HB2	1.89	0.55
1:A:447:ILE:HG22	1:A:450:TYR:CZ	2.42	0.55
1:A:35:ILE:HA	1:A:38:THR:HG23	1.88	0.55
2:B:915:TRP:CD1	2:B:920:PRO:HA	2.42	0.55
2:B:331:LEU:HD23	2:B:338:ASP:HB3	1.88	0.55
1:A:319:LYS:HA	1:A:437:ARG:HH21	1.72	0.55
1:A:404:VAL:HG12	1:A:405:ILE:HG13	1.88	0.55
2:B:142:VAL:HB	2:B:155:PRO:HG3	1.90	0.54
2:B:115:ASN:HB2	2:B:328:TYR:CZ	2.43	0.54
2:B:150:LEU:HD22	2:B:788:PHE:CZ	2.43	0.54
2:B:753:ARG:O	2:B:754:ASN:HB2	2.08	0.54
2:B:610:LEU:HD23	2:B:612:TRP:HE1	1.73	0.54
2:B:221:SER:HB2	2:B:305:ILE:HD12	1.88	0.53
2:B:377:ILE:HD12	2:B:378:ILE:H	1.71	0.53
1:A:43:ASN:ND2	3:C:4:FRU:O1	2.34	0.53
2:B:352:LEU:HB2	2:B:357:LEU:HD12	1.90	0.53
2:B:316:SER:OG	2:B:317:GLU:N	2.41	0.53
1:A:48:LEU:HD23	1:A:493:PHE:HE2	1.74	0.53
2:B:766:GLY:HA2	2:B:863:LEU:HA	1.90	0.53
1:A:226:ASN:O	1:A:230:LEU:HD12	2.09	0.53
1:A:407:TYR:O	1:A:410:VAL:HG22	2.09	0.53
1:A:439:ARG:NH2	1:A:484:GLU:OE2	2.42	0.53
2:B:712:TYR:HD1	2:B:744:GLN:HG2	1.72	0.53
2:B:370:GLU:HB3	2:B:422:TYR:CE2	2.43	0.52
1:A:406:ARG:NH1	1:A:488:GLU:OE2	2.43	0.52
1:A:54:ARG:HG2	1:A:74:LEU:O	2.08	0.52
1:A:122:ARG:NH1	1:A:125:GLU:OE2	2.40	0.52
1:A:45:SER:C	1:A:47:SER:H	2.12	0.52
1:A:250:GLU:HB3	1:A:255:MET:HE2	1.91	0.52
1:A:444:THR:O	1:A:448:PHE:N	2.43	0.52
2:B:950:LYS:NZ	2:B:994:ASP:OD1	2.36	0.51
1:A:152:MET:HG3	1:A:156:ALA:HB3	1.92	0.51
1:A:35:ILE:HD12	1:A:100:ARG:CZ	2.41	0.51
2:B:585:LYS:H	2:B:585:LYS:CD	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:HD22	1:A:508:TYR:HD1	1.58	0.51
2:B:101:VAL:HG13	2:B:182:LEU:HD12	1.93	0.51
1:A:518:ILE:HG13	1:A:519:TYR:N	2.25	0.51
1:A:124:ALA:HB1	1:A:181:ALA:HA	1.93	0.51
2:B:690:GLN:HG2	2:B:713:LYS:HA	1.92	0.51
1:A:61:GLY:HA2	1:A:373:TYR:CD2	2.46	0.50
2:B:850:ASN:O	2:B:852:ILE:HG23	2.11	0.50
2:B:232:LEU:HG	2:B:907:LYS:O	2.12	0.50
