Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 04:28 AM EDT

PDB ID	:	1JMO
Title	:	Crystal Structure of the Heparin Cofactor II-S195A Thrombin Complex
Authors	:	Baglin, T.P.; Carrell, R.W.; Esmon, C.T.; Huntington, J.A.
Deposited on	:	2001-07-19
Resolution	:	2.20 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

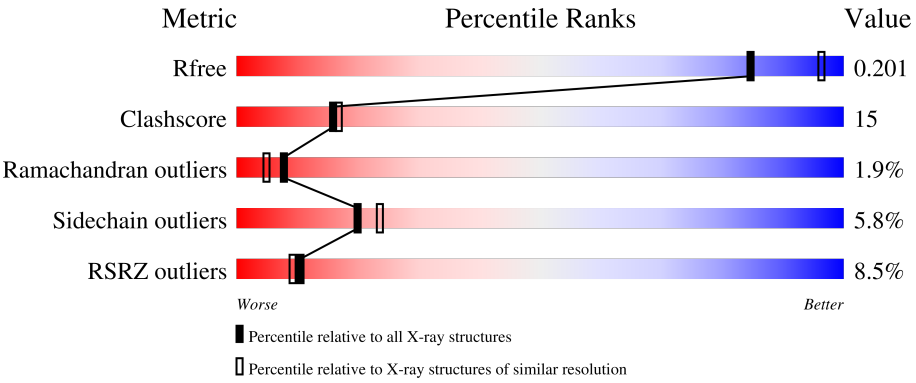
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	L	48	8% 79% 15%
2	H	260	7% 77% 21%
3	A	480	8% 58% 25% 6% 11%
4	B	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1	X	-	-	X
4	NAG	B	2	-	-	-	X
6	MPD	H	2004	-	-	-	X
7	NAG	A	481	-	-	-	X
7	NAG	A	482	X	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6235 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 Thrombin, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	47	378	237	61	79	1	0	0	0

- Molecule 2 is a protein called Thrombin, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	259	2092	1334	370	374	14	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	195	ALA	SER	engineered mutation	UNP P00734

- Molecule 3 is a protein called HEPARIN COFACTOR II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	427	3460	2203	591	644	22	81	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	TYS	TYR	modified residue	UNP P05546
A	73	TYS	TYR	modified residue	UNP P05546

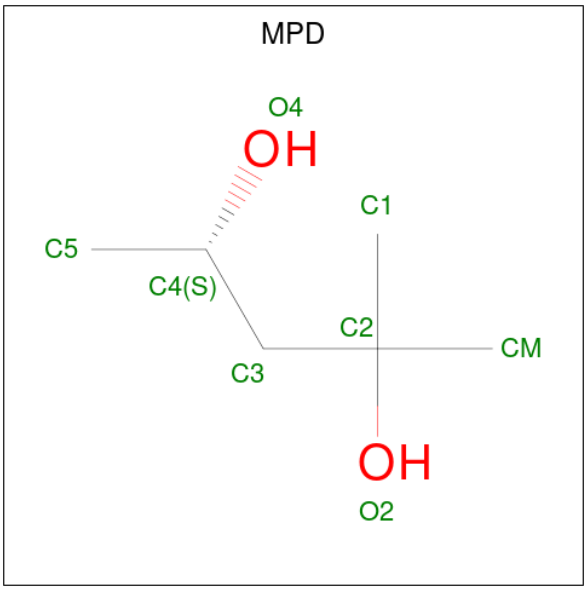
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

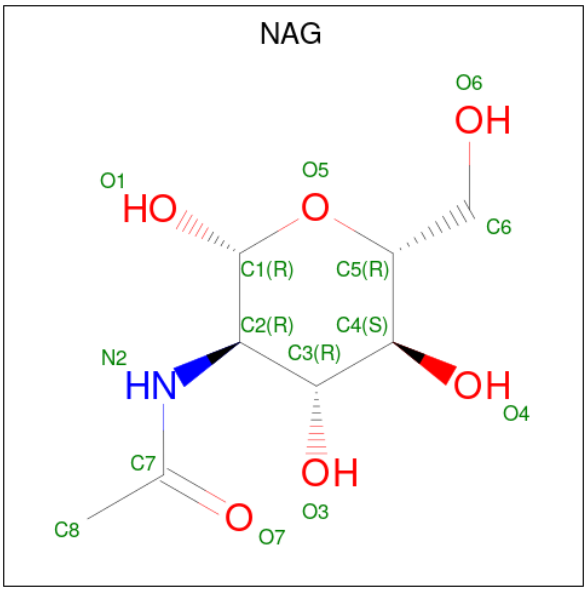
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Na 1 1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 8 6 2	0	0
6	H	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

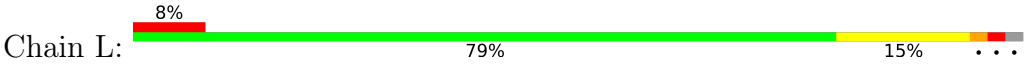
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	39	Total O 39 39	0	0
8	H	83	Total O 83 83	0	0
8	A	86	Total O 86 86	0	0

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.

