Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:32 AM EDT

PDB ID	:	1NCC
Title	:	CRYSTAL STRUCTURES OF TWO MUTANT NEURAMINIDASE-ANTIBODY COMPLEXES WITH AMINO ACID SUBSTITUTIONS IN THE INTERFACE
Authors	:	Tulip, W.R.; Varghese, J.N.; Colman, P.M.
Deposited on	:	1992-01-21
Resolution	:	2.50 Å(reported)

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

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

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

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

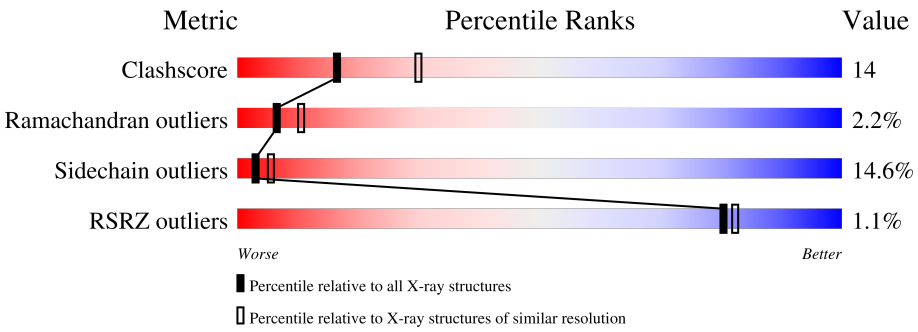
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	N	389	53% 35% 11% •
2	L	214	% 52% 36% 11% •
3	H	221	3% 55% 39% 5% •
4	A	6	67% 33%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6508 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 INFLUENZA A SUBTYPE N9 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	N	389	3078	1920	542	593	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	368	ARG	ILE	conflict	UNP P03472

- Molecule 2 is a protein called IGG2A-KAPPA NC41 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	214	1667	1043	280	336	8	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	20	THR	SER	conflict	EMBL Y11589
L	21	ILE	VAL	conflict	EMBL Y11589
L	28	ASP	ILE	conflict	EMBL Y11589
L	30	SER	GLY	conflict	EMBL Y11589
L	32	ALA	ASN	conflict	EMBL Y11589
L	34	VAL	ALA	conflict	EMBL Y11589
L	46	LEU	ALA	conflict	EMBL Y11589
L	50	TRP	SER	conflict	EMBL Y11589
L	53	THR	TYR	conflict	EMBL Y11589
L	55	HIS	TYR	conflict	EMBL Y11589
L	56	ILE	SER	conflict	EMBL Y11589
L	63	ALA	THR	conflict	EMBL Y11589
L	71	TYR	PHE	conflict	EMBL Y11589
L	77	SER	ASN	conflict	EMBL Y11589
L	80	ALA	SER	conflict	EMBL Y11589

Continued on next page...

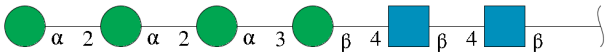
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	85	LEU	GLU	conflict	EMBL Y11589
L	87	TYR	PHE	conflict	EMBL Y11589
L	91	HIS	TYR	conflict	EMBL Y11589
L	92	TYR	ASN	conflict	EMBL Y11589
L	93	SER	ARG	conflict	EMBL Y11589
L	94	PRO	TYR	conflict	EMBL Y11589

- Molecule 3 is a protein called IGG2A-KAPPA NC41 FAB (HEAVY CHAIN).

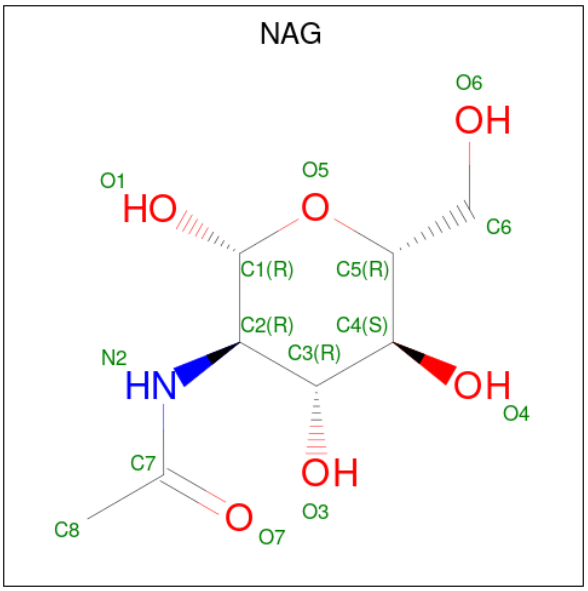
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	221	1662	1048	273	334	7	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	6	72	40	2	30	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