2:B:333:VAL:HG21	2:B:1005:PRO:HB3	1.93	0.50
2:B:283:ASP:OD2	2:B:287:THR:HG22	2.12	0.50
2:B:599:TRP:HE1	2:B:604:GLU:HG3	1.77	0.50
2:B:571:LEU:HG	2:B:572:SER:N	2.26	0.50
1:A:52:ASP:CG	1:A:489:SER:HA	2.32	0.50
2:B:179:ILE:HG12	2:B:202:ILE:HG12	1.94	0.50
2:B:610:LEU:H	2:B:610:LEU:HD12	1.77	0.50
2:B:619:ARG:HH12	2:B:709:GLU:HG2	1.76	0.50
1:A:347:MET:HG2	1:A:376:TYR:CD1	2.47	0.49
2:B:873:ASP:OD1	2:B:873:ASP:N	2.45	0.49
1:A:48:LEU:HG	1:A:140:LEU:HD21	1.94	0.49
1:A:295:ILE:HG13	1:A:295:ILE:O	2.11	0.49
2:B:961:PRO:HG2	2:B:964:ILE:HG13	1.95	0.49
2:B:600:ARG:HG3	2:B:617:LYS:HE3	1.93	0.49
2:B:652:GLN:O	2:B:652:GLN:HG3	2.12	0.49
2:B:934:ASN:O	2:B:937:ARG:HD2	2.11	0.49
1:A:346:GLY:HA3	1:A:379:LEU:HD21	1.94	0.49
2:B:258:GLY:O	2:B:278:LEU:HA	2.13	0.49
2:B:459:PHE:CD1	2:B:534:MET:HE2	2.48	0.49
2:B:861:TYR:CZ	2:B:880:GLY:HA3	2.48	0.49
1:A:422:ASN:HB2	1:A:470:GLN:OE1	2.12	0.49
2:B:643:TYR:HB3	2:B:645:THR:HG23	1.95	0.49
1:A:81:ASN:HB2	1:A:84:ASP:OD1	2.12	0.48
1:A:250:GLU:HB3	1:A:255:MET:CE	2.43	0.48
2:B:106:VAL:HG11	2:B:177:GLU:O	2.13	0.48
1:A:118:LEU:O	1:A:121:GLN:N	2.47	0.48
2:B:420:ASN:HB3	2:B:458:TYR:CD1	2.44	0.48
2:B:587:HIS:CD2	2:B:684:LYS:HB3	2.48	0.48
2:B:949:LEU:O	2:B:985:ILE:HG22	2.13	0.48
1:A:410:VAL:HA	1:A:413:MET:HE2	1.95	0.48
2:B:1012:LEU:HD12	2:B:1014:ILE:HG13	1.95	0.48
2:B:857:PRO:HB3	2:B:884:VAL:HG13	1.94	0.48
2:B:149:THR:OG1	2:B:150:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:858:SER:O	2:B:859:PHE:CD2	2.67	0.48
2:B:124:ARG:HD3	2:B:877:PHE:CE1	2.48	0.48
2:B:825:GLN:HE21	2:B:828:ALA:HB2	1.79	0.48
1:A:257:PHE:CE1	1:A:380:LYS:HD3	2.49	0.47
2:B:818:GLU:OE1	2:B:834:ARG:NH1	2.47	0.47
1:A:118:LEU:O	1:A:120:ASN:N	2.48	0.47
1:A:45:SER:C	1:A:47:SER:N	2.67	0.47
