Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 05:19 AM EDT

PDB ID	:	4LNV
Title	:	Crystal Structure of TEP1s
Authors	:	Le, B.V.; Williams, M.; Logarajah, S.; Baxter, R.H.G.
Deposited on	:	2013-07-12
Resolution	:	3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

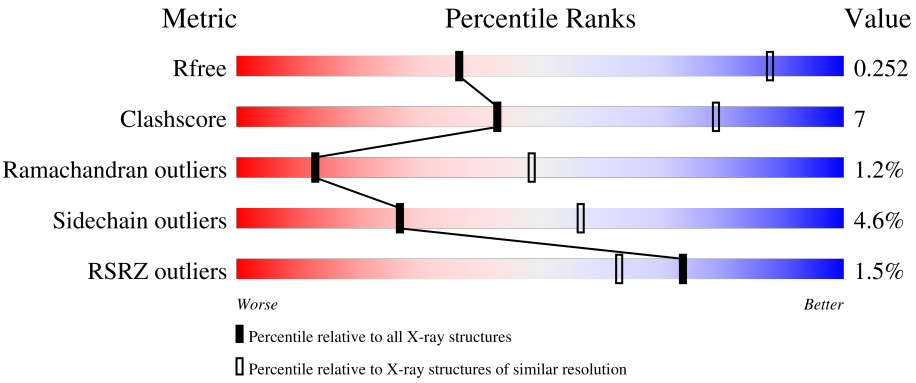
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1323	2% 79% 16%
1	B	1323	64% 15% 20%
1	C	1323	79% 16%
2	D	2	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27034 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 Thioester-containing protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1276	Total	C	N	O	S	0	0	0
			9704	6210	1583	1866	45			
1	B	1063	Total	C	N	O	S	0	0	0
			7461	4750	1225	1454	32			
1	C	1276	Total	C	N	O	S	0	0	0
			9631	6163	1573	1850	45			

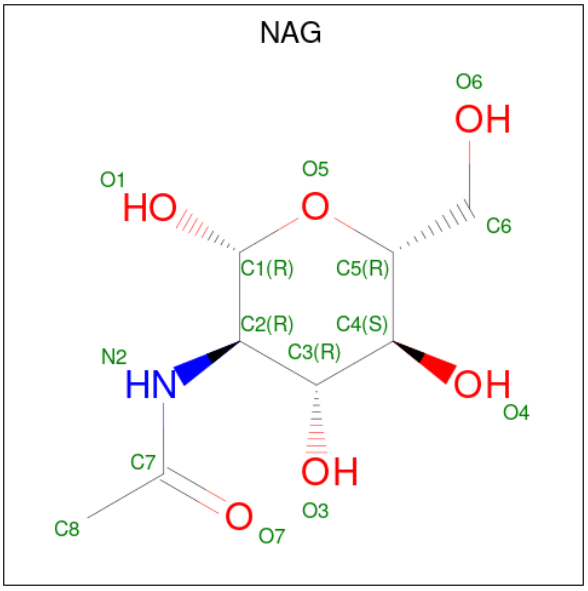
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1339	HIS	-	expression tag	UNP Q9GYW4
A	1340	HIS	-	expression tag	UNP Q9GYW4
A	1341	HIS	-	expression tag	UNP Q9GYW4
A	1342	HIS	-	expression tag	UNP Q9GYW4
A	1343	HIS	-	expression tag	UNP Q9GYW4
A	1344	HIS	-	expression tag	UNP Q9GYW4
B	1339	HIS	-	expression tag	UNP Q9GYW4
B	1340	HIS	-	expression tag	UNP Q9GYW4
B	1341	HIS	-	expression tag	UNP Q9GYW4
B	1342	HIS	-	expression tag	UNP Q9GYW4
B	1343	HIS	-	expression tag	UNP Q9GYW4
B	1344	HIS	-	expression tag	UNP Q9GYW4
C	1339	HIS	-	expression tag	UNP Q9GYW4
C	1340	HIS	-	expression tag	UNP Q9GYW4
C	1341	HIS	-	expression tag	UNP Q9GYW4
C	1342	HIS	-	expression tag	UNP Q9GYW4
C	1343	HIS	-	expression tag	UNP Q9GYW4
C	1344	HIS	-	expression tag	UNP Q9GYW4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

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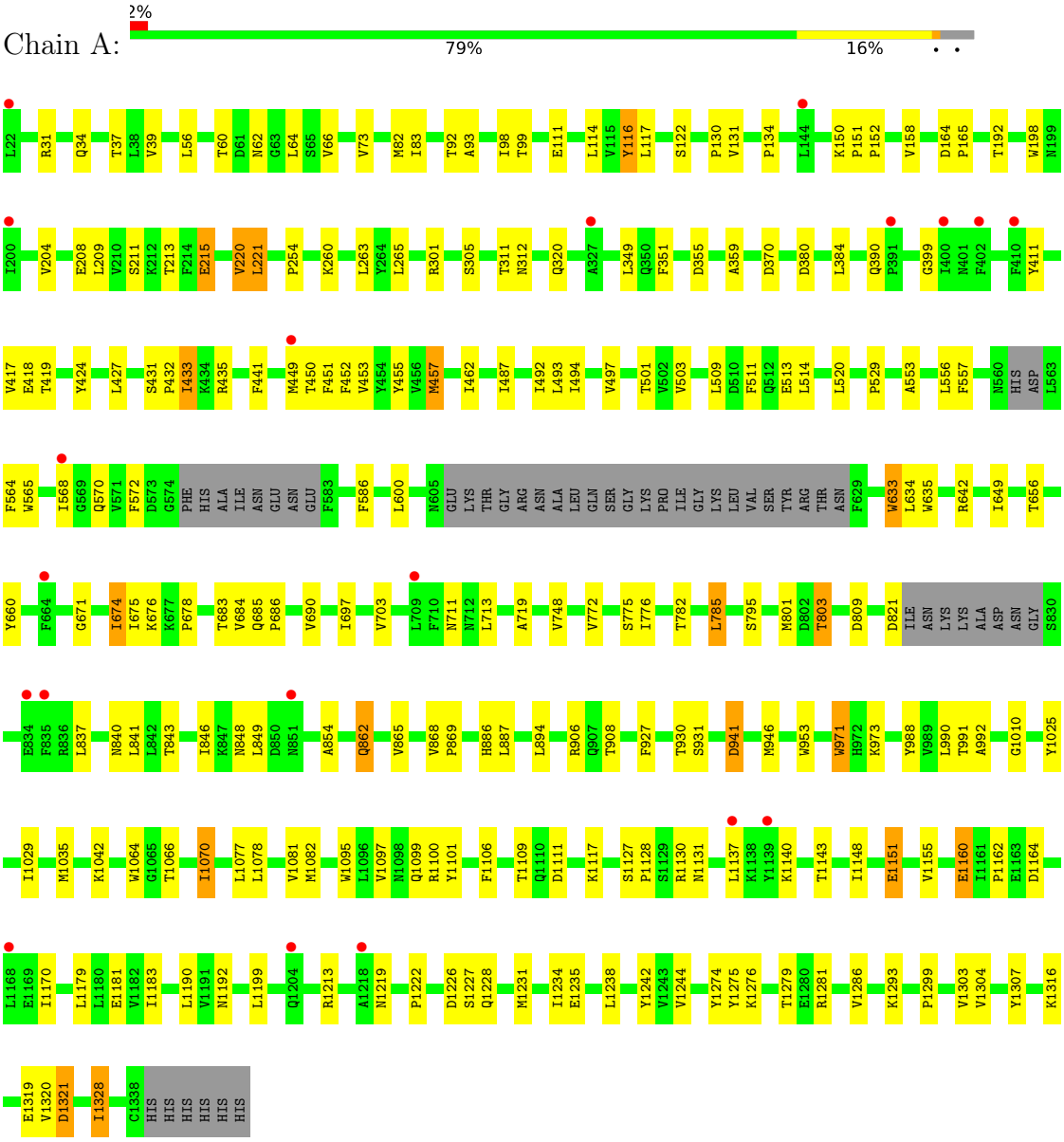
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0

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.