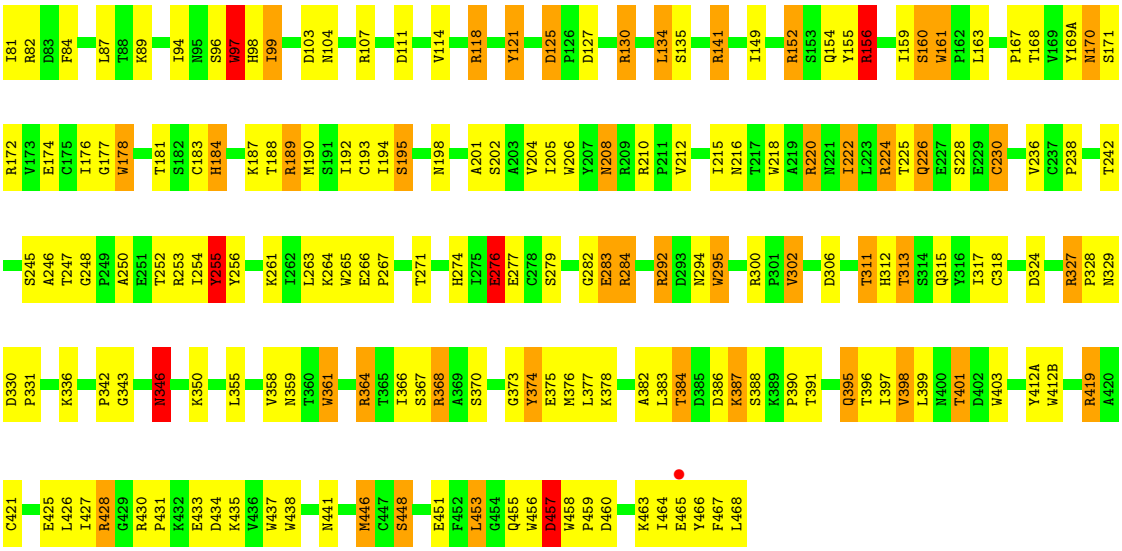
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	1	Total Ca 1 1	0	0

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.

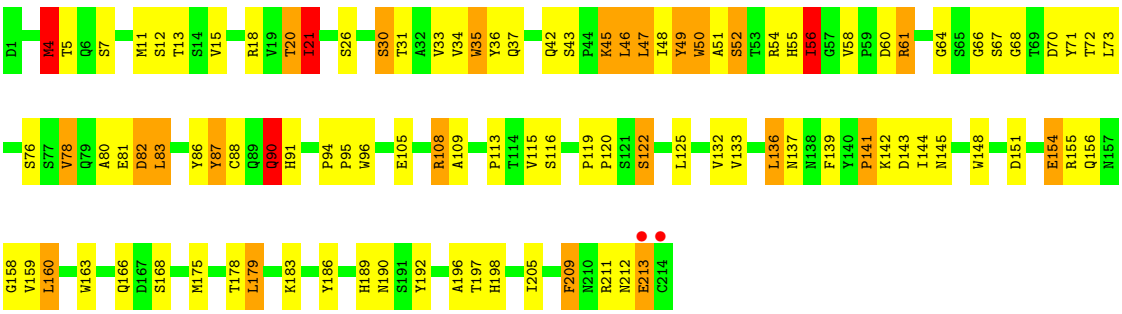
• Molecule 1: INFLUENZA A SUBTYPE N9 NEURAMINIDASE

Chain N: 53% 35% 11%



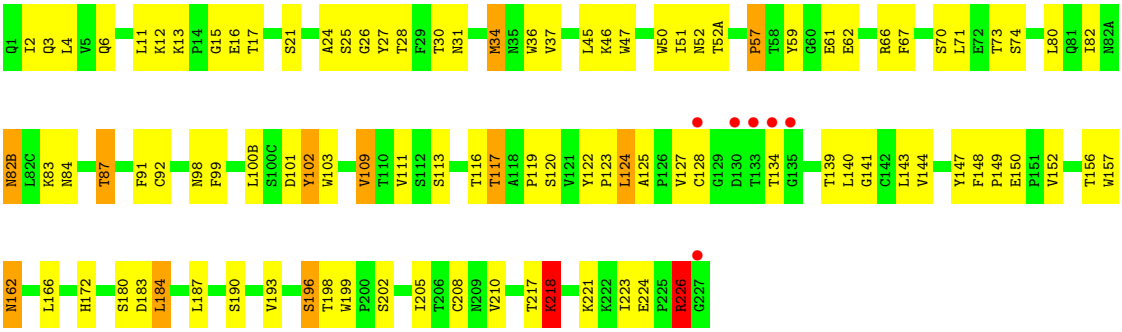
• Molecule 2: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)