1:A:155:ASP:OD1	2:B:734:ARG:NH2	2.32	0.47
1:A:48:LEU:HD23	1:A:493:PHE:CE2	2.48	0.47
1:A:100:ARG:NE	2:B:730:GLU:OE2	2.41	0.47
2:B:881:VAL:HG12	2:B:884:VAL:HG13	1.95	0.47
1:A:319:LYS:HE3	1:A:463:TYR:HA	1.97	0.47
2:B:648:SER:OG	2:B:651:GLY:O	2.21	0.47
2:B:808:ILE:HA	2:B:940:THR:HG23	1.96	0.47
1:A:138:LYS:HD3	1:A:171:TRP:CD2	2.49	0.47
1:A:99:THR:HG21	2:B:730:GLU:N	2.20	0.47
2:B:945:ASN:OD1	2:B:947:SER:OG	2.26	0.47
1:A:225:ILE:HG22	1:A:230:LEU:HD11	1.94	0.47
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.70	0.47
1:A:502:LYS:HG2	1:A:506:ASN:HD22	1.80	0.47
2:B:502:ARG:HB2	2:B:564:SER:OG	2.15	0.47
2:B:791:ASN:OD1	2:B:804:GLN:HG2	2.15	0.47
2:B:832:ARG:HD3	2:B:935:GLU:OE1	2.15	0.47
2:B:369:SER:OG	2:B:421:ARG:HD3	2.15	0.47
1:A:133:ALA:O	1:A:137:LEU:HB2	2.15	0.46
1:A:266:GLU:OE1	1:A:439:ARG:NH1	2.44	0.46
2:B:708:LEU:HG	2:B:709:GLU:N	2.31	0.46
2:B:553:SER:O	2:B:554:LEU:HD23	2.16	0.46
2:B:145:ARG:NH2	2:B:747:GLU:OE1	2.44	0.46
1:A:325:TYR:CE2	1:A:326:ASP:HB2	2.50	0.46
1:A:491:ARG:O	1:A:494:ASP:HB2	2.15	0.46
1:A:162:ASN:OD1	1:A:546:TYR:HA	2.15	0.46
2:B:377:ILE:CD1	2:B:378:ILE:HG12	2.45	0.46
2:B:568:ARG:HB2	2:B:569:TYR:CD1	2.51	0.46
2:B:825:GLN:HG2	2:B:828:ALA:HB2	1.97	0.46
1:A:61:GLY:HA2	1:A:373:TYR:CG	2.50	0.46
2:B:190:ILE:HD12	2:B:560:LYS:CB	2.46	0.46
1:A:43:ASN:OD1	3:C:5:FRU:O3	2.21	0.45
2:B:320:SER:OG	2:B:321:SER:N	2.49	0.45
2:B:370:GLU:HG2	2:B:372:GLN:HG2	1.97	0.45
2:B:959:THR:HG22	2:B:974:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:ALA:HB3	2:B:592:PHE:CE2	2.51	0.45
1:A:42:ILE:HB	1:A:290:LEU:HG	1.98	0.45
2:B:866:TYR:O	2:B:867:LEU:HD23	2.16	0.45
1:A:116:TYR:O	1:A:118:LEU:N	2.50	0.45
1:A:266:GLU:HG3	1:A:407:TYR:HB3	1.99	0.45
2:B:411:ARG:HD2	2:B:411:ARG:HA	1.74	0.45
2:B:434:ASN:HA	2:B:444:ARG:HB2	1.97	0.45