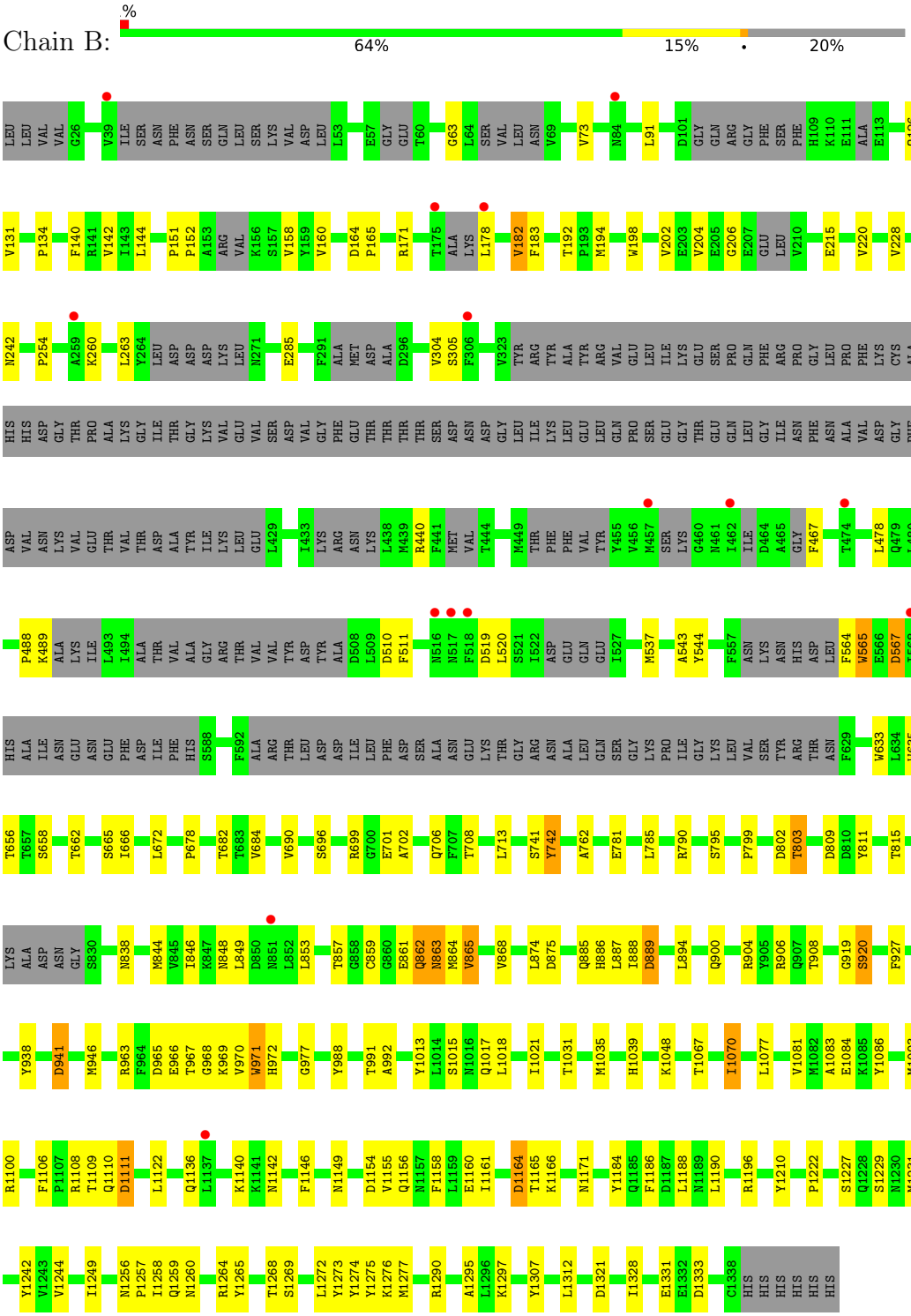
• Molecule 1: Thioester-containing protein I

Chain A:



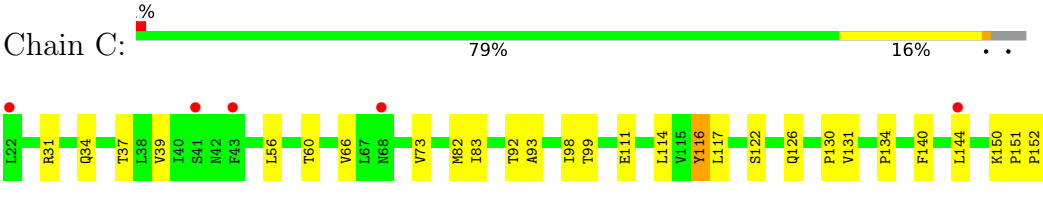
• Molecule 1: Thioester-containing protein I

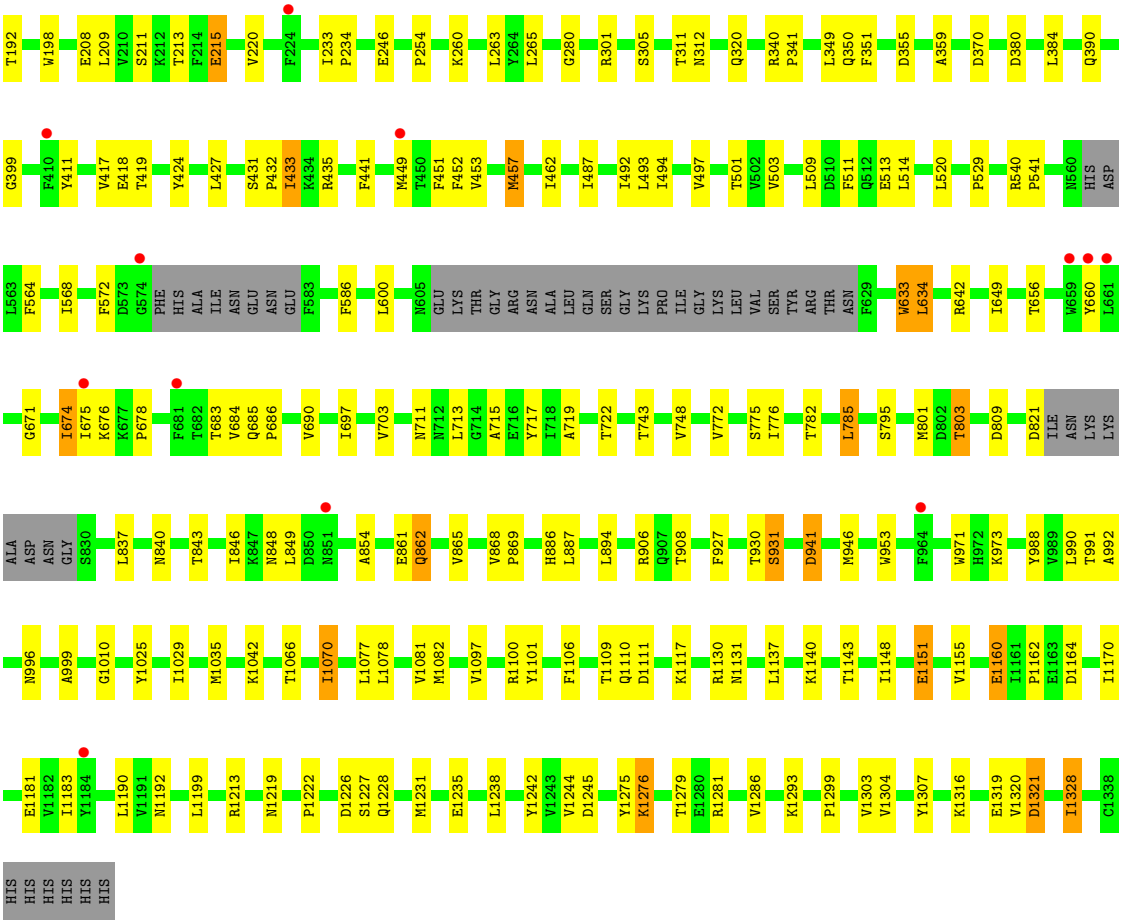
Chain B:



• Molecule 1: Thioester-containing protein I

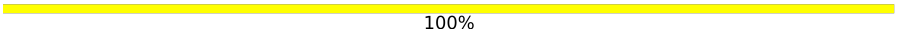
Chain C:





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	196.47Å 196.47Å 225.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 3.70 49.12 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.12-3.70) 99.7 (49.12-3.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.89	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.67Å)	Xtriage
Refinement program	REFMAC refmac_5.7.0025	Depositor
R, R_{free}	0.237 , 0.276 0.215 , 0.252	Depositor DCC
R_{free} test set	4584 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	147.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 111.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.196 for h,-k,-l	Xtriage
Reported twinning fraction	0.504 for H, K, L 0.496 for K, H, -L	Depositor
Outliers	2 of 90746 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27034	wwPDB-VP
Average B, all atoms (Å^2)	157.0	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 23.99 % 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 4.1834e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.41	6/9902 (0.1%)	0.53	0/13515
1	B	0.42	3/7592 (0.0%)	0.52	0/10410
1	C	0.40	2/9825 (0.0%)	0.52	0/13417
All	All	0.41	11/27319 (0.0%)	0.53	0/37342