Chain L: % 52% 36% 11%



• Molecule 3: IGG2A-KAPPA NC41 FAB (HEAVY CHAIN)

Chain H: 3% 55% 39% 5%



• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 67% 33%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.00Å 167.00Å 124.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 49.7 (8.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , (Not available) 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 47.9	EDS
L-test for twinning[1]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6508	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	N	1.16	6/3161 (0.2%)	1.99	113/4304 (2.6%)
2	L	1.00	0/1708	1.88	42/2323 (1.8%)
3	H	1.02	0/1704	1.91	45/2323 (1.9%)
All	All	1.09	6/6573 (0.1%)	1.94	200/8950 (2.2%)

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	N	0	6
2	L	0	3
All	All	0	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	97	TRP	CG-CD2	-6.30	1.32	1.43
1	N	327	ARG	CZ-NH2	5.77	1.40	1.33
1	N	284	ARG	CZ-NH2	5.49	1.40	1.33
1	N	456	TRP	NE1-CE2	-5.23	1.30	1.37
1	N	283	GLU	CD-OE2	-5.08	1.20	1.25
1	N	195	SER	CA-CB	-5.04	1.45	1.52

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	284	ARG	CD-NE-CZ	-11.46	107.56	123.60
3	H	36	TRP	CD1-CG-CD2	10.48	114.68	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	130	ARG	NE-CZ-NH2	-10.33	115.14	120.30
1	N	218	TRP	CD1-CG-CD2	10.24	114.49	106.30
3	H	34	MET	CG-SD-CE	-10.18	83.92	100.20
2	L	163	TRP	CD1-CG-CD2	9.64	114.01	106.30
1	N	189	ARG	NE-CZ-NH2	-9.55	115.53	120.30
3	H	157	TRP	CD1-CG-CD2	9.50	113.90	106.30
3	H	99	PHE	CB-CG-CD1	-9.43	114.20	120.80
3	H	36	TRP	CE2-CD2-CG	-9.42	99.76	107.30
1	N	210	ARG	NE-CZ-NH2	-9.41	115.60	120.30
2	L	96	TRP	CD1-CG-CD2	9.23	113.68	106.30
1	N	152	ARG	NE-CZ-NH2	-9.22	115.69	120.30
3	H	101	ASP	CB-CG-OD1	9.21	126.58	118.30
2	L	96	TRP	CE2-CD2-CG	-9.15	99.98	107.30
2	L	189	HIS	CA-CB-CG	-8.88	98.51	113.60
1	N	456	TRP	CG-CD2-CE3	8.64	141.67	133.90
3	H	36	TRP	CG-CD2-CE3	8.61	141.65	133.90
2	L	96	TRP	CB-CG-CD1	-8.61	115.81	127.00
1	N	218	TRP	CE2-CD2-CG	-8.58	100.44	107.30
1	N	403	TRP	CD1-CG-CD2	8.57	113.16	106.30
2	L	148	TRP	CD1-CG-CD2	8.57	113.15	106.30
2	L	35	TRP	CD1-CG-CD2	8.56	113.15	106.30
2	L	54	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	N	438	TRP	CE2-CD2-CG	-8.40	100.58	107.30
1	N	265	TRP	CD1-CG-CD2	8.40	113.02	106.30
2	L	163	TRP	CE2-CD2-CG	-8.34	100.63	107.30
2	L	20	THR	N-CA-CB	-8.27	94.58	110.30
3	H	157	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	N	107	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	N	172	ARG	NE-CZ-NH2	-8.19	116.21	120.30
2	L	50	TRP	CD1-CG-CD2	8.16	112.83	106.30
3	H	103	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	N	327	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	N	438	TRP	CD1-CG-CD2	8.06	112.75	106.30