1:A:304:PRO:HB3	1:A:487:MET:SD	2.57	0.45
2:B:612:TRP:CD1	2:B:612:TRP:N	2.85	0.45
1:A:99:THR:HG21	2:B:730:GLU:HB3	1.99	0.45
2:B:878:TRP:CE3	2:B:949:LEU:HD21	2.52	0.45
1:A:473:ALA:HA	1:A:476:MET:SD	2.56	0.45
2:B:857:PRO:HB3	2:B:884:VAL:CG1	2.47	0.45
1:A:330:TYR:CZ	1:A:332:VAL:HA	2.52	0.45
1:A:84:ASP:HB2	1:A:87:ILE:HD12	1.99	0.45
2:B:150:LEU:HD22	2:B:788:PHE:CE2	2.52	0.45
2:B:590:ALA:HB3	2:B:592:PHE:CZ	2.51	0.45
2:B:718:ILE:HG22	2:B:720:THR:OG1	2.17	0.45
2:B:794:LYS:HB2	2:B:805:VAL:HG21	1.99	0.45
2:B:195:ALA:O	2:B:198:GLY:N	2.48	0.44
2:B:832:ARG:NH1	2:B:935:GLU:OE2	2.50	0.44
1:A:134:HIS:HB3	1:A:174:ILE:HG12	1.99	0.44
1:A:87:ILE:HG22	1:A:535:PRO:HG3	1.98	0.44
2:B:404:TRP:HB3	2:B:405:PRO:HD2	1.99	0.44
2:B:528:ILE:HB	2:B:533:TYR:CG	2.52	0.44
1:A:330:TYR:CZ	1:A:337:VAL:HG21	2.52	0.44
1:A:42:ILE:HD13	1:A:395:TYR:CZ	2.52	0.44
2:B:258:GLY:O	2:B:278:LEU:HD12	2.17	0.44
1:A:300:ASP:CG	1:A:303:LYS:HZ2	2.20	0.44
3:C:1:FRU:H62	3:C:7:FRU:O6	2.17	0.44
2:B:131:THR:HG23	2:B:141:THR:OG1	2.17	0.44
2:B:837:ASP:OD2	2:B:840:HIS:HA	2.18	0.44
1:A:55:SER:HB3	1:A:492:PHE:HB2	2.00	0.44
2:B:108:GLU:HA	2:B:111:LYS:HD3	1.98	0.44
1:A:95:TYR:CE2	1:A:137:LEU:HD21	2.53	0.44
2:B:322:PHE:HE2	2:B:324:SER:HB3	1.83	0.44
2:B:566:ALA:C	2:B:568:ARG:H	2.22	0.43
2:B:791:ASN:ND2	2:B:804:GLN:HG2	2.33	0.43
2:B:246:VAL:O	2:B:249:GLY:N	2.38	0.43
2:B:328:TYR:CE2	2:B:330:ASN:HB2	2.53	0.43
2:B:422:TYR:HA	2:B:456:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HG13	1:A:78:LYS:H	1.84	0.43
1:A:451:LYS:HD3	1:A:451:LYS:C	2.38	0.43
1:A:479:TRP:O	1:A:483:VAL:HG22	2.18	0.43
1:A:96:GLN:HB2	2:B:730:GLU:HB2	2.00	0.43
2:B:791:ASN:HD21	2:B:804:GLN:HG2	1.83	0.43
1:A:23:GLU:HG3	1:A:23:GLU:H	1.50	0.43
1:A:138:LYS:HE3	1:A:170:GLN:HB3	2.01	0.43