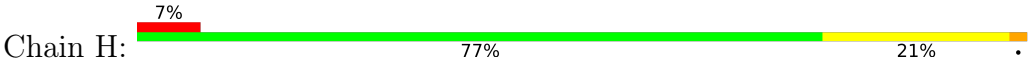
• Molecule 1: Thrombin, light chain

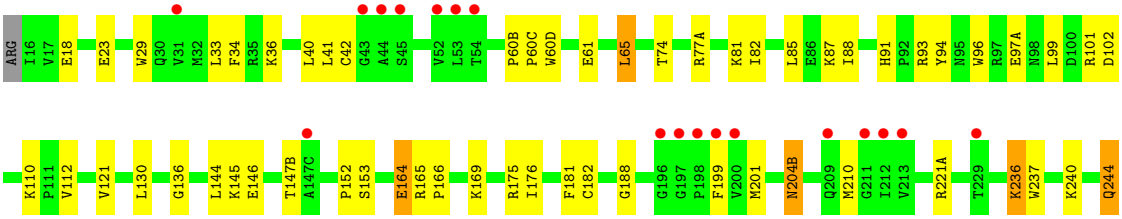
Chain L:



• Molecule 2: Thrombin, heavy chain

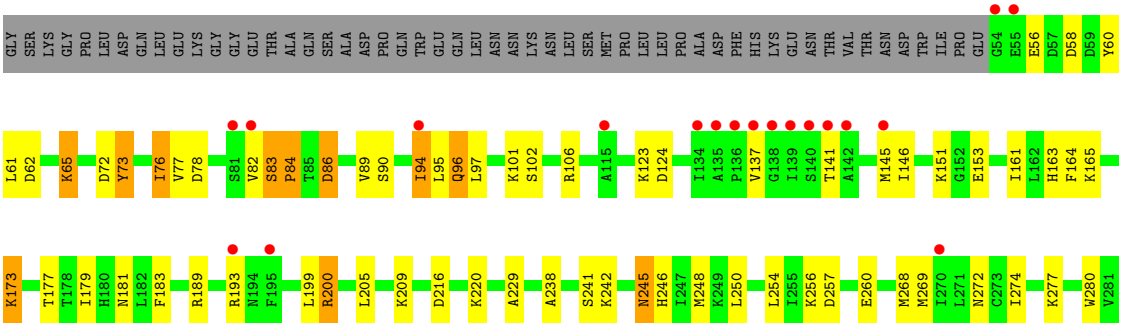
Chain H:

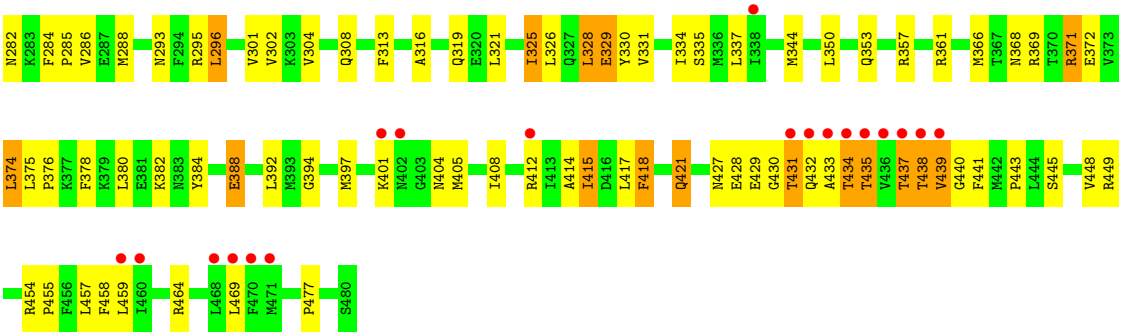




• Molecule 3: HEPARIN COFACTOR II

Chain A:





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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	152.31Å 152.31Å 126.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.44 – 2.20 29.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.44-2.20) 91.2 (29.43-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.211 0.189 , 0.201	Depositor DCC
R_{free} test set	983 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: MPD, TYS, NAG, NA

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	L	0.40	0/385	0.77	1/516 (0.2%)
2	H	0.35	0/2147	0.65	0/2902
3	A	0.34	0/3491	0.63	1/4704 (0.0%)
All	All	0.35	0/6023	0.64	2/8122 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	14(L)	ASP	N-CA-C	7.17	130.36	111.00
3	A	229	ALA	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	378	0	356	6	0
2	H	2092	0	2063	43	0
3	A	3460	0	3464	132	0
4	B	28	0	25	1	0
5	H	1	0	0	0	0
6	A	24	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	16	0	28	4	0
7	A	28	0	26	6	0
8	A	86	0	0	5	0
8	H	83	0	0	1	0
8	L	39	0	0	0	0
All	All	6235	0	6004	173	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 15.