2	L	35	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	N	412(B)	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	N	437	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	N	456	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	N	253	ARG	N-CA-CB	-7.84	96.49	110.60
1	N	111	ASP	O-C-N	-7.76	110.28	122.70
1	N	302	VAL	CG1-CB-CG2	-7.70	98.58	110.90
2	L	96	TRP	CG-CD2-CE3	7.69	140.82	133.90
1	N	456	TRP	CD1-CG-CD2	7.67	112.43	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	50	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	N	437	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	N	403	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	N	169(A)	TYR	CB-CG-CD2	-7.52	116.49	121.00
3	H	199	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	N	292	ARG	NE-CZ-NH2	-7.46	116.57	120.30
3	H	36	TRP	CB-CG-CD1	-7.43	117.34	127.00
3	H	50	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	N	438	TRP	CG-CD2-CE3	7.28	140.45	133.90
1	N	163	LEU	CA-CB-CG	7.14	131.73	115.30
1	N	253	ARG	CA-CB-CG	7.12	129.06	113.40
1	N	361	TRP	CE2-CD2-CG	-7.08	101.63	107.30
2	L	148	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	N	306	ASP	CB-CG-OD1	7.04	124.63	118.30
1	N	265	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	N	327	ARG	N-CA-CB	-6.97	98.06	110.60
1	N	163	LEU	CB-CG-CD2	-6.93	99.22	111.00
1	N	255	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	N	97	TRP	CE2-CD2-CG	-6.90	101.78	107.30
3	H	103	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	N	178	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	N	97	TRP	CD1-CG-CD2	6.82	111.75	106.30
1	N	368	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	N	226	GLN	N-CA-C	6.76	129.26	111.00
3	H	103	TRP	CG-CD1-NE1	-6.76	103.34	110.10
1	N	161	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	N	178	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	N	457	ASP	O-C-N	-6.69	111.99	122.70
1	N	218	TRP	CG-CD1-NE1	-6.69	103.41	110.10
1	N	97	TRP	CD2-CE3-CZ3	-6.66	110.14	118.80
1	N	121	TYR	CA-CB-CG	6.65	126.04	113.40
1	N	412(B)	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	N	103	ASP	CB-CG-OD1	6.61	124.25	118.30
2	L	211	ARG	NE-CZ-NH2	-6.61	117.00	120.30
3	H	199	TRP	CE2-CD2-CG	-6.61	102.02	107.30
3	H	50	TRP	CD1-CG-CD2	6.60	111.58	106.30
1	N	97	TRP	CE2-CD2-CE3	6.59	126.61	118.70
3	H	30	THR	N-CA-CB	-6.59	97.78	110.30
3	H	109	VAL	CG1-CB-CG2	-6.50	100.50	110.90
3	H	152	VAL	CG1-CB-CG2	-6.50	100.50	110.90
2	L	36	TYR	CB-CG-CD2	-6.47	117.11	121.00
1	N	403	TRP	CG-CD1-NE1	-6.45	103.66	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	184	HIS	CA-C-N	6.42	131.32	117.20
1	N	206	TRP	CE2-CD2-CG	-6.41	102.17	107.30
1	N	111	ASP	CA-C-N	6.39	131.26	117.20
1	N	152	ARG	CG-CD-NE	-6.38	98.40	111.80
1	N	198	ASN	CB-CG-ND2	6.24	131.67	116.70
3	H	36	TRP	CG-CD1-NE1	-6.22	103.88	110.10
2	L	18	ARG	NE-CZ-NH1	6.18	123.39	120.30
3	H	82(B)	ASN	CA-C-N	-6.18	103.61	117.20
1	N	161	TRP	CD1-CG-CD2	6.12	111.20	106.30