2:B:307:GLN:HG2	2:B:328:TYR:CD1	2.53	0.43
1:A:217:GLY:H	1:A:223:THR:HG21	1.83	0.43
1:A:303:LYS:HB3	1:A:303:LYS:HE3	1.90	0.43
1:A:347:MET:HG2	1:A:376:TYR:CE1	2.54	0.42
1:A:139:GLN:HB3	1:A:493:PHE:CZ	2.54	0.42
2:B:253:ASN:HD21	2:B:261:TYR:H	1.66	0.42
2:B:253:ASN:ND2	2:B:260:ALA:HA	2.33	0.42
2:B:291:ALA:O	2:B:387:ALA:HA	2.18	0.42
2:B:299:ILE:HG21	2:B:410:PRO:HB2	2.01	0.42
2:B:353:ILE:O	2:B:353:ILE:HG22	2.19	0.42
1:A:35:ILE:HB	1:A:100:ARG:HD2	2.01	0.42
1:A:516:CYS:SG	1:A:518:ILE:HG12	2.59	0.42
1:A:406:ARG:NH2	1:A:484:GLU:OE2	2.52	0.42
1:A:433:ILE:HG23	1:A:480:GLU:HG2	2.01	0.42
2:B:580:SER:O	2:B:588:ARG:HD3	2.20	0.42
2:B:771:TYR:CZ	2:B:856:THR:HG23	2.55	0.42
1:A:139:GLN:HB3	1:A:493:PHE:CE1	2.55	0.42
1:A:428:ASP:O	1:A:432:LEU:HG	2.20	0.42
2:B:150:LEU:HD12	2:B:718:ILE:HG21	2.01	0.42
2:B:258:GLY:C	2:B:278:LEU:HD12	2.39	0.42
2:B:458:TYR:CE2	2:B:479:LYS:HD3	2.55	0.42
2:B:216:PHE:CE1	2:B:218:ALA:HB2	2.53	0.42
3:C:2:FRU:H5	3:C:3:FRU:H62	2.01	0.42
1:A:304:PRO:HG2	1:A:376:TYR:HB3	2.01	0.42
2:B:741:MET:HG3	2:B:775:ILE:HA	2.02	0.42
2:B:150:LEU:HA	2:B:150:LEU:HD23	1.90	0.41
2:B:191:TYR:CE1	2:B:201:ILE:HD11	2.55	0.41
2:B:459:PHE:HD1	2:B:534:MET:HE2	1.85	0.41
1:A:319:LYS:HA	1:A:437:ARG:NH2	2.34	0.41
2:B:621:SER:HB2	2:B:692:ASN:HB3	2.03	0.41
2:B:583:PHE:HD1	2:B:683:ILE:HG13	1.85	0.41
2:B:143:ARG:CZ	2:B:153:ASN:HB2	2.51	0.41
2:B:493:THR:HA	2:B:505:VAL:O	2.21	0.41
1:A:138:LYS:HA	1:A:144:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:LYS:HD3	1:A:526:GLU:HB2	2.03	0.41
2:B:463:TYR:HB2	2:B:465:GLU:OE1	2.20	0.41
2:B:450:ASP:HB3	2:B:485:LYS:HB2	2.02	0.41
1:A:345:VAL:HG12	1:A:347:MET:HG3	2.02	0.41
2:B:741:MET:HG3	2:B:775:ILE:HG12	2.02	0.41
1:A:512:GLU:OE2	1:A:515:ARG:NH1	2.54	0.41