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TRP	CD2-CE2	5.30	1.47	1.41
1	A	198	TRP	CD2-CE2	5.27	1.47	1.41
1	A	971	TRP	CD2-CE2	5.24	1.47	1.41
1	B	971	TRP	CD2-CE2	5.24	1.47	1.41
1	C	953	TRP	CD2-CE2	5.08	1.47	1.41
1	A	953	TRP	CD2-CE2	5.07	1.47	1.41
1	A	635	TRP	CD2-CE2	5.06	1.47	1.41
1	A	565	TRP	CD2-CE2	5.04	1.47	1.41
1	A	633	TRP	CD2-CE2	5.03	1.47	1.41
1	B	565	TRP	CD2-CE2	5.03	1.47	1.41
1	C	198	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1064	TRP	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	9704	0	9100	130	0
1	B	7461	0	6369	101	0
1	C	9631	0	8983	126	0
2	D	28	0	25	0	0
3	A	98	0	91	0	0
3	B	14	0	13	0	0
3	C	98	0	91	3	0
All	All	27034	0	24672	352	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 (352) 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)
3:C:1402:NAG:H4	3:C:1403:NAG:H5	1.59	0.84
1:A:62:ASN:HB3	1:B:970:VAL:HG23	1.63	0.79
1:C:862:GLN:HA	1:C:1109:THR:HG21	1.64	0.79
1:A:1100:ARG:HG2	1:A:1106:PHE:HE1	1.48	0.77
1:A:1100:ARG:HG2	1:A:1106:PHE:CE1	2.20	0.77
1:A:862:GLN:HA	1:A:1109:THR:HG21	1.66	0.76
1:C:1100:ARG:HG2	1:C:1106:PHE:CE1	2.23	0.74
1:A:568:ILE:HG12	1:A:674:ILE:HD11	1.69	0.74
1:C:1293:LYS:HB3	1:C:1328:ILE:HG12	1.69	0.74
1:C:1131:ASN:H	1:C:1151:GLU:HB3	1.52	0.74
1:A:1131:ASN:H	1:A:1151:GLU:HB3	1.53	0.73
1:A:1238:LEU:HD11	1:A:1244:VAL:HG13	1.68	0.73
1:A:971:TRP:HB2	1:A:1231:MET:HB2	1.71	0.73
1:A:1293:LYS:HB3	1:A:1328:ILE:HG12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:HE2	1:A:462:ILE:HG12	1.71	0.73
1:C:971:TRP:HB2	1:C:1231:MET:HB2	1.71	0.72
1:A:1070:ILE:HD12	1:A:1070:ILE:H	1.54	0.72
1:C:1238:LEU:HD11	1:C:1244:VAL:HG13	1.71	0.72
1:C:568:ILE:HG12	1:C:674:ILE:HD11	1.72	0.72
1:C:424:TYR:HA	1:C:503:VAL:HG11	1.72	0.72
1:C:131:VAL:HG12	1:C:215:GLU:HB3	1.72	0.71
1:C:1100:ARG:HG2	1:C:1106:PHE:HE1	1.53	0.71
1:C:457:MET:HE2	1:C:462:ILE:HG12	1.72	0.71
1:A:424:TYR:HA	1:A:503:VAL:HG11	1.72	0.70
1:B:1260:ASN:HB3	1:B:1273:TYR:HB2	1.71	0.70
1:A:131:VAL:HG12	1:A:215:GLU:HB3	1.75	0.69
1:A:927:PHE:O	1:A:931:SER:HB2	1.92	0.69
1:B:158:VAL:HG12	1:B:204:VAL:HG22	1.76	0.68
1:B:803:THR:HG21	1:B:1100:ARG:HH21	1.59	0.68
1:C:927:PHE:O	1:C:931:SER:HB2	1.93	0.67
1:B:853:LEU:HD11	1:B:865:VAL:HG11	1.75	0.67
1:C:1070:ILE:HD12	1:C:1070:ILE:H	1.61	0.66
1:A:435:ARG:HH11	1:A:514:LEU:HD11	1.61	0.66
1:C:435:ARG:HH11	1:C:514:LEU:HD11	1.61	0.66
1:A:351:PHE:HB3	1:A:359:ALA:HB3	1.76	0.65
1:A:795:SER:HA	1:A:1190:LEU:HD13	1.79	0.65
1:B:1210:TYR:HD1	1:B:1290:ARG:HD2	1.61	0.65
1:A:62:ASN:O	1:B:969:LYS:HA	1.96	0.65
1:A:930:THR:HG21	1:A:992:ALA:HB1	1.78	0.65
1:B:713:LEU:HD11	1:B:781:GLU:HG3	1.78	0.64
1:C:930:THR:HG21	1:C:992:ALA:HB1	1.78	0.64
1:B:171:ARG:HA	1:B:941:ASP:HB3	1.80	0.64
1:C:351:PHE:HB3	1:C:359:ALA:HB3	1.79	0.64
1:A:31:ARG:HB3	1:A:34:GLN:HB2	1.80	0.62
1:A:64:LEU:HD11	1:B:977:GLY:HA2	1.81	0.62
1:A:840:ASN:HB3	1:A:843:THR:HG23	1.80	0.62
1:A:553:ALA:O	1:A:556:LEU:HB2	2.00	0.62
1:B:857:THR:HG21	1:B:865:VAL:HG21	1.81	0.62
1:C:116:TYR:HD1	1:C:117:LEU:N	1.98	0.62
1:A:1035:MET:HB3	1:A:1082:MET:HG2	1.82	0.62
1:C:990:LEU:HD21	1:C:1010:GLY:HA3	1.82	0.62
1:B:128:ASP:HB3	1:B:635:TRP:CZ3	2.34	0.61
1:C:840:ASN:HB3	1:C:843:THR:HG23	1.81	0.61
1:C:31:ARG:HB3	1:C:34:GLN:HB2	1.81	0.60
1:B:838:ASN:ND2	1:B:844:MET:HG2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LEU:HD21	1:C:586:PHE:CE1	2.37	0.60
1:A:116:TYR:HD1	1:A:117:LEU:N	1.99	0.60
1:C:887:LEU:HD21	1:C:1155:VAL:HG23	1.84	0.60
1:A:887:LEU:HD21	1:A:1155:VAL:HG23	1.84	0.59
1:A:990:LEU:HD21	1:A:1010:GLY:HA3	1.83	0.59
1:B:658:SER:HA	1:B:682:THR:HA	1.84	0.59
1:B:861:GLU:OE2	1:B:1110:GLN:HG2	2.01	0.59
1:C:795:SER:HA	1:C:1190:LEU:HD13	1.83	0.59
1:A:862:GLN:HG2	1:A:1307:TYR:CZ	2.38	0.59
1:C:719:ALA:HB2	1:C:776:ILE:HG22	1.83	0.59
1:A:493:LEU:HD21	1:A:586:PHE:CE1	2.38	0.59
1:B:1070:ILE:HD12	1:B:1070:ILE:H	1.68	0.59
1:C:862:GLN:HG2	1:C:1307:TYR:CZ	2.37	0.59
1:C:837:LEU:HD21	1:C:1148:ILE:CD1	2.33	0.59
1:C:427:LEU:HD13	1:C:494:ILE:HD12	1.85	0.58
1:B:164:ASP:HB2	1:B:165:PRO:CD	2.32	0.58
1:C:1078:LEU:HD21	1:C:1117:LYS:HG2	1.86	0.57
1:B:846:ILE:HG21	1:B:887:LEU:HD22	1.85	0.57
1:B:1108:ARG:O	1:B:1111:ASP:HB2	2.04	0.57
1:C:1035:MET:HB3	1:C:1082:MET:HG2	1.86	0.57
1:C:399:GLY:HA2	1:C:411:TYR:HE1	1.69	0.57
1:B:142:VAL:HB	1:B:183:PHE:HB3	1.87	0.57
1:A:427:LEU:HD13	1:A:494:ILE:HD12	1.87	0.57
1:B:565:TRP:CD1	1:B:678:PRO:HG3	2.39	0.57
1:A:390:GLN:HE22	1:C:380:ASP:HA	1.69	0.57
1:B:164:ASP:HB2	1:B:165:PRO:HD2	1.87	0.57
1:A:837:LEU:HD21	1:A:1148:ILE:CD1	2.34	0.56
1:A:399:GLY:HA2	1:A:411:TYR:HE1	1.71	0.56
1:A:868:VAL:HG21	1:A:927:PHE:HZ	1.72	0.55
1:B:1238:LEU:HD11	1:B:1244:VAL:HG13	1.88	0.55
1:A:1078:LEU:HD21	1:A:1117:LYS:HG2	1.88	0.55
1:C:492:ILE:HB	1:C:509:LEU:HD11	1.87	0.55
1:A:868:VAL:HG21	1:A:927:PHE:CZ	2.42	0.55
1:B:666:ILE:HG12	1:B:672:LEU:HD12	1.89	0.54
1:A:1111:ASP:OD1	1:A:1111:ASP:N	2.40	0.54
1:A:719:ALA:HB2	1:A:776:ILE:HG22	1.89	0.54
1:C:868:VAL:HG21	1:C:927:PHE:HZ	1.72	0.54
1:B:254:PRO:HD2	1:B:690:VAL:HG11	1.89	0.54
1:B:795:SER:HA	1:B:1190:LEU:HD13	1.89	0.54
1:B:1239:PRO:HG2	1:B:1242:TYR:CD1	2.42	0.54
1:C:431:SER:HB2	1:C:432:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1242:TYR:OH	1:C:1320:VAL:HG11	2.08	0.54
1:A:656:THR:OG1	1:A:685:GLN:HG2	2.08	0.53
1:A:1242:TYR:OH	1:A:1320:VAL:HG11	2.07	0.53
1:C:656:THR:OG1	1:C:685:GLN:HG2	2.09	0.53
1:A:39:VAL:HG22	1:A:82:MET:HG2	1.90	0.53
1:C:846:ILE:HA	1:C:849:LEU:HG	1.89	0.53
1:A:431:SER:HB2	1:A:432:PRO:HD2	1.90	0.53
1:A:492:ILE:HB	1:A:509:LEU:HD11	1.88	0.53
1:C:868:VAL:HG21	1:C:927:PHE:CZ	2.43	0.53