1	N	364	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	N	446	MET	CA-CB-CG	6.08	123.63	113.30
3	H	99	PHE	N-CA-CB	6.05	121.49	110.60
2	L	95	PRO	CA-C-N	-6.03	103.94	117.20
3	H	208	CYS	CA-CB-SG	-6.02	103.16	114.00
1	N	313	THR	CA-CB-CG2	-6.02	103.97	112.40
1	N	236	VAL	CA-CB-CG2	-6.00	101.90	110.90
2	L	73	LEU	CA-CB-CG	5.97	129.03	115.30
2	L	160	LEU	CA-CB-CG	5.95	128.97	115.30
1	N	279	SER	N-CA-CB	-5.92	101.62	110.50
1	N	224	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	N	256	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	N	125	ASP	CB-CG-OD1	5.85	123.57	118.30
1	N	361	TRP	CD1-CG-CD2	5.85	110.98	106.30
3	H	47	TRP	CE2-CD2-CG	-5.82	102.64	107.30
1	N	208	ASN	CA-C-N	-5.82	104.39	117.20
1	N	456	TRP	CG-CD1-NE1	-5.80	104.30	110.10
2	L	4	MET	CA-CB-CG	-5.79	103.45	113.30
1	N	324	ASP	CB-CG-OD2	5.79	123.51	118.30
3	H	99	PHE	CB-CA-C	-5.78	98.84	110.40
3	H	103	TRP	CG-CD2-CE3	5.77	139.09	133.90
2	L	56	ILE	CA-C-N	-5.77	104.67	116.20
1	N	468	LEU	CA-C-O	-5.75	108.01	120.10
1	N	104	ASN	CB-CG-ND2	5.75	130.51	116.70
1	N	163	LEU	CB-CG-CD1	5.75	120.78	111.00
2	L	35	TRP	CG-CD2-CE3	5.75	139.07	133.90
3	H	157	TRP	CG-CD1-NE1	-5.75	104.35	110.10
3	H	62	GLU	CA-CB-CG	5.74	126.03	113.40
1	N	412(B)	TRP	CB-CG-CD1	-5.74	119.54	127.00
3	H	50	TRP	NE1-CE2-CZ2	-5.74	124.09	130.40
1	N	127	ASP	CA-CB-CG	-5.74	100.78	113.40
1	N	277	GLU	N-CA-CB	-5.74	100.28	110.60
3	H	30	THR	CA-CB-OG1	-5.74	96.96	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	456	TRP	O-C-N	5.73	131.87	122.70
3	H	122	TYR	CB-CG-CD2	-5.72	117.57	121.00
3	H	157	TRP	CG-CD2-CE3	5.72	139.05	133.90
2	L	90	GLN	N-CA-CB	-5.72	100.31	110.60
2	L	108	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	L	21	ILE	CA-C-N	-5.71	104.64	117.20
3	H	218	LYS	CA-C-N	-5.71	104.65	117.20
1	N	236	VAL	CG1-CB-CG2	-5.65	101.86	110.90
2	L	86	TYR	CB-CG-CD2	-5.65	117.61	121.00
3	H	196	SER	N-CA-CB	-5.65	102.02	110.50
1	N	104	ASN	OD1-CG-ND2	-5.63	108.95	121.90
1	N	374	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	N	398	VAL	CG1-CB-CG2	-5.61	101.93	110.90
1	N	295	TRP	CD1-CG-CD2	5.59	110.77	106.30
1	N	279	SER	CB-CA-C	5.57	120.69	110.10
1	N	284	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	N	264	LYS	CA-CB-CG	5.56	125.63	113.40
2	L	4	MET	CG-SD-CE	-5.55	91.32	100.20
1	N	218	TRP	CG-CD2-CE3	5.54	138.89	133.90
3	H	98	ASN	CB-CG-ND2	5.54	129.99	116.70
1	N	103	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	N	295	TRP	CE2-CD2-CG	-5.49	102.91	107.30
1	N	230	CYS	CA-C-N	5.49	129.28	117.20
1	N	456	TRP	CB-CG-CD1	-5.48	119.88	127.00
1	N	156	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	N	438	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	N	181	THR	N-CA-C	-5.42	96.38	111.00
3	H	47	TRP	CD1-CG-CD2	5.41	110.63	106.30
1	N	412(A)	TYR	CA-CB-CG	-5.40	103.14	113.40
1	N	81	ILE	N-CA-C	-5.37	96.51	111.00
1	N	401	THR	CA-CB-CG2	-5.36	104.89	112.40