2:B:506:MET:HG2	2:B:507:ILE:N	2.36	0.41
2:B:382:LEU:O	2:B:906:ASN:HB3	2.19	0.41
1:A:118:LEU:O	1:A:119:LYS:C	2.59	0.41
2:B:451:TYR:HH	2:B:482:HIS:CE1	2.39	0.41
1:A:191:GLU:OE2	1:A:194:ARG:NH1	2.54	0.41
1:A:514:SER:HB2	1:A:515:ARG:HD2	2.03	0.41
2:B:364:THR:HG22	2:B:428:PHE:HB3	2.03	0.41
2:B:458:TYR:HE2	2:B:479:LYS:HD3	1.86	0.41
2:B:500:LYS:HB2	2:B:501:HIS:CD2	2.56	0.41
1:A:5:LEU:HD11	2:B:555:VAL:HG21	2.03	0.41
2:B:579:GLY:HA2	2:B:588:ARG:O	2.21	0.41
1:A:230:LEU:HB2	1:A:421:LEU:HD21	2.03	0.40
2:B:182:LEU:HD23	2:B:187:SER:O	2.21	0.40
2:B:425:TRP:O	2:B:452:ALA:HA	2.20	0.40
1:A:348:PRO:HA	1:A:360:ILE:O	2.21	0.40
1:A:448:PHE:CG	1:A:449:ASN:N	2.89	0.40
2:B:242:TRP:CG	2:B:273:LEU:HD13	2.57	0.40
1:A:342:PHE:CZ	1:A:456:VAL:HG21	2.57	0.40
2:B:295:TRP:CZ3	2:B:410:PRO:HD2	2.56	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	550/580 (95%)	506 (92%)	38 (7%)	6 (1%)	14 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	919/1041 (88%)	823 (90%)	88 (10%)	8 (1%)	17 52
All	All	1469/1621 (91%)	1329 (90%)	126 (9%)	14 (1%)	15 49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	LYS
1	A	298	CYS
1	A	528	LYS
2	B	604	GLU
1	A	46	PHE
1	A	289	GLY
2	B	100	ALA
2	B	642	ASN
2	B	859	PHE
2	B	898	SER
1	A	142	LYS
2	B	196	ALA
2	B	605	ASN
2	B	353	ILE

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	473/495 (96%)	465 (98%)	8 (2%)	60 83
2	B	766/869 (88%)	734 (96%)	32 (4%)	30 62
All	All	1239/1364 (91%)	1199 (97%)	40 (3%)	39 69

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	41	ASP

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Mol	Chain	Res	Type
1	A	59	TYR
1	A	138	LYS
1	A	184	ASN
1	A	203	TYR
1	A	298	CYS
1	A	540	SER
2	B	219	SER
2	B	224	MET
2	B	228	LYS
2	B	313	SER
2	B	316	SER
2	B	321	SER
2	B	361	GLN
2	B	408	ARG
2	B	444	ARG