1:A:803:THR:HB	1:A:1097:VAL:HG12	1.90	0.53
1:B:941:ASP:N	1:B:941:ASP:OD1	2.42	0.53
1:C:39:VAL:HG22	1:C:82:MET:HG2	1.90	0.53
1:A:93:ALA:HA	1:A:116:TYR:HD2	1.74	0.53
1:C:1100:ARG:HA	1:C:1106:PHE:HD1	1.74	0.53
1:A:1160:GLU:O	1:A:1162:PRO:HD3	2.10	0.52
1:A:98:ILE:CG1	1:A:114:LEU:HD11	2.40	0.52
1:C:98:ILE:CG1	1:C:114:LEU:HD11	2.39	0.52
1:C:803:THR:HB	1:C:1097:VAL:HG12	1.92	0.52
1:B:864:MET:HB3	1:B:868:VAL:HG23	1.91	0.52
1:A:349:LEU:O	1:A:384:LEU:HA	2.10	0.52
1:B:1222:PRO:HB3	1:B:1227:SER:HA	1.91	0.52
1:C:93:ALA:HA	1:C:116:TYR:HD2	1.75	0.52
1:A:390:GLN:NE2	1:C:380:ASP:HA	2.25	0.52
1:B:228:VAL:HG21	1:B:304:VAL:HG21	1.91	0.52
1:A:449:MET:CE	1:A:452:PHE:HB3	2.40	0.51
1:C:449:MET:CE	1:C:452:PHE:HB3	2.40	0.51
1:C:1111:ASP:OD1	1:C:1111:ASP:N	2.43	0.51
1:B:696:SER:HA	1:B:790:ARG:O	2.10	0.51
1:B:862:GLN:O	1:B:865:VAL:HG22	2.11	0.51
1:B:885:GLN:HA	1:B:888:ILE:HD12	1.93	0.51
1:C:1213:ARG:HA	1:C:1286:VAL:O	2.11	0.51
1:A:846:ILE:HA	1:A:849:LEU:HG	1.92	0.51
1:A:887:LEU:HD21	1:A:1155:VAL:CG2	2.41	0.51
1:B:182:VAL:HG22	1:B:666:ILE:HD12	1.93	0.51
1:A:1100:ARG:HA	1:A:1106:PHE:HD1	1.74	0.50
1:B:886:HIS:O	1:B:889:ASP:HB2	2.11	0.50
1:B:1265:TYR:O	1:B:1268:THR:HB	2.11	0.50
1:C:887:LEU:HD21	1:C:1155:VAL:CG2	2.42	0.50
1:C:1299:PRO:HB3	1:C:1319:GLU:HG2	1.94	0.50
1:B:1013:TYR:O	1:B:1017:GLN:HG3	2.12	0.50
1:C:1160:GLU:O	1:C:1162:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:GLN:HA	1:B:1109:THR:HG21	1.94	0.50
1:A:150:LYS:HA	1:A:671:GLY:HA2	1.94	0.50
1:B:544:TYR:O	1:B:665:SER:HA	2.11	0.50
1:A:1222:PRO:HB3	1:A:1227:SER:HA	1.93	0.50
1:B:702:ALA:HB3	1:B:1295:ALA:HB3	1.92	0.50
1:A:99:THR:HG23	1:A:111:GLU:HB3	1.94	0.50
1:C:433:ILE:HG22	1:C:511:PHE:HE1	1.76	0.50
3:C:1406:NAG:O7	3:C:1406:NAG:H3	2.11	0.50
1:B:701:GLU:HG2	1:B:1297:LYS:HA	1.94	0.50
1:A:451:PHE:HZ	1:A:497:VAL:HG23	1.77	0.49
1:A:433:ILE:HG22	1:A:511:PHE:HE1	1.77	0.49
1:B:699:ARG:HA	1:B:762:ALA:HB3	1.95	0.49
1:B:919:GLY:O	1:B:920:SER:C	2.50	0.49
1:A:1213:ARG:HA	1:A:1286:VAL:O	2.12	0.49
1:C:1199:LEU:HD22	1:C:1304:VAL:HG23	1.94	0.49
1:A:164:ASP:HB2	1:A:165:PRO:CD	2.42	0.49
1:B:489:LYS:HA	1:B:510:ASP:HA	1.93	0.49
1:C:164:ASP:HB2	1:C:165:PRO:CD	2.43	0.49
1:A:164:ASP:HB2	1:A:165:PRO:HD2	1.95	0.49
1:A:1299:PRO:HB3	1:A:1319:GLU:HG2	1.94	0.49
1:A:656:THR:HA	1:A:683:THR:O	2.13	0.49
1:B:126:GLN:O	1:B:140:PHE:HA	2.13	0.49
1:C:1222:PRO:HB3	1:C:1227:SER:HA	1.95	0.49
1:C:656:THR:HA	1:C:683:THR:O	2.13	0.49
1:A:854:ALA:HB2	1:A:1101:TYR:OH	2.13	0.49
1:C:37:THR:HA	1:C:83:ILE:O	2.13	0.48
1:C:99:THR:HG23	1:C:111:GLU:HB3	1.94	0.48
1:C:150:LYS:HA	1:C:671:GLY:HA2	1.95	0.48
1:B:741:SER:O	1:B:742:TYR:HB2	2.13	0.48
1:C:501:THR:HG22	1:C:600:LEU:HB2	1.95	0.48
1:A:501:THR:HG22	1:A:600:LEU:HB2	1.95	0.48
1:C:451:PHE:HZ	1:C:497:VAL:HG23	1.79	0.48
1:C:775:SER:HB3	1:C:782:THR:HG22	1.95	0.48
1:A:775:SER:HB3	1:A:782:THR:HG22	1.94	0.48
1:A:37:THR:HA	1:A:83:ILE:O	2.13	0.48
1:B:966:GLU:HG3	1:B:968:GLY:O	2.12	0.48
1:C:349:LEU:O	1:C:384:LEU:HA	2.14	0.48
1:B:144:LEU:HD12	1:B:178:LEU:HD11	1.96	0.48
1:B:543:ALA:HB3	1:B:640:ILE:HD12	1.96	0.48
1:B:1186:PHE:HB3	1:B:1188:LEU:HD21	1.95	0.48
1:A:772:VAL:HB	1:A:785:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:HA	1:A:1106:PHE:CD1	2.50	0.47
1:C:803:THR:HG23	1:C:1181:GLU:HG2	1.95	0.47
1:A:1219:ASN:HB3	1:A:1281:ARG:HA	1.97	0.47
1:C:164:ASP:HB2	1:C:165:PRO:HD2	1.97	0.47
1:A:906:ARG:CZ	1:A:946:MET:HG2	2.45	0.47
1:B:260:LYS:HB2	1:B:305:SER:HB2	1.96	0.47
1:A:660:TYR:CZ	1:A:678:PRO:HG2	2.50	0.47
1:A:660:TYR:OH	1:A:678:PRO:HG2	2.15	0.47
1:B:874:LEU:HB3	1:B:938:TYR:CE1	2.50	0.47
1:C:772:VAL:HB	1:C:785:LEU:HD12	1.97	0.46
1:C:837:LEU:HD21	1:C:1148:ILE:HD11	1.98	0.46
1:C:1100:ARG:HA	1:C:1106:PHE:CD1	2.50	0.46
1:B:927:PHE:O	1:B:931:SER:HB2	2.14	0.46
1:C:854:ALA:HB2	1:C:1101:TYR:OH	2.14	0.46
1:B:1077:LEU:HD11	1:B:1122:LEU:HD22	1.96	0.46
1:A:220:VAL:O	1:A:221:LEU:HB2	2.15	0.46
1:A:380:ASP:HA	1:C:390:GLN:HE22	1.80	0.46
1:C:1192:ASN:OD1	1:C:1316:LYS:HA	2.15	0.46
1:A:457:MET:SD	1:A:457:MET:N	2.89	0.46
1:A:1070:ILE:H	1:A:1070:ILE:CD1	2.16	0.46
1:A:1199:LEU:HD22	1:A:1304:VAL:HG23	1.98	0.46
1:A:656:THR:HG23	1:A:684:VAL:HA	1.98	0.46
1:B:160:VAL:HG22	1:B:202:VAL:HG22	1.98	0.45
1:A:941:ASP:OD1	1:A:941:ASP:N	2.50	0.45
1:B:1095:TRP:O	1:B:1099:GLN:HG2	2.16	0.45
1:A:801:MET:HG3	1:A:1183:ILE:HG12	1.99	0.45
1:C:311:THR:O	1:C:312:ASN:HB2	2.16	0.45
1:A:520:LEU:HB3	1:A:675:ILE:HG21	1.99	0.45
1:B:131:VAL:HA	1:B:215:GLU:O	2.17	0.45
1:C:846:ILE:C	1:C:848:ASN:H	2.20	0.45
1:A:1192:ASN:OD1	1:A:1316:LYS:HA	2.16	0.45
1:C:1137:LEU:HD12	1:C:1170:ILE:HG12	1.98	0.45
3:C:1402:NAG:O4	3:C:1403:NAG:N2	2.49	0.45
1:C:208:GLU:OE2	1:C:211:SER:HB2	2.17	0.45
1:A:803:THR:HG23	1:A:1181:GLU:HG2	1.97	0.45
1:A:846:ILE:C	1:A:848:ASN:H	2.19	0.45
1:A:862:GLN:O	1:A:865:VAL:HG22	2.17	0.45
1:B:1258:ILE:HD13	1:B:1272:LEU:HD13	1.98	0.45
1:C:449:MET:HE2	1:C:452:PHE:HB3	1.99	0.45
1:C:801:MET:HG3	1:C:1183:ILE:HG12	1.99	0.45
1:A:529:PRO:HB3	1:A:683:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LEU:HD21	1:A:1148:ILE:HD11	1.99	0.45
1:B:1013:TYR:O	1:B:1017:GLN:CG	2.65	0.45
1:C:417:VAL:O	1:C:419:THR:HG23	2.17	0.44
1:A:301:ARG:HD3	1:A:320:GLN:HE22	1.81	0.44
1:B:1106:PHE:HB3	1:B:1111:ASP:HB3	2.00	0.44
1:A:449:MET:HE2	1:A:452:PHE:HB3	1.98	0.44
1:B:1231:MET:O	1:B:1307:TYR:HB2	2.17	0.44
1:C:846:ILE:HG21	1:C:887:LEU:HD22	1.99	0.44
1:C:996:ASN:HB2	1:C:999:ALA:HB3	1.98	0.44
1:A:1077:LEU:O	1:A:1081:VAL:HG23	2.17	0.44
1:B:1015:SER:HB2	1:B:1039:HIS:CE1	2.53	0.44
1:A:1231:MET:O	1:A:1307:TYR:HB2	2.18	0.44
1:B:564:PHE:HA	1:B:567:ASP:OD2	2.18	0.44