1	N	218	TRP	CB-CG-CD1	-5.35	120.04	127.00
2	L	213	GLU	CA-C-N	-5.34	105.44	117.20
3	H	50	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	N	361	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	N	99	ILE	CB-CA-C	-5.33	100.94	111.60
3	H	152	VAL	CA-CB-CG2	-5.33	102.91	110.90
1	N	253	ARG	CB-CA-C	5.32	121.05	110.40
2	L	46	LEU	CB-CG-CD1	-5.29	102.01	111.00
2	L	30	SER	N-CA-CB	-5.28	102.58	110.50
1	N	364	ARG	CA-CB-CG	5.28	125.02	113.40
1	N	428	ARG	NE-CZ-NH2	5.28	122.94	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	466	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	N	312	HIS	N-CA-C	5.26	125.21	111.00
1	N	313	THR	OG1-CB-CG2	5.26	122.10	110.00
3	H	157	TRP	CB-CG-CD1	-5.26	120.17	127.00
2	L	148	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	N	403	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	N	421	CYS	CA-CB-SG	5.22	123.40	114.00
3	H	66	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	N	311	THR	CA-CB-OG1	-5.16	98.16	109.00
1	N	204	VAL	CA-CB-CG2	-5.16	103.17	110.90
2	L	35	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	N	276	GLU	CA-CB-CG	-5.14	102.10	113.40
1	N	403	TRP	CG-CD2-CE3	5.13	138.51	133.90
2	L	82	ASP	CB-CG-OD1	5.11	122.90	118.30
2	L	136	LEU	N-CA-C	-5.11	97.19	111.00
3	H	172	HIS	N-CA-C	-5.11	97.21	111.00
1	N	384	THR	CA-CB-CG2	-5.11	105.25	112.40
1	N	206	TRP	CD1-CG-CD2	5.10	110.38	106.30
3	H	99	PHE	CB-CG-CD2	5.06	124.34	120.80
2	L	163	TRP	CG-CD1-NE1	-5.05	105.05	110.10
2	L	35	TRP	CB-CG-CD1	-5.04	120.44	127.00
2	L	54	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	H	50	TRP	CB-CG-CD1	-5.04	120.45	127.00
2	L	49	TYR	CB-CG-CD1	-5.03	117.98	121.00
2	L	20	THR	CA-CB-OG1	-5.03	98.45	109.00
3	H	199	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	N	361	TRP	CB-CG-CD1	-5.01	120.48	127.00
1	N	382	ALA	CB-CA-C	-5.01	102.59	110.10
2	L	190	ASN	CA-C-N	5.01	128.21	117.20
3	H	101	ASP	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	56	ILE	Mainchain
2	L	87	TYR	Sidechain
2	L	94	PRO	Peptide
1	N	155	TYR	Sidechain
1	N	248	GLY	Peptide
1	N	255	TYR	Sidechain
1	N	284	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	N	327	ARG	Sidechain
1	N	457	ASP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	3078	0	2905	101	0
2	L	1667	0	1598	43	0
3	H	1662	0	1611	46	0
4	A	72	0	61	1	0
5	N	28	0	26	1	0
6	N	1	0	0	0	0
All	All	6508	0	6201	182	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 14.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:426:LEU:HD23	1:N:460:ASP:HB2	1.40	1.03
2:L:145:ASN:HB3	2:L:197:THR:HB	1.53	0.91
1:N:426:LEU:HD23	1:N:460:ASP:CB	2.00	0.91
1:N:188:THR:HG21	1:N:208:ASN:HB2	1.60	0.82
1:N:426:LEU:HD23	1:N:460:ASP:CA	2.10	0.81
3:H:2:ILE:HA	3:H:26:GLY:HA3	1.64	0.80
1:N:141:ARG:HH21	1:N:467:PHE:HA	1.47	0.77
1:N:401:THR:HB	3:H:52:ASN:ND2	2.00	0.76
1:N:373:GLY:HA2	1:N:398:VAL:HG13	1.70	0.72
1:N:426:LEU:CD2	1:N:460:ASP:CA	2.68	0.72