2	B	455	GLN
2	B	471	ASN
2	B	497	GLU
2	B	537	ASP
2	B	565	TYR
2	B	567	ASP
2	B	574	THR
2	B	581	SER
2	B	585	LYS
2	B	612	TRP
2	B	614	ASP
2	B	617	LYS
2	B	674	LYS
2	B	700	PHE
2	B	762	TYR
2	B	817	ASP
2	B	869	TYR
2	B	874	LEU
2	B	895	ASP
2	B	937	ARG
2	B	972	ARG
2	B	980	GLN
2	B	1012	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
2	B	366	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FRU	C	1	3	11,12,12	0.86	1 (9%)	10,18,18	1.69	2 (20%)
3	FRU	C	2	3	11,11,12	0.54	0	15,15,18	1.06	2 (13%)
3	FRU	C	3	3	11,11,12	0.46	0	15,15,18	1.04	0
3	FRU	C	4	3	11,11,12	0.38	0	15,15,18	0.99	1 (6%)
3	FRU	C	5	3	11,11,12	0.56	0	15,15,18	1.43	2 (13%)
3	FRU	C	6	3	11,11,12	0.63	0	15,15,18	1.31	3 (20%)
3	FRU	C	7	3	11,11,12	0.57	0	15,15,18	1.10	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
3	FRU	C	1	3	-	1/5/24/24	0/1/1/1
3	FRU	C	2	3	-	0/4/20/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	C	3	3	-	2/4/20/24	0/1/1/1
3	FRU	C	4	3	-	4/4/20/24	0/1/1/1
3	FRU	C	5	3	-	2/4/20/24	0/1/1/1
3	FRU	C	6	3	-	4/4/20/24	0/1/1/1
3	FRU	C	7	3	-	4/4/20/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FRU	O2-C2	2.07	1.44	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	FRU	O6-C6-C5	-4.06	97.37	111.29
3	C	5	FRU	C1-C2-C3	-3.29	107.17	115.09
3	C	6	FRU	C1-C2-C3	-2.88	108.15	115.09
3	C	5	FRU	C4-C3-C2	2.59	107.67	102.64
3	C	4	FRU	C1-C2-C3	-2.43	109.23	115.09
3	C	2	FRU	O5-C2-C1	2.26	114.10	109.21
3	C	6	FRU	O4-C4-C3	-2.23	104.60	111.82
3	C	1	FRU	O5-C5-C4	2.19	110.95	105.49
3	C	2	FRU	C4-C3-C2	-2.13	98.51	102.64
3	C	6	FRU	C3-C4-C5	2.12	106.75	102.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	7	FRU	O1-C1-C2-C3
3	C	7	FRU	O1-C1-C2-O5
3	C	5	FRU	O1-C1-C2-C3
3	C	5	FRU	O1-C1-C2-O5
3	C	4	FRU	O5-C5-C6-O6
3	C	7	FRU	C4-C5-C6-O6