1:C:520:LEU:HB3	1:C:675:ILE:HG21	2.00	0.44
1:C:686:PRO:HB3	1:C:713:LEU:HD21	2.00	0.44
1:B:930:THR:HG21	1:B:992:ALA:HB1	2.00	0.44
1:B:1196:ARG:HB2	1:B:1312:LEU:CD2	2.47	0.44
1:C:254:PRO:HD2	1:C:690:VAL:HG11	1.98	0.44
1:C:350:GLN:HA	1:C:384:LEU:HD23	2.00	0.44
1:C:427:LEU:HD11	1:C:441:PHE:CD2	2.53	0.44
1:A:433:ILE:HD13	1:A:509:LEU:HA	1.99	0.44
1:A:846:ILE:HG21	1:A:887:LEU:HD22	1.99	0.44
1:C:260:LYS:HB2	1:C:305:SER:HB2	2.00	0.44
1:C:1235:GLU:HB3	1:C:1303:VAL:HG12	2.00	0.44
1:A:427:LEU:HD11	1:A:441:PHE:CD2	2.53	0.44
1:B:233:ILE:HA	1:B:234:PRO:HD3	1.87	0.44
1:B:1161:ILE:HG23	1:B:1161:ILE:O	2.17	0.44
1:A:906:ARG:NH1	1:A:946:MET:HG2	2.33	0.43
1:A:973:LYS:NZ	1:A:1226:ASP:OD1	2.51	0.43
1:B:988:TYR:O	1:B:991:THR:HB	2.18	0.43
1:B:1021:ILE:O	1:B:1048:LYS:NZ	2.47	0.43
1:A:260:LYS:HB2	1:A:305:SER:HB2	2.00	0.43
1:B:1264:ARG:HG3	1:B:1269:SER:HB3	2.00	0.43
1:C:868:VAL:HB	1:C:869:PRO:HD3	2.00	0.43
1:C:1219:ASN:HB3	1:C:1281:ARG:HA	2.00	0.43
1:C:1077:LEU:O	1:C:1081:VAL:HG23	2.17	0.43
1:A:417:VAL:O	1:A:419:THR:HG23	2.18	0.43
1:C:529:PRO:HB3	1:C:683:THR:HB	2.00	0.43
1:A:487:ILE:HD13	1:A:511:PHE:CE2	2.53	0.43
1:B:656:THR:HG23	1:B:684:VAL:HA	2.00	0.43
1:C:862:GLN:O	1:C:865:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:PRO:HB3	1:A:713:LEU:HD21	2.00	0.43
1:A:868:VAL:HB	1:A:869:PRO:HD3	2.00	0.43
1:B:1184:TYR:CD1	1:B:1184:TYR:N	2.86	0.43
1:C:92:THR:HA	1:C:116:TYR:HE2	1.83	0.43
1:C:719:ALA:HB2	1:C:776:ILE:CG2	2.48	0.43
1:A:254:PRO:HD2	1:A:690:VAL:HG11	2.00	0.43
1:A:988:TYR:O	1:A:991:THR:HB	2.17	0.43
1:A:1222:PRO:CB	1:A:1227:SER:HA	2.48	0.43
1:C:656:THR:HG23	1:C:684:VAL:HA	1.99	0.43
1:A:92:THR:HA	1:A:116:TYR:HE2	1.82	0.43
1:B:488:PRO:HA	1:B:511:PHE:HB2	2.01	0.43
1:B:1257:PRO:HB2	1:B:1259:GLN:HE21	1.82	0.43
1:C:722:THR:HG23	1:C:743:THR:OG1	2.19	0.43
1:A:311:THR:O	1:A:312:ASN:HB2	2.19	0.43
1:A:1235:GLU:HB3	1:A:1303:VAL:HG12	2.00	0.43
1:B:969:LYS:H	1:B:969:LYS:HD2	1.84	0.43
1:C:60:THR:HG23	1:C:66:VAL:CG2	2.49	0.43
1:C:697:ILE:HG21	1:C:703:VAL:HG21	2.01	0.43
1:A:263:LEU:HD21	1:A:265:LEU:HG	2.00	0.43
1:B:848:ASN:O	1:B:849:LEU:C	2.58	0.43
1:C:973:LYS:NZ	1:C:1226:ASP:OD1	2.51	0.43
1:B:862:GLN:O	1:B:864:MET:N	2.52	0.42
1:C:1231:MET:O	1:C:1307:TYR:HB2	2.19	0.42
1:A:116:TYR:CD1	1:A:117:LEU:N	2.83	0.42
1:A:1137:LEU:HD12	1:A:1170:ILE:HG12	2.01	0.42
1:B:1259:GLN:HG3	1:B:1275:TYR:CD2	2.54	0.42
1:C:116:TYR:CD1	1:C:117:LEU:N	2.83	0.42
1:B:242:ASN:OD1	1:B:285:GLU:HG3	2.19	0.42
1:C:233:ILE:HA	1:C:234:PRO:HD3	1.85	0.42
1:C:660:TYR:CZ	1:C:678:PRO:HG2	2.54	0.42
1:A:122:SER:HA	1:A:209:LEU:HD11	2.01	0.42
1:B:1154:ASP:O	1:B:1156:GLN:N	2.47	0.42
1:C:660:TYR:OH	1:C:678:PRO:HG2	2.20	0.42
1:B:862:GLN:HB3	1:B:1109:THR:HG21	2.02	0.42
1:C:122:SER:HA	1:C:209:LEU:HD11	2.02	0.42
1:C:301:ARG:HD3	1:C:320:GLN:HE22	1.84	0.42
1:A:151:PRO:HA	1:A:152:PRO:HD3	1.92	0.42
1:C:711:ASN:HB3	1:C:748:VAL:HG12	2.01	0.42
1:C:906:ARG:CZ	1:C:946:MET:HG2	2.49	0.42
1:C:1320:VAL:CG1	1:C:1321:ASP:N	2.81	0.42
1:C:433:ILE:HD13	1:C:509:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:906:ARG:NH1	1:C:946:MET:HG2	2.35	0.42
1:C:1025:TYR:CE1	1:C:1029:ILE:HD11	2.55	0.41
1:B:1295:ALA:HB2	1:B:1328:ILE:HG13	2.01	0.41
1:C:941:ASP:OD1	1:C:941:ASP:N	2.51	0.41
1:C:1222:PRO:CB	1:C:1227:SER:HA	2.50	0.41
1:A:1228:GLN:HE22	1:B:63:GLY:C	2.23	0.41
1:B:1229:SER:OG	1:B:1277:MET:N	2.54	0.41
1:C:457:MET:SD	1:C:457:MET:N	2.93	0.41
1:A:158:VAL:HG12	1:A:204:VAL:HG22	2.01	0.41
1:A:841:LEU:HA	1:A:1179:LEU:HD11	2.02	0.41
1:A:1025:TYR:CE1	1:A:1029:ILE:HD11	2.55	0.41
1:A:1127:SER:HA	1:A:1128:PRO:HD3	1.91	0.41
1:B:1031:THR:O	1:B:1035:MET:HG2	2.21	0.41
1:C:340:ARG:HA	1:C:341:PRO:HD3	1.89	0.41
1:A:60:THR:HG23	1:A:66:VAL:CG2	2.50	0.41
1:A:1320:VAL:CG1	1:A:1321:ASP:N	2.83	0.41
1:C:540:ARG:HA	1:C:541:PRO:HD2	1.93	0.41
1:A:697:ILE:HG21	1:A:703:VAL:HG21	2.02	0.41
1:B:862:GLN:HG2	1:B:1307:TYR:CZ	2.55	0.41
1:B:1258:ILE:HG12	1:B:1274:TYR:CZ	2.55	0.41
1:C:151:PRO:HA	1:C:152:PRO:HD3	1.91	0.41
1:C:246:GLU:HA	1:C:280:GLY:O	2.20	0.41
1:C:263:LEU:HD21	1:C:265:LEU:HG	2.02	0.41
1:C:861:GLU:OE2	1:C:1110:GLN:HG2	2.21	0.41
1:A:208:GLU:OE2	1:A:211:SER:HB2	2.21	0.41
1:B:151:PRO:HA	1:B:152:PRO:HD3	1.92	0.41
1:B:971:TRP:HB2	1:B:1231:MET:HB2	2.02	0.41
1:C:988:TYR:O	1:C:991:THR:HB	2.20	0.41
1:A:455:TYR:HB3	1:A:457:MET:HE3	2.02	0.41
1:A:1070:ILE:HD12	1:A:1070:ILE:N	2.30	0.41
1:B:440:ARG:HA	1:B:478:LEU:O	2.20	0.41
1:B:1146:PHE:CE2	1:B:1158:PHE:HB3	2.56	0.41
1:A:1095:TRP:O	1:A:1099:GLN:HG2	2.20	0.41
1:A:1100:ARG:CG	1:A:1106:PHE:HE1	2.24	0.41
1:A:1131:ASN:N	1:A:1151:GLU:HB3	2.30	0.41
1:B:194:MET:HE3	1:B:904:ARG:HA	2.03	0.40
1:B:1256:ASN:HA	1:B:1257:PRO:HD3	1.84	0.40
1:C:633:TRP:CD1	1:C:634:LEU:N	2.89	0.40
1:A:711:ASN:HB3	1:A:748:VAL:HG12	2.02	0.40
1:B:1136:GLN:HB3	1:B:1171:ASN:HB2	2.02	0.40
1:C:1228:GLN:CD	1:C:1276:LYS:HD3	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:THR:HG22	1:B:678:PRO:HB3	2.03	0.40
1:C:126:GLN:O	1:C:140:PHE:HA	2.22	0.40
1:B:906:ARG:NH1	1:B:946:MET:HG2	2.37	0.40
1:B:1083:ALA:O	1:B:1084:GLU:HB2	2.21	0.40
1:B:1093:MET:HB2	1:B:1122:LEU:HD23	2.02	0.40
1:C:715:ALA:HB3	1:C:717:TYR:CZ	2.57	0.40
1:A:380:ASP:HA	1:C:390:GLN:NE2	2.36	0.40
1:A:1234:ILE:HD12	1:A:1274:TYR:HE2	1.86	0.40
1:B:520:LEU:HA	1:B:537:MET:HA	2.04	0.40
1:B:1081:VAL:HG13	1:B:1086:TYR:HE1	1.86	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	1266/1323 (96%)	1154 (91%)	101 (8%)	11 (1%)	17	54
1	B	1011/1323 (76%)	898 (89%)	94 (9%)	19 (2%)	8	40
1	C	1266/1323 (96%)	1157 (91%)	97 (8%)	12 (1%)	17	54
All	All	3543/3969 (89%)	3209 (91%)	292 (8%)	42 (1%)	13	48