1:N:194:ILE:HD11	1:N:225:THR:HB	1.75	0.69
3:H:11:LEU:HD22	3:H:149:PRO:HG3	1.75	0.69
3:H:6:GLN:HE22	3:H:91:PHE:HA	1.58	0.68
1:N:361:TRP:HE1	1:N:378:LYS:HZ3	1.41	0.67
1:N:387:LYS:HB2	1:N:387:LYS:NZ	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:MET:SD	2:L:90:GLN:HB2	2.36	0.66
1:N:399:LEU:HD12	1:N:457:ASP:OD2	1.98	0.63
3:H:210:VAL:O	3:H:218:LYS:HA	1.98	0.63
3:H:84:ASN:HA	3:H:111:VAL:HB	1.81	0.63
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.80	0.62
3:H:117:THR:O	3:H:147:TYR:HA	1.98	0.62
1:N:361:TRP:HE1	1:N:378:LYS:NZ	1.98	0.62
3:H:123:PRO:HD3	3:H:221:LYS:HG3	1.82	0.61
2:L:133:VAL:HG22	2:L:178:THR:HG23	1.83	0.61
3:H:34:MET:HB2	3:H:51:ILE:HG22	1.82	0.61
1:N:374:TYR:HB3	1:N:397:ILE:HB	1.83	0.61
1:N:168:THR:H	1:N:170:ASN:HD21	1.49	0.60
3:H:184:LEU:H	3:H:184:LEU:HD22	1.65	0.60
1:N:328:PRO:HG3	1:N:343:GLY:HA3	1.84	0.60
2:L:34:VAL:HG23	2:L:91:HIS:CD2	2.37	0.60
1:N:368:ARG:HH12	2:L:55:HIS:CD2	2.19	0.59
1:N:426:LEU:CD2	1:N:460:ASP:N	2.65	0.59
1:N:426:LEU:CD2	1:N:460:ASP:HA	2.33	0.59
1:N:97:TRP:HZ3	1:N:361:TRP:CE3	2.21	0.58
3:H:12:LYS:O	3:H:111:VAL:HA	2.03	0.58
1:N:149:ILE:HD12	1:N:430:ARG:HB3	1.87	0.57
3:H:2:ILE:HD12	3:H:27:TYR:HB3	1.86	0.57
1:N:118:ARG:HA	1:N:441:ASN:ND2	2.19	0.56
2:L:83:LEU:HD13	2:L:166:GLN:HB3	1.87	0.56
2:L:141:PRO:HD2	2:L:198:HIS:CE1	2.40	0.56
3:H:144:VAL:HB	3:H:187:LEU:HB3	1.88	0.56
3:H:15:GLY:O	3:H:82(B):ASN:HA	2.04	0.56
1:N:94:ILE:HD12	1:N:359:ASN:HD21	1.71	0.56
2:L:144:ILE:HD12	2:L:198:HIS:HB2	1.88	0.56
3:H:148:PHE:CE2	3:H:149:PRO:HB3	2.41	0.56
1:N:149:ILE:HD11	1:N:431:PRO:HD3	1.87	0.56
1:N:401:THR:HB	3:H:52:ASN:HD21	1.70	0.56
3:H:17:THR:HA	3:H:82:ILE:O	2.06	0.56
2:L:122:SER:HA	2:L:125:LEU:HD12	1.87	0.56
3:H:2:ILE:HB	3:H:102:TYR:CD2	2.41	0.56
1:N:118:ARG:HA	1:N:441:ASN:HD22	1.71	0.55
1:N:135:SER:HB2	1:N:159:ILE:HD13	1.88	0.55
1:N:152:ARG:HG2	1:N:178:TRP:CG	2.40	0.55
3:H:34:MET:HB2	3:H:51:ILE:CG2	2.36	0.55
1:N:428:ARG:HH21	1:N:464:ILE:HG12	1.71	0.55
1:N:168:THR:H	1:N:170:ASN:ND2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2:ILE:HG23	3:H:27:TYR:HD1	1.72	0.55
1:N:451:GLU:HB2	1:N:453:LEU:HD21	1.88	0.54
2:L:125:LEU:O	2:L:183:LYS:HD3	2.08	0.54
2:L:45:LYS:HD2	2:L:46:LEU:N	2.23	0.54
1:N:366:ILE:HD13	3:H:31:ASN:HD21	1.73	0.54
1:N:426:LEU:HD23	1:N:460:ASP:N	2.23	0.53
1:N:205:ILE:HD11	1:N:215:ILE:HD12	1.89	0.53
1:N:170:ASN:HD22	1:N:171:SER:N	2.07	0.53
3:H:162:ASN:OD1	3:H:205:ILE:HA	2.07	0.53
1:N:97:TRP:H	1:N:395:GLN:HE21	1.55	0.53
1:N:188:THR:CG2	1:N:208:ASN:HB2	2.37	0.53
1:N:294:ASN:O	1:N:346:ASN:HA	2.09	0.53
2:L:66:GLY:HA3	2:L:71:TYR:CD1	2.44	0.52
2:L:108:ARG:HG2	2:L:109:ALA:H	1.72	0.52
1:N:121:TYR:CB	1:N:228:SER:HA	2.39	0.52
1:N:84:PHE:O	5:N:475(A):NAG:H82	2.08	0.52
1:N:378:LYS:O	1:N:390:PRO:HA	2.09	0.52
1:N:176:ILE:O	1:N:193:CYS:HB3	2.09	0.52
1:N:96:SER:OG	1:N:453:LEU:HG	2.10	0.52
1:N:386:ASP:OD1	1:N:387:LYS:NZ	2.43	0.51