All (173) 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:A:96:GLN:HE21	3:A:357:ARG:HH22	1.03	0.99
2:H:61:GLU:HG2	2:H:87:LYS:HA	1.51	0.92
2:H:181:PHE:HA	6:H:2003:MPD:H53	1.52	0.89
3:A:96:GLN:HE21	3:A:357:ARG:NH2	1.75	0.84
3:A:151:LYS:HB2	3:A:404:ASN:ND2	1.93	0.83
4:B:1:NAG:H62	4:B:2:NAG:O5	1.83	0.79
3:A:448:VAL:HG12	8:A:2057:HOH:O	1.84	0.78
3:A:439:VAL:HG12	3:A:440:GLY:H	1.52	0.75
1:L:14(A):LYS:HG3	2:H:23:GLU:OE2	1.87	0.75
3:A:321:LEU:HD22	3:A:353:GLN:NE2	2.01	0.75
3:A:372:GLU:HB2	3:A:449:ARG:HG2	1.70	0.74
1:L:14(J):TYR:O	1:L:14(L):ASP:N	2.21	0.73
3:A:325:ILE:HD13	3:A:326:LEU:N	2.03	0.73
3:A:76:ILE:HD13	3:A:77:VAL:N	2.03	0.73
3:A:368:ASN:HB2	7:A:482:NAG:HN2	1.54	0.72
2:H:77(A):ARG:HG3	2:H:77(A):ARG:HH11	1.55	0.71
3:A:448:VAL:HG11	8:A:2072:HOH:O	1.92	0.70
3:A:151:LYS:HB2	3:A:404:ASN:HD21	1.58	0.69
3:A:248:MET:SD	3:A:256:LYS:HB3	2.33	0.69
3:A:325:ILE:HD11	3:A:337:LEU:CD1	2.23	0.68
3:A:439:VAL:HG12	3:A:440:GLY:N	2.09	0.67
2:H:61:GLU:CG	2:H:87:LYS:HA	2.25	0.66
3:A:401:LYS:HG2	3:A:414:ALA:HB2	1.77	0.66
2:H:81:LYS:HG2	2:H:112:VAL:HG23	1.80	0.64
1:L:1(T):ALA:O	1:L:1(Q):GLU:HG2	1.98	0.64
3:A:137:VAL:O	3:A:141:THR:HG23	1.97	0.64
3:A:96:GLN:NE2	3:A:357:ARG:HH22	1.87	0.64
2:H:85:LEU:HD13	2:H:88:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:295:ARG:HG2	3:A:344:MET:CE	2.28	0.63
3:A:368:ASN:CB	7:A:482:NAG:HN2	2.12	0.63
3:A:454:ARG:HH11	3:A:454:ARG:HG3	1.64	0.63
3:A:268:MET:HE2	3:A:415:ILE:HB	1.82	0.61
3:A:62:ASP:OD2	3:A:65:LYS:HB2	2.01	0.61
3:A:329:GLU:OE2	3:A:335:SER:HB3	2.00	0.60
3:A:293:ASN:HB3	3:A:301:VAL:HG21	1.83	0.60
2:H:42:CYS:SG	3:A:445:SER:HB2	2.42	0.60
3:A:200:ARG:HH11	3:A:200:ARG:HG3	1.66	0.59
3:A:308:GLN:HG3	3:A:374:LEU:HD22	1.82	0.59
3:A:295:ARG:O	3:A:455:PRO:HD3	2.03	0.59
3:A:153:GLU:HB3	3:A:397:MET:SD	2.42	0.59
3:A:325:ILE:HD11	3:A:337:LEU:HD11	1.84	0.58
3:A:321:LEU:HD22	3:A:353:GLN:HE21	1.68	0.58
2:H:97(A):GLU:OE2	2:H:175:ARG:HD3	2.03	0.58
2:H:169:LYS:HA	2:H:176:ILE:HD12	1.85	0.57
3:A:330:TYR:HB2	3:A:334:ILE:HG13	1.86	0.57
3:A:325:ILE:HD13	3:A:325:ILE:C	2.24	0.57
3:A:173:LYS:HB3	3:A:173:LYS:NZ	2.20	0.57
3:A:285:PRO:HG2	3:A:288:MET:CG	2.35	0.57
3:A:368:ASN:CG	7:A:482:NAG:HN2	2.09	0.56
3:A:435:THR:HG22	3:A:437:THR:HG22	1.87	0.56
3:A:96:GLN:NE2	3:A:357:ARG:NH2	2.51	0.56
2:H:77(A):ARG:HG3	2:H:77(A):ARG:NH1	2.21	0.56
2:H:36:LYS:HG3	2:H:65:LEU:CD2	2.36	0.55
3:A:433:ALA:O	3:A:434:THR:OG1	2.18	0.55
2:H:153:SER:HB2	3:A:56:GLU:HG3	1.89	0.55
3:A:285:PRO:HG2	3:A:288:MET:HG3	1.89	0.54
2:H:36:LYS:HG3	2:H:65:LEU:HD22	1.91	0.53
3:A:304:VAL:HG11	3:A:477:PRO:HG2	1.91	0.53
3:A:293:ASN:HB3	3:A:301:VAL:CG2	2.39	0.53
1:L:14(A):LYS:HD2	1:L:14(B):THR:HG23	1.91	0.53
3:A:193:ARG:HG2	3:A:193:ARG:HH11	1.74	0.53
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.91	0.53
3:A:286:VAL:HG12	3:A:428:GLU:HG3	1.90	0.53
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.44	0.53
2:H:99:LEU:HG	3:A:441:PHE:HZ	1.73	0.52
3:A:382:LYS:O	3:A:421:GLN:HG2	2.09	0.52
3:A:58:ASP:O	3:A:295:ARG:NH1	2.43	0.52
3:A:163:HIS:HA	8:A:2078:HOH:O	2.08	0.52
3:A:331:VAL:HG21	3:A:431:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:325:ILE:HD11	3:A:337:LEU:HG	1.92	0.52
3:A:368:ASN:HB2	7:A:482:NAG:N2	2.23	0.52
3:A:435:THR:CG2	3:A:437:THR:HG22	2.39	0.52
2:H:82:ILE:HD13	3:A:61:LEU:HD13	1.92	0.52
2:H:240:LYS:HD2	6:H:2004:MPD:HM2	1.92	0.52
3:A:200:ARG:HG3	3:A:200:ARG:NH1	2.25	0.52
3:A:432:GLN:HG2	3:A:433:ALA:H	1.75	0.52
3:A:369:ARG:O	3:A:371:ARG:HD2	2.10	0.51
3:A:238:ALA:O	3:A:242:LYS:HG3	2.11	0.51
3:A:141:THR:HG22	3:A:183:PHE:CD1	2.46	0.51
2:H:99:LEU:O	2:H:102:ASP:HB2	2.11	0.50
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.46	0.50
3:A:439:VAL:CG1	3:A:440:GLY:H	2.17	0.50
2:H:144:LEU:HD21	2:H:152:PRO:HB3	1.93	0.49
3:A:257:ASP:HB3	3:A:260:GLU:HG3	1.94	0.49
3:A:401:LYS:CG	3:A:414:ALA:HB2	2.42	0.49
3:A:209:LYS:HE2	8:A:2063:HOH:O	2.11	0.49
3:A:350:LEU:CD1	3:A:457:LEU:HD12	2.43	0.49
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.15	0.48
2:H:99:LEU:HD11	3:A:443:PRO:HB3	1.95	0.48
3:A:325:ILE:HD11	3:A:337:LEU:CG	2.43	0.48
2:H:165:ARG:HB2	2:H:166:PRO:HD3	1.94	0.48