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	642	ARG
1	A	1160	GLU
1	C	642	ARG
1	C	1160	GLU
1	A	418	GLU
1	A	676	LYS
1	A	1140	LYS

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Mol	Chain	Res	Type
1	A	1164	ASP
1	A	1321	ASP
1	B	73	VAL
1	B	91	LEU
1	B	742	TYR
1	B	811	TYR
1	B	863	ASN
1	B	920	SER
1	B	1140	LYS
1	B	1160	GLU
1	B	1164	ASP
1	B	1321	ASP
1	B	1331	GLU
1	C	418	GLU
1	C	676	LYS
1	C	1140	LYS
1	C	1164	ASP
1	C	1321	ASP
1	B	1155	VAL
1	A	355	ASP
1	B	220	VAL
1	B	1018	LEU
1	B	1166	LYS
1	C	355	ASP
1	B	134	PRO
1	C	1245	ASP
1	B	206	GLY
1	C	134	PRO
1	A	130	PRO
1	A	220	VAL
1	C	220	VAL
1	A	134	PRO
1	C	130	PRO
1	B	799	PRO
1	B	130	PRO

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	997/1177 (85%)	957 (96%)	40 (4%)	31	60
1	B	670/1177 (57%)	627 (94%)	43 (6%)	17	48
1	C	979/1177 (83%)	940 (96%)	39 (4%)	31	60
All	All	2646/3531 (75%)	2524 (95%)	122 (5%)	27	57

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	73	VAL
1	A	116	TYR
1	A	192	THR
1	A	213	THR
1	A	215	GLU
1	A	221	LEU
1	A	370	ASP
1	A	433	ILE
1	A	450	THR
1	A	453	VAL
1	A	457	MET
1	A	513	GLU
1	A	557	PHE
1	A	564	PHE
1	A	570	GLN
1	A	572	PHE
1	A	633	TRP
1	A	634	LEU
1	A	649	ILE
1	A	674	ILE
1	A	785	LEU
1	A	803	THR
1	A	809	ASP
1	A	821	ASP
1	A	862	GLN
1	A	886	HIS
1	A	894	LEU
1	A	908	THR
1	A	941	ASP
1	A	1042	LYS
1	A	1066	THR

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Mol	Chain	Res	Type
1	A	1070	ILE
1	A	1130	ARG
1	A	1143	THR
1	A	1151	GLU
1	A	1275	TYR
1	A	1276	LYS
1	A	1279	THR
1	A	1328	ILE
1	B	182	VAL
1	B	192	THR
1	B	263	LEU
1	B	467	PHE
1	B	519	ASP
1	B	567	ASP
1	B	633	TRP
1	B	640	ILE
1	B	655	THR
1	B	706	GLN
1	B	708	THR
1	B	785	LEU
1	B	802	ASP
1	B	803	THR
1	B	809	ASP
1	B	815	THR
1	B	859	CYS
1	B	862	GLN
1	B	863	ASN
1	B	865	VAL
1	B	875	ASP
1	B	889	ASP
1	B	894	LEU
1	B	900	GLN
1	B	908	THR
1	B	931	SER
1	B	934	THR
1	B	941	ASP
1	B	963	ARG
1	B	965	ASP
1	B	967	THR
1	B	972	HIS
1	B	1067	THR
1	B	1070	ILE

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Mol	Chain	Res	Type
1	B	1111	ASP
1	B	1142	ASN
1	B	1149	ASN
1	B	1164	ASP
1	B	1165	THR
1	B	1237	THR
1	B	1249	ILE
1	B	1276	LYS
1	B	1333	ASP
1	C	56	LEU
1	C	73	VAL
1	C	116	TYR
1	C	144	LEU
1	C	192	THR
1	C	213	THR
1	C	215	GLU
1	C	370	ASP
1	C	433	ILE
1	C	453	VAL
1	C	457	MET
1	C	487	ILE
1	C	513	GLU
1	C	564	PHE
1	C	572	PHE
1	C	633	TRP
1	C	634	LEU
1	C	649	ILE
1	C	674	ILE
1	C	785	LEU
1	C	803	THR
1	C	809	ASP
1	C	821	ASP
1	C	862	GLN
1	C	886	HIS
1	C	894	LEU
1	C	908	THR
1	C	931	SER
1	C	941	ASP
1	C	1042	LYS
1	C	1066	THR
1	C	1070	ILE
1	C	1130	ARG