3:H:125:ALA:HB2	3:H:223:ILE:HG23	1.91	0.51
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.45	0.51
3:H:116:THR:HG22	3:H:149:PRO:HD3	1.92	0.51
1:N:387:LYS:HB2	1:N:387:LYS:HZ3	1.74	0.51
1:N:161:TRP:CE3	1:N:167:PRO:HB3	2.46	0.51
1:N:376:MET:O	1:N:377:LEU:HD23	2.11	0.51
1:N:226:GLN:O	1:N:350:LYS:NZ	2.45	0.50
1:N:97:TRP:N	1:N:395:GLN:HE21	2.08	0.50
3:H:4:LEU:CD2	3:H:24:ALA:HA	2.42	0.50
3:H:83:LYS:O	3:H:111:VAL:HG21	2.12	0.50
2:L:83:LEU:O	2:L:83:LEU:HG	2.11	0.49
1:N:271:THR:OG1	1:N:315:GLN:HA	2.12	0.49
2:L:196:ALA:HB3	2:L:205:ILE:HB	1.93	0.49
3:H:183:ASP:HB3	3:H:184:LEU:HD13	1.94	0.49
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.94	0.49
2:L:52:SER:HA	2:L:64:GLY:HA3	1.95	0.49
1:N:97:TRP:H	1:N:395:GLN:NE2	2.11	0.49
1:N:121:TYR:CG	1:N:228:SER:HA	2.48	0.49
3:H:2:ILE:HG23	3:H:27:TYR:CD1	2.47	0.49
1:N:130:ARG:HE	1:N:160:SER:HB2	1.78	0.48
2:L:34:VAL:HA	2:L:48:ILE:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:318:CYS:HB3	1:N:386:ASP:HA	1.96	0.48
3:H:3:GLN:HB2	3:H:25:SER:HB2	1.95	0.48
1:N:367:SER:HB3	1:N:370:SER:O	2.14	0.47
2:L:49:TYR:CD1	3:H:100(B):LEU:HD21	2.48	0.47
1:N:184:HIS:HA	1:N:189:ARG:HA	1.96	0.47
3:H:67:PHE:CE1	3:H:82:ILE:HG23	2.50	0.47
3:H:37:VAL:HA	3:H:46:LYS:O	2.14	0.47
1:N:84:PHE:CD1	1:N:187:LYS:HG3	2.50	0.47
1:N:114:VAL:HG13	1:N:167:PRO:O	2.15	0.47
1:N:246:ALA:HA	1:N:274:HIS:NE2	2.30	0.46
2:L:37:GLN:HB2	2:L:47:LEU:HD21	1.96	0.46
1:N:195:SER:O	1:N:201:ALA:HA	2.15	0.46
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.97	0.46
1:N:189:ARG:HG2	1:N:190:MET:O	2.16	0.46
1:N:395:GLN:HA	1:N:455:GLN:NE2	2.31	0.46
3:H:124:LEU:HB2	3:H:141:GLY:C	2.36	0.46
1:N:224:ARG:HG2	1:N:224:ARG:HH11	1.81	0.46
2:L:34:VAL:HG23	2:L:91:HIS:HD2	1.80	0.46
2:L:45:LYS:HD2	2:L:46:LEU:H	1.80	0.46
2:L:15:VAL:HA	2:L:78:VAL:O	2.16	0.45
1:N:463:LYS:C	1:N:465:GLU:H	2.19	0.45
1:N:426:LEU:CD2	1:N:460:ASP:HB2	2.29	0.45
3:H:57:PRO:HB2	3:H:59:TYR:CE1	2.51	0.45
2:L:186:TYR:HA	2:L:192:TYR:OH	2.17	0.45
1:N:426:LEU:HD21	1:N:460:ASP:N	2.32	0.45
1:N:216:ASN:ND2	1:N:220:ARG:HH21	2.15	0.45
2:L:46:LEU:HD11	3:H:100(B):LEU:HD23	1.99	0.45
2:L:87:TYR:CD2	3:H:45:LEU:HD12	2.52	0.45
1:N:373:GLY:HA2	1:N:398:VAL:O	2.17	0.44
1:N:366:ILE:HG12	1:N:375:GLU:HG2	1.99	0.44
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.51	0.44
2:L:154:GLU:CD	2:L:154:GLU:H	2.20	0.44
2:L:155:ARG:HG2	2:L:179:LEU:HD11	2.00	0.44
3:H:127:VAL:O	3:H:128:CYS:HB2	2.16	0.44
1:N:428:ARG:NH2	1:N:433:GLU:OE2	2.51	0.44
2:L:49:TYR:HD2	2:L:50:TRP:HD1	1.65	0.44
1:N:134:LEU:HB3	1:N:156:ARG:NH1	2.33	0.44
3:H:166:LEU:HD12	3:H:166:LEU:HA	1.84	0.44
1:N:98:HIS:O	1:N:446:MET:HB3	2.17	0.43
2:L:4:MET:HG2	2:L:88:CYS:SG	2.59	0.43
1:N:121:TYR:HB3	1:N:228:SER:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:245:SER:O	1:N:250:ALA:HB2	2.19	0.43
1:N:238:PRO:HA	1:N:255:TYR:O	2.18	0.43
1:N:266:GLU:HA	1:N:267:PRO:HD3	1.86	0.43
1:N:355:LEU:HD13	1:N:383