3:A:325:ILE:HD12	3:A:366:MET:SD	2.52	0.48
2:H:201:MET:SD	2:H:210:MET:HG3	2.54	0.47
2:H:164:GLU:H	2:H:164:GLU:CD	2.17	0.47
3:A:164:PHE:HB3	3:A:179:ILE:CD1	2.44	0.47
3:A:189:ARG:NH1	3:A:464:ARG:HD3	2.30	0.47
3:A:269:MET:HA	3:A:415:ILE:HD13	1.97	0.47
3:A:177:THR:HG22	3:A:181:ASN:ND2	2.29	0.47
3:A:295:ARG:HG2	3:A:344:MET:SD	2.55	0.47
3:A:62:ASP:CG	3:A:65:LYS:HB2	2.35	0.47
3:A:418:PHE:CD2	3:A:418:PHE:C	2.87	0.47
3:A:418:PHE:C	3:A:418:PHE:HD2	2.18	0.47
3:A:284:PHE:O	3:A:428:GLU:HB2	2.14	0.46
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.97	0.46
3:A:76:ILE:HD12	3:A:78:ASP:OD1	2.15	0.46
3:A:384:TYR:HD2	6:A:2002:MPD:HM1	1.81	0.46
3:A:141:THR:HG22	3:A:183:PHE:CE1	2.51	0.46
3:A:295:ARG:HG2	3:A:344:MET:HE1	1.98	0.46
3:A:438:THR:HG23	3:A:438:THR:O	2.16	0.45
3:A:280:TRP:CZ3	3:A:328:LEU:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:237:TRP:HB2	6:H:2004:MPD:H53	1.97	0.45
3:A:164:PHE:HB3	3:A:179:ILE:HD13	1.98	0.45
3:A:246:HIS:O	3:A:250:LEU:HG	2.17	0.45
3:A:295:ARG:HB3	3:A:454:ARG:HG2	1.97	0.45
3:A:73:TYS:HE2	3:A:73:TYS:O2	2.15	0.45
2:H:29:TRP:CG	2:H:121:VAL:HB	2.52	0.45
3:A:350:LEU:C	3:A:350:LEU:HD13	2.37	0.45
3:A:405:MET:HE1	3:A:408:ILE:HD12	1.99	0.45
3:A:454:ARG:HG3	3:A:454:ARG:NH1	2.31	0.45
3:A:375:LEU:HD12	3:A:376:PRO:HD2	1.98	0.45
2:H:60(B):PRO:HB2	2:H:60(C):PRO:HD3	1.99	0.45
3:A:434:THR:O	3:A:435:THR:O	2.35	0.45
2:H:244:GLN:HG3	2:H:245:PHE:CD2	2.53	0.44
3:A:216:ASP:O	3:A:220:LYS:HD3	2.16	0.44
3:A:102:SER:O	3:A:106:ARG:HG3	2.17	0.44
2:H:145:LYS:NZ	2:H:147(B):THR:OG1	2.48	0.44
3:A:296:LEU:HD13	3:A:302:VAL:HG12	1.99	0.44
3:A:440:GLY:O	3:A:441:PHE:C	2.56	0.44
3:A:412:ARG:HG2	3:A:412:ARG:HH11	1.83	0.44
3:A:161:ILE:HD11	3:A:394:GLY:HA3	2.00	0.44
3:A:321:LEU:HG	3:A:361:ARG:HH22	1.83	0.44
3:A:427:ASN:HB2	3:A:428:GLU:OE1	2.18	0.44
3:A:388:GLU:HB2	8:A:2036:HOH:O	2.18	0.43
2:H:145:LYS:HE3	2:H:145:LYS:HB2	1.74	0.43
3:A:412:ARG:HG2	3:A:412:ARG:NH1	2.33	0.43
3:A:368:ASN:CG	7:A:482:NAG:N2	2.67	0.43
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.54	0.43
3:A:428:GLU:H	3:A:428:GLU:CD	2.22	0.43
2:H:74:THR:HB	3:A:58:ASP:HA	2.00	0.43
3:A:388:GLU:OE1	3:A:388:GLU:HA	2.18	0.43
2:H:240:LYS:HB2	6:H:2004:MPD:HM2	2.01	0.43
3:A:282:ASN:HD22	3:A:313:PHE:HE1	1.66	0.43
2:H:93:ARG:HB2	2:H:101:ARG:HD2	2.01	0.42
2:H:61:GLU:H	2:H:61:GLU:CD	2.22	0.42
3:A:193:ARG:HG2	3:A:193:ARG:NH1	2.35	0.42
3:A:316:ALA:HB2	3:A:366:MET:HA	2.02	0.42
3:A:316:ALA:HB2	3:A:366:MET:HG2	2.01	0.42
3:A:337:LEU:O	3:A:458:PHE:HA	2.19	0.42
3:A:94:ILE:C	3:A:95:LEU:HD22	2.40	0.42
3:A:145:MET:HE1	3:A:205:LEU:HD22	2.00	0.42
3:A:241:SER:O	3:A:245:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:LEU:HD12	2:H:41:LEU:N	2.35	0.42
3:A:368:ASN:CB	7:A:482:NAG:N2	2.82	0.42
2:H:236:LYS:HB2	8:H:2042:HOH:O	2.19	0.41
3:A:378:PHE:HD1	3:A:380:LEU:HD13	1.85	0.41
3:A:274:ILE:N	3:A:274:ILE:HD12	2.34	0.41
2:H:110:LYS:NZ	3:A:72:ASP:OD1	2.54	0.41
3:A:415:ILE:HD12	3:A:417:LEU:H	1.86	0.41
3:A:97:LEU:O	3:A:101:LYS:HG3	2.21	0.41
3:A:123:LYS:HG3	3:A:124:ASP:N	2.35	0.41
3:A:257:ASP:HB3	3:A:260:GLU:CG	2.50	0.41
3:A:350:LEU:HD12	3:A:457:LEU:CD1	2.51	0.41
1:L:14(A):LYS:HG3	1:L:14(A):LYS:H	1.71	0.41
2:H:60(D):TRP:CH2	3:A:443:PRO:HG2	2.56	0.41
3:A:430:GLY:O	3:A:431:THR:O	2.39	0.41
2:H:146:GLU:OE2	2:H:221(A):ARG:NH2	2.54	0.41
3:A:277:LYS:NZ	3:A:429:GLU:OE2	2.52	0.41
3:A:401:LYS:O	3:A:412:ARG:NH1	2.54	0.41
3:A:165:LYS:HE2	3:A:165:LYS:HB3	1.82	0.40
3:A:448:VAL:HG13	3:A:448:VAL:O	2.20	0.40
3:A:405:MET:CE	3:A:408:ILE:HD12	2.51	0.40
3:A:94:ILE:HG22	3:A:95:LEU:N	2.35	0.40
3:A:95:LEU:C	3:A:97:LEU:H	2.24	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	L	45/48 (94%)	42 (93%)	1 (2%)	2 (4%)	2 1
2	H	257/260 (99%)	245 (95%)	12 (5%)	0	100 100
3	A	423/480 (88%)	394 (93%)	17 (4%)	12 (3%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	725/788 (92%)	681 (94%)	30 (4%)	14 (2%)	8 5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(L)	ASP
3	A	82	VAL
3	A	84	PRO
3	A	431	THR
3	A	434	THR
3	A	435	THR
3	A	438	THR
1	L	14(K)	ILE
3	A	94	ILE
3	A	83	SER
3	A	86	ASP
3	A	90	SER
3	A	439	VAL
3	A	89	VAL