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Mol	Chain	Res	Type
1	C	1143	THR
1	C	1151	GLU
1	C	1275	TYR
1	C	1276	LYS
1	C	1279	THR
1	C	1328	ILE

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

Mol	Chain	Res	Type
1	A	271	ASN
1	A	283	GLN
1	A	320	GLN
1	A	390	GLN
1	A	1136	GLN
1	A	1171	ASN
1	A	1228	GLN
1	A	1324	ASN
1	B	1039	HIS
1	B	1098	ASN
1	B	1256	ASN
1	B	1259	GLN
1	C	271	ASN
1	C	283	GLN
1	C	320	GLN
1	C	1136	GLN
1	C	1171	ASN
1	C	1324	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

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.71	0	17,19,21	1.83	4 (23%)
2	NAG	D	2	2	14,14,15	0.45	0	17,19,21	0.95	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C2-N2-C7	4.53	129.35	122.90
2	D	1	NAG	O5-C1-C2	-3.26	106.13	111.29
2	D	1	NAG	C4-C3-C2	3.03	115.46	111.02
2	D	1	NAG	C3-C4-C5	2.44	114.59	110.24
2	D	2	NAG	C1-O5-C5	2.43	115.48	112.19

There are no chirality outliers.

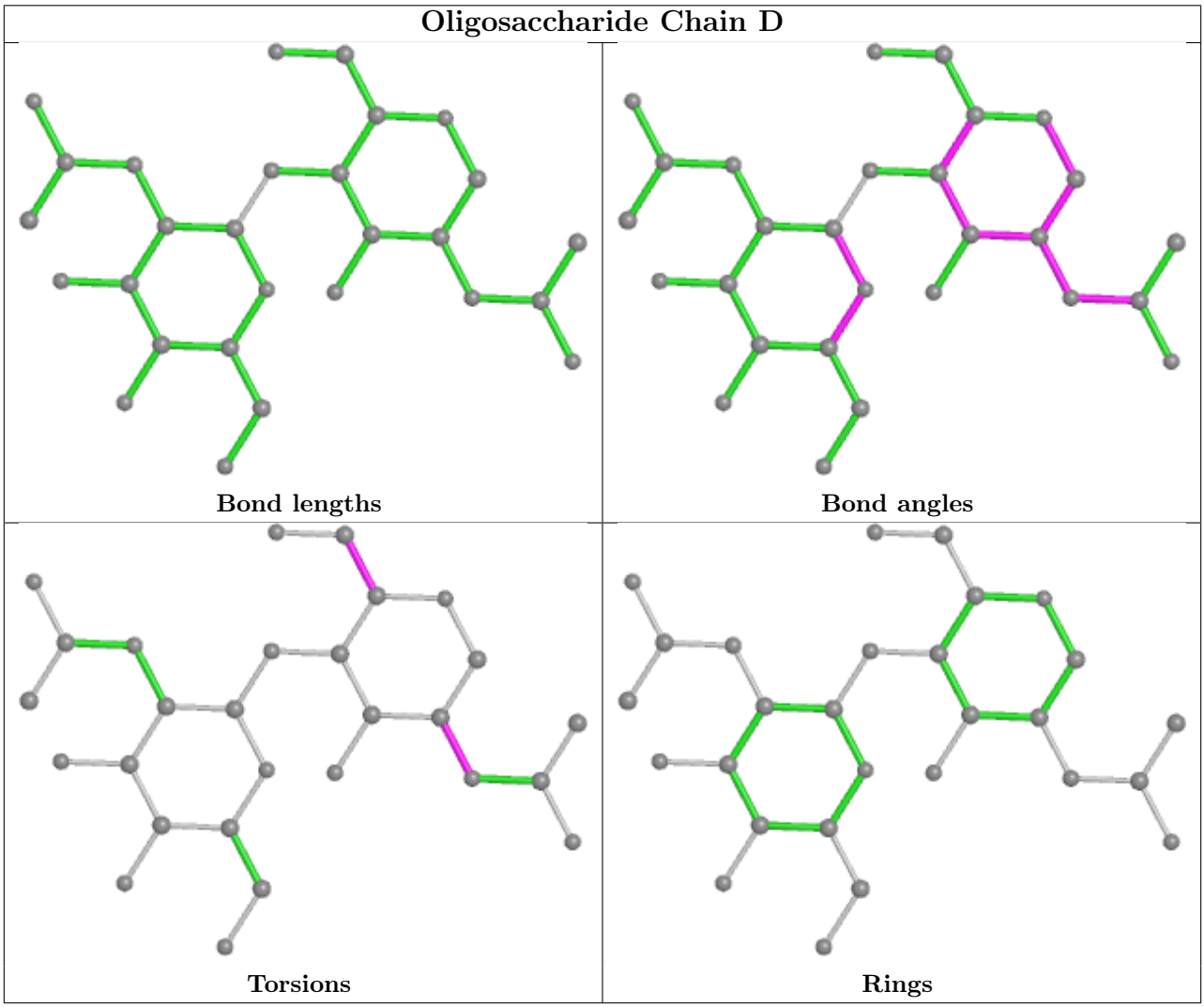
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7

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.