3	C	7	FRU	O5-C5-C6-O6
3	C	3	FRU	O1-C1-C2-O5
3	C	6	FRU	O1-C1-C2-C3
3	C	4	FRU	O1-C1-C2-O5
3	C	3	FRU	O1-C1-C2-C3

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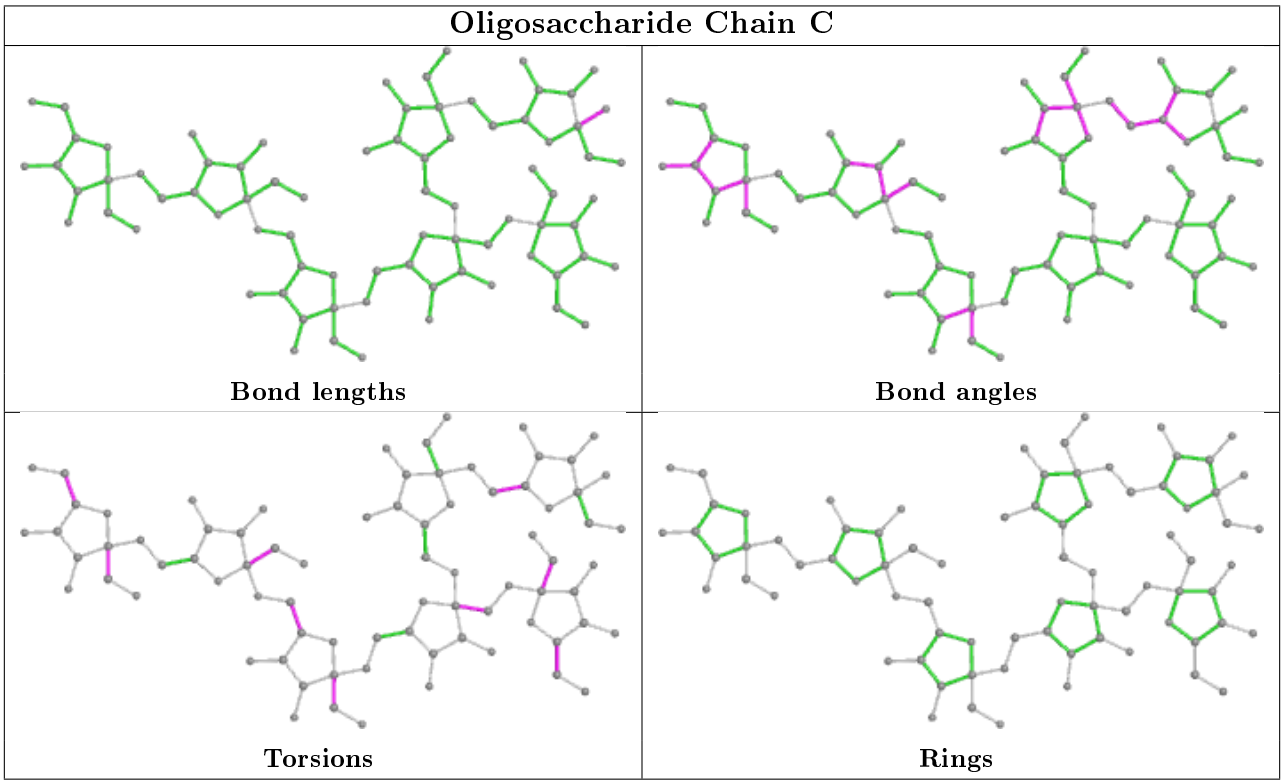
Mol	Chain	Res	Type	Atoms
3	C	4	FRU	C4-C5-C6-O6
3	C	4	FRU	O1-C1-C2-C3
3	C	6	FRU	O1-C1-C2-O5
3	C	6	FRU	C4-C5-C6-O6
3	C	1	FRU	C4-C5-C6-O6
3	C	6	FRU	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	7	FRU	1	0
3	C	2	FRU	1	0
3	C	3	FRU	1	0
3	C	1	FRU	1	0
3	C	5	FRU	1	0
3	C	4	FRU	1	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	552/580 (95%)	-0.13	1 (0%)	95	90	40, 64, 91, 150	0
2	B	921/1041 (88%)	0.03	3 (0%)	94	88	40, 68, 117, 161	0
All	All	1473/1621 (90%)	-0.03	4 (0%)	94	88	40, 66, 110, 161	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1016	PHE	2.6
2	B	598	GLY	2.4
2	B	498	VAL	2.2
1	A	2	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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, 95^{th} 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
3	FRU	C	6	11/12	0.72	0.29	64,79,99,102	0
3	FRU	C	7	11/12	0.80	0.37	68,100,112,116	0
3	FRU	C	1	12/12	0.85	0.23	82,93,112,112	0
3	FRU	C	5	11/12	0.91	0.33	56,73,93,99	0
3	FRU	C	2	11/12	0.94	0.22	52,73,89,90	0

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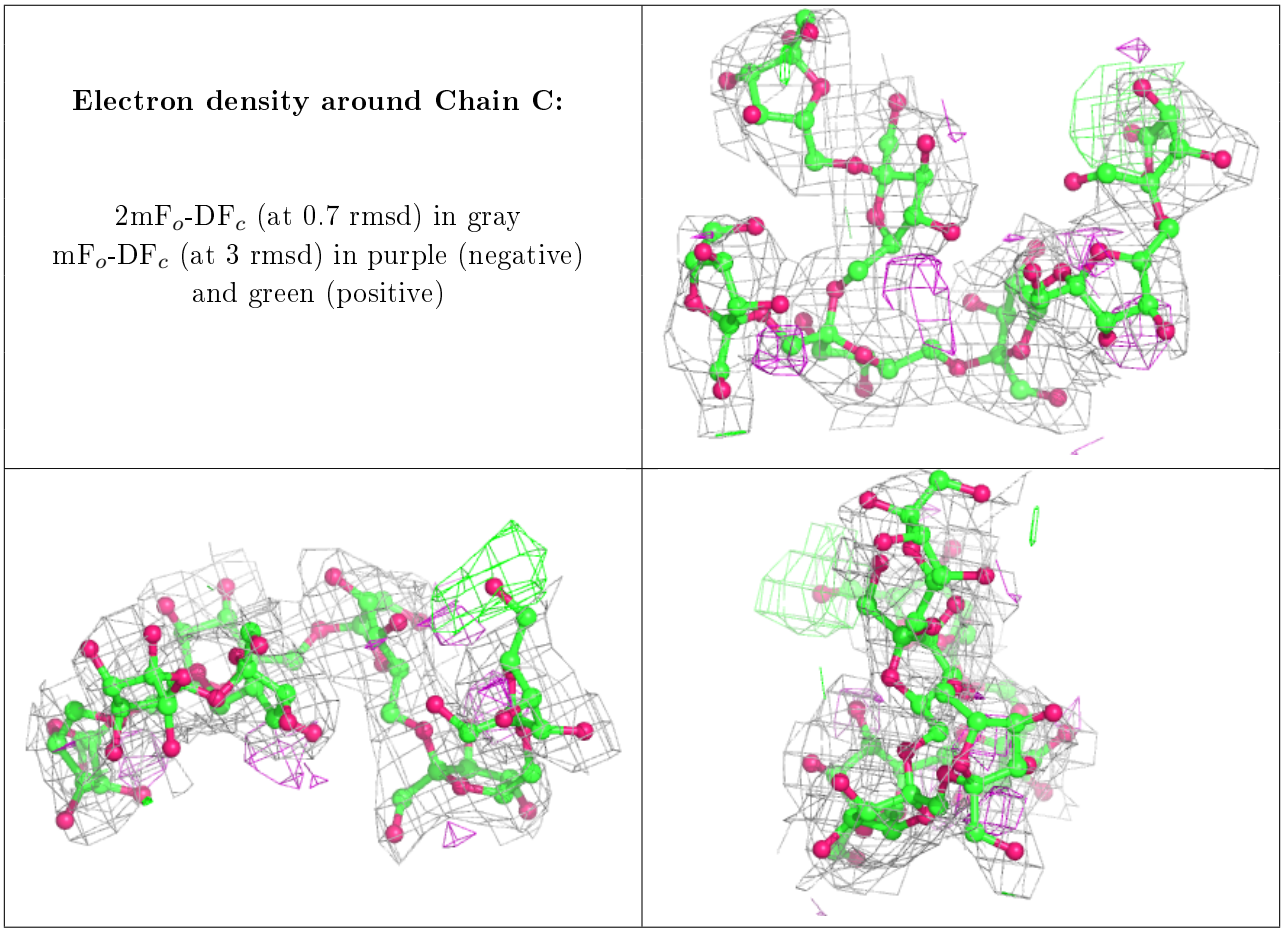
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FRU	C	3	11/12	0.97	0.20	54,64,80,90	0
3	FRU	C	4	11/12	0.97	0.18	29,35,43,46	0

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 C:

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



6.4 Ligands

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
4	CL	A	601	1/1	0.98	0.35	77,77,77,77	0
5	MG	B	1101	1/1	0.98	0.18	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.