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	L	41/42 (98%)	40 (98%)	1 (2%)	49 62
2	H	224/225 (100%)	215 (96%)	9 (4%)	31 40
3	A	385/431 (89%)	357 (93%)	28 (7%)	14 15
All	All	650/698 (93%)	612 (94%)	38 (6%)	20 23

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14(A)	LYS
2	H	33	LEU

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Mol	Chain	Res	Type
2	H	34	PHE
2	H	65	LEU
2	H	130	LEU
2	H	164	GLU
2	H	182	CYS
2	H	204(B)	ASN
2	H	236	LYS
2	H	244	GLN
3	A	65	LYS
3	A	76	ILE
3	A	83	SER
3	A	84	PRO
3	A	86	ASP
3	A	96	GLN
3	A	146	ILE
3	A	173	LYS
3	A	199	LEU
3	A	200	ARG
3	A	245	ASN
3	A	254	LEU
3	A	272	ASN
3	A	296	LEU
3	A	319	GLN
3	A	325	ILE
3	A	328	LEU
3	A	329	GLU
3	A	371	ARG
3	A	374	LEU
3	A	388	GLU
3	A	392	LEU
3	A	415	ILE
3	A	418	PHE
3	A	421	GLN
3	A	437	THR
3	A	459	LEU
3	A	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	1(O)	GLN
2	H	71	HIS