5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1406	1	14,14,15	0.29	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	2002	1	14,14,15	0.50	0	17,19,21	0.87	0
3	NAG	C	1404	1	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
3	NAG	B	1401	1	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
3	NAG	C	1407	1	14,14,15	0.59	0	17,19,21	1.36	3 (17%)
3	NAG	A	2009	1	14,14,15	0.80	1 (7%)	17,19,21	1.65	4 (23%)
3	NAG	C	1401	1	14,14,15	0.51	0	17,19,21	1.16	1 (5%)
3	NAG	C	1403	-	14,14,15	0.48	0	17,19,21	1.63	4 (23%)
3	NAG	C	1402	1	14,14,15	0.49	0	17,19,21	0.69	0
3	NAG	C	1405	1	14,14,15	0.49	0	17,19,21	1.13	1 (5%)
3	NAG	A	2001	1	14,14,15	0.53	0	17,19,21	1.12	1 (5%)
3	NAG	A	2004	-	14,14,15	0.45	0	17,19,21	0.90	1 (5%)
3	NAG	A	2003	1	14,14,15	0.48	0	17,19,21	0.87	0
3	NAG	A	2005	1	14,14,15	0.62	0	17,19,21	2.28	5 (29%)
3	NAG	A	2008	1	14,14,15	0.43	0	17,19,21	2.54	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1406	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2009	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1403	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2004	-	-	1/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2005	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2008	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2009	NAG	C1-C2	2.20	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2008	NAG	C1-O5-C5	9.60	125.20	112.19
3	A	2005	NAG	C1-O5-C5	6.21	120.61	112.19
3	A	2009	NAG	C4-C3-C2	4.56	117.70	111.02
3	A	2005	NAG	C2-N2-C7	4.47	129.27	122.90
3	C	1403	NAG	C1-O5-C5	4.12	117.77	112.19
3	C	1405	NAG	C1-O5-C5	3.45	116.87	112.19
3	C	1407	NAG	C4-C3-C2	3.44	116.06	111.02
3	A	2001	NAG	O5-C5-C6	3.35	112.46	107.20
3	C	1401	NAG	C1-O5-C5	3.26	116.60	112.19
3	A	2005	NAG	O5-C1-C2	2.85	115.79	111.29
3	A	2009	NAG	C1-O5-C5	2.75	115.91	112.19
3	B	1401	NAG	C1-O5-C5	2.72	115.87	112.19
3	C	1403	NAG	C3-C4-C5	2.71	115.07	110.24
3	A	2004	NAG	C1-O5-C5	2.67	115.81	112.19
3	C	1403	NAG	C4-C3-C2	2.60	114.83	111.02
3	C	1407	NAG	C1-O5-C5	2.42	115.47	112.19
3	C	1404	NAG	C1-O5-C5	2.40	115.44	112.19
3	A	2008	NAG	C4-C3-C2	-2.34	107.59	111.02
3	A	2008	NAG	O5-C5-C4	2.29	116.40	110.83
3	A	2005	NAG	C1-C2-N2	2.15	114.17	110.49
3	A	2005	NAG	O7-C7-N2	2.11	125.83	121.95
3	A	2009	NAG	C2-N2-C7	2.04	125.80	122.90
3	C	1407	NAG	C3-C4-C5	2.02	113.84	110.24
3	A	2009	NAG	O5-C5-C6	2.02	110.36	107.20
3	C	1403	NAG	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1401	NAG	C4-C5-C6-O6
3	B	1401	NAG	O5-C5-C6-O6
3	C	1402	NAG	C4-C5-C6-O6
3	A	2005	NAG	O5-C5-C6-O6
3	A	2008	NAG	O5-C5-C6-O6
3	A	2001	NAG	O5-C5-C6-O6
3	C	1405	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1407	NAG	O5-C5-C6-O6
3	C	1406	NAG	C4-C5-C6-O6
3	C	1402	NAG	O5-C5-C6-O6
3	C	1406	NAG	O5-C5-C6-O6
3	C	1403	NAG	O5-C5-C6-O6
3	A	2001	NAG	C4-C5-C6-O6
3	A	2005	NAG	C1-C2-N2-C7
3	C	1403	NAG	C4-C5-C6-O6
3	A	2008	NAG	C4-C5-C6-O6
3	A	2005	NAG	C4-C5-C6-O6
3	A	2009	NAG	C4-C5-C6-O6
3	A	2003	NAG	O5-C5-C6-O6
3	A	2004	NAG	O5-C5-C6-O6
3	C	1405	NAG	C4-C5-C6-O6
3	C	1407	NAG	C4-C5-C6-O6
3	A	2009	NAG	O5-C5-C6-O6
3	A	2002	NAG	C4-C5-C6-O6
3	C	1406	NAG	C3-C2-N2-C7
3	A	2002	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1406	NAG	1	0
3	C	1403	NAG	2	0
3	C	1402	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	1276/1323 (96%)	0.07	20 (1%)	72	61	113, 151, 175, 200	0
1	B	1063/1323 (80%)	0.04	17 (1%)	72	61	125, 165, 200, 200	0
1	C	1276/1323 (96%)	0.01	17 (1%)	77	67	123, 160, 191, 200	0
All	All	3615/3969 (91%)	0.04	54 (1%)	73	63	113, 157, 194, 200	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	PRO	3.0
1	C	660	TYR	3.0
1	A	410	PHE	2.9
1	B	84	ASN	2.8
1	B	241	VAL	2.8
1	B	457	MET	2.7
1	A	144	LEU	2.7
1	B	39	VAL	2.7
1	B	259	ALA	2.7
1	A	851	ASN	2.6
1	A	834	GLU	2.6
1	C	144	LEU	2.6
1	B	474	THR	2.5
1	A	1139	TYR	2.5
1	B	516	ASN	2.5
1	C	22	LEU	2.4
1	B	462	ILE	2.4
1	B	178	LEU	2.4
1	C	410	PHE	2.3
1	A	449	MET	2.3
1	A	22	LEU	2.3
1	C	851	ASN	2.3
1	A	835	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	306	PHE	2.3
1	C	661	LEU	2.2
1	C	41	SER	2.2
1	A	568	ILE	2.2
1	A	400	ILE	2.2
1	C	964	PHE	2.2
1	A	200	ILE	2.2
1	C	681	PHE	2.2
1	A	391	PRO	2.1
1	B	568	ILE	2.1
1	A	709	LEU	2.1
1	B	1137	LEU	2.1
1	B	851	ASN	2.1
1	A	1137	LEU	2.1
1	A	402	PHE	2.1
1	B	517	ASN	2.1
1	C	224	PHE	2.1
1	C	1184	TYR	2.1
1	C	68	ASN	2.1
1	B	518	PHE	2.1
1	A	1204	GLN	2.1
1	C	574	GLY	2.1
1	C	675	ILE	2.1
1	C	43	PHE	2.1
1	C	659	TRP	2.0
1	A	1218	ALA	2.0
1	B	175	THR	2.0
1	A	327	ALA	2.0
1	A	1168	LEU	2.0
1	C	449	MET	2.0
1	A	664	PHE	2.0

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

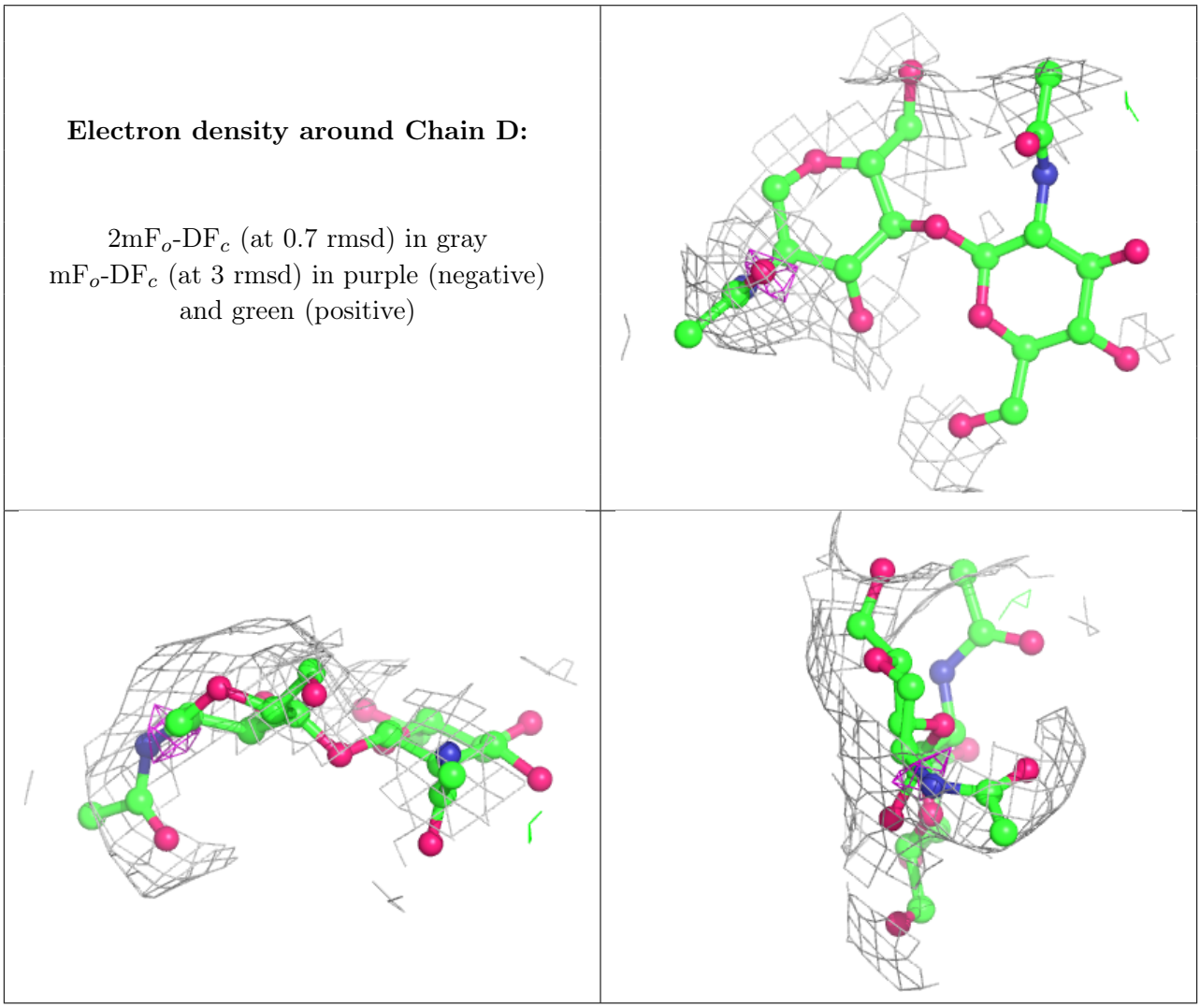
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
2	NAG	D	1	14/15	0.87	0.28	167,168,169,170	0
2	NAG	D	2	14/15	0.92	0.12	169,171,172,173	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.



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
3	NAG	C	1401	14/15	0.76	0.26	166,167,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	2008	14/15	0.78	0.27	152,152,152,153	0
3	NAG	C	1407	14/15	0.79	0.24	168,169,169,169	0
3	NAG	A	2005	14/15	0.80	0.22	170,172,173,173	0
3	NAG	A	2009	14/15	0.81	0.22	166,168,168,168	0
3	NAG	B	1401	14/15	0.81	0.14	175,176,176,176	0
3	NAG	C	1406	14/15	0.82	0.22	174,175,176,176	0
3	NAG	C	1404	14/15	0.84	0.18	173,174,175,175	0
3	NAG	C	1405	14/15	0.84	0.16	162,163,163,164	0
3	NAG	A	2002	14/15	0.84	0.20	156,157,158,158	0
3	NAG	A	2001	14/15	0.84	0.20	165,168,168,169	0
3	NAG	A	2003	14/15	0.86	0.15	160,160,161,162	0
3	NAG	A	2004	14/15	0.87	0.13	177,177,178,178	0
3	NAG	C	1403	14/15	0.90	0.13	183,185,185,185	0
3	NAG	C	1402	14/15	0.91	0.14	166,166,167,168	0

6.5 Other polymers (i)

There are no such residues in this entry.