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Mol	Chain	Res	Type
2	H	156	GLN
2	H	204(B)	ASN
2	H	239	GLN
2	H	244	GLN
3	A	96	GLN
3	A	181	ASN
3	A	353	GLN
3	A	363	GLN
3	A	404	ASN
3	A	411	GLN
3	A	447	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TYS	A	60	3	15,16,17	3.55	2 (13%)	18,22,24	0.78	0
3	TYS	A	73	3	15,16,17	3.87	2 (13%)	18,22,24	0.73	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	TYS	A	60	3	-	1/10/11/13	0/1/1/1
3	TYS	A	73	3	-	2/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	73	TYS	OH-S	-10.96	1.41	1.58
3	A	73	TYS	OH-CZ	-9.94	1.26	1.42
3	A	60	TYS	OH-S	-9.58	1.43	1.58
3	A	60	TYS	OH-CZ	-9.46	1.27	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	73	TYS	CE1-CZ-OH-S
3	A	73	TYS	CE2-CZ-OH-S
3	A	60	TYS	CZ-OH-S-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	73	TYS	1	0

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
4	NAG	B	1	2,4	14,14,15	0.91	0	17,19,21	0.88	1 (5%)
4	NAG	B	2	4	14,14,15	0.61	0	17,19,21	1.04	2 (11%)

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
4	NAG	B	1	2,4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	NAG	O5-C1-C2	-2.30	107.66	111.29
4	B	1	NAG	O4-C4-C5	2.18	114.70	109.30
4	B	2	NAG	C2-N2-C7	-2.10	119.92	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1	NAG	C1

All (5) torsion outliers are listed below:

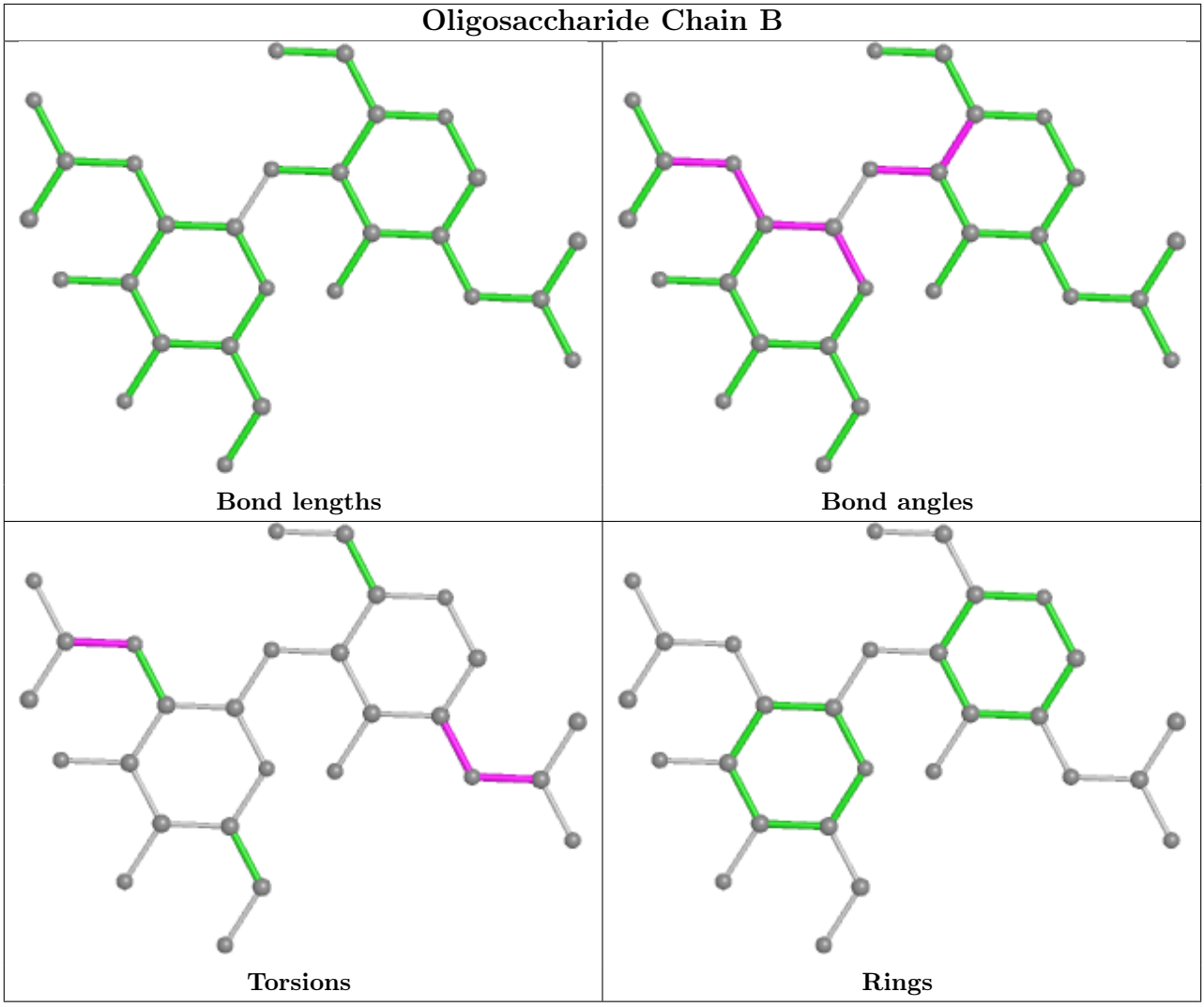
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C3-C2-N2-C7
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	1	0
4	B	2	NAG	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 (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	MPD	A	2002	-	7,7,7	0.57	0	9,10,10	0.46	0
7	NAG	A	481	3	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
6	MPD	A	2005	-	7,7,7	0.47	0	9,10,10	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MPD	A	2001	-	7,7,7	0.51	0	9,10,10	0.58	0
7	NAG	A	482	3	14,14,15	0.74	0	17,19,21	0.82	1 (5%)
6	MPD	H	2003	-	7,7,7	0.40	0	9,10,10	0.47	0
6	MPD	H	2004	-	7,7,7	0.40	0	9,10,10	0.50	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
6	MPD	A	2002	-	-	0/5/5/5	-
7	NAG	A	481	3	-	2/6/23/26	0/1/1/1
6	MPD	A	2001	-	-	1/5/5/5	-
7	NAG	A	482	3	1/1/5/7	4/6/23/26	0/1/1/1
6	MPD	A	2005	-	-	0/5/5/5	-
6	MPD	H	2003	-	-	2/5/5/5	-
6	MPD	H	2004	-	-	2/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	481	NAG	C2-N2-C7	-2.08	119.95	122.90
7	A	482	NAG	C2-N2-C7	-2.07	119.96	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	482	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	481	NAG	C8-C7-N2-C2
7	A	481	NAG	O7-C7-N2-C2
7	A	482	NAG	C8-C7-N2-C2
7	A	482	NAG	O7-C7-N2-C2
7	A	482	NAG	C4-C5-C6-O6
6	H	2003	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	H	2004	MPD	O2-C2-C3-C4
7	A	482	NAG	O5-C5-C6-O6
6	H	2003	MPD	C1-C2-C3-C4
6	H	2004	MPD	C1-C2-C3-C4
6	A	2001	MPD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2002	MPD	1	0
7	A	482	NAG	6	0
6	H	2003	MPD	1	0
6	H	2004	MPD	3	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	L	47/48 (97%)	-0.14	4 (8%) 10 9	36, 46, 78, 100	0
2	H	259/260 (99%)	-0.02	19 (7%) 15 14	32, 45, 63, 76	1 (0%)
3	A	414/480 (86%)	0.18	38 (9%) 9 7	40, 54, 85, 123	6 (1%)
All	All	720/788 (91%)	0.09	61 (8%) 10 9	32, 51, 79, 123	7 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	82	VAL	8.6
1	L	14(M)	GLY	7.2
3	A	81	SER	6.9
3	A	434	THR	6.6
3	A	436	VAL	5.7
3	A	435	THR	5.4
3	A	437	THR	5.1
3	A	401	LYS	5.0
3	A	54	GLY	4.9
3	A	433	ALA	4.7
3	A	94	ILE	4.3
2	H	53	LEU	4.1
2	H	212	ILE	4.0
3	A	439	VAL	3.8
3	A	438	THR	3.8
3	A	139	ILE	3.5
3	A	468	LEU	3.4
3	A	134	ILE	3.4
3	A	460	ILE	3.4
3	A	402	ASN	3.3
3	A	195	PHE	3.2
3	A	137	VAL	3.2
2	H	247	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	198	PRO	3.2
3	A	142	ALA	3.1
2	H	44	ALA	3.1
2	H	197	GLY	3.1
3	A	55	GLU	3.1
3	A	135	ALA	3.0
1	L	1(Q)	GLU	2.9
2	H	200	VAL	2.9
2	H	213	VAL	2.9
2	H	147(C)	ALA	2.8
2	H	229	THR	2.8
2	H	45	SER	2.7
3	A	136	PRO	2.7
1	L	1(S)	THR	2.7
3	A	115	ALA	2.6
3	A	470	PHE	2.6
3	A	432	GLN	2.5
3	A	431	THR	2.5
2	H	196	GLY	2.5
3	A	141	THR	2.5
3	A	412	ARG	2.5
2	H	43	GLY	2.5
3	A	138	GLY	2.4
2	H	31	VAL	2.4
2	H	199	PHE	2.4
3	A	193	ARG	2.4
2	H	54	THR	2.4
3	A	338	ILE	2.3
2	H	211	GLY	2.3
3	A	469	LEU	2.3
3	A	459	LEU	2.3
1	L	14(L)	ASP	2.2
3	A	140	SER	2.2
3	A	145	MET	2.1
3	A	270	ILE	2.1
2	H	52	VAL	2.1
3	A	471	MET	2.1
2	H	209	GLN	2.0

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, 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	TYS	A	60	16/17	0.91	0.11	46,49,73,75	0
3	TYS	A	73	16/17	0.96	0.11	65,74,83,84	0

6.3 Carbohydrates (i)

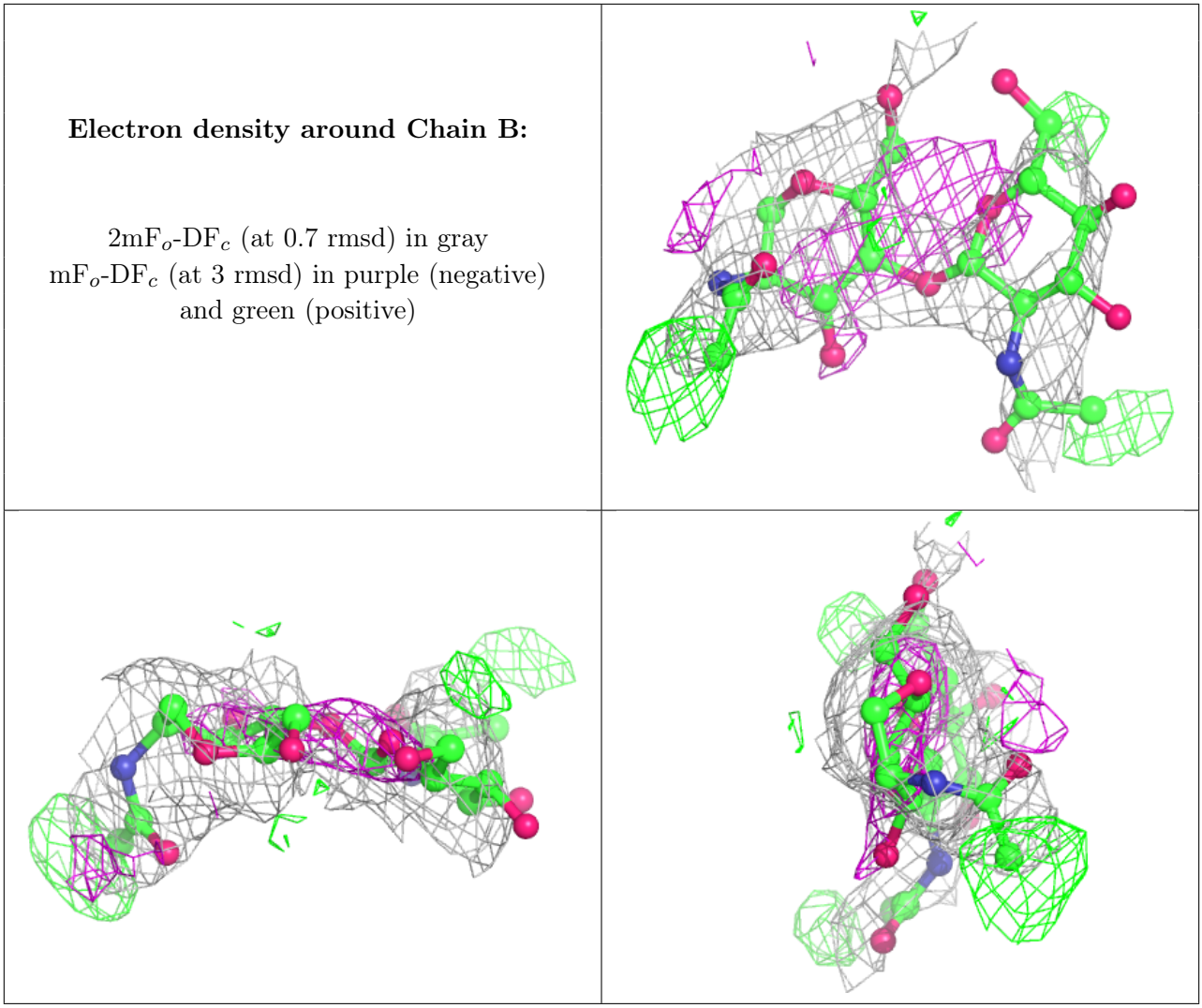
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NAG	B	1	14/15	0.71	0.45	99,105,109,115	0
4	NAG	B	2	14/15	0.71	0.56	119,123,124,125	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 B:

$2mF_o$-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, 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
7	NAG	A	481	14/15	0.40	0.54	103,107,111,111	0
7	NAG	A	482	14/15	0.63	0.50	101,104,105,105	0
6	MPD	A	2002	8/8	0.70	0.36	117,118,118,119	0
6	MPD	H	2003	8/8	0.72	0.37	80,82,82,83	0
6	MPD	A	2005	8/8	0.78	0.39	116,117,117,117	0
6	MPD	H	2004	8/8	0.79	0.63	129,130,131,131	0
6	MPD	A	2001	8/8	0.88	0.33	110,111,111,111	0
5	NA	H	501	1/1	0.96	0.10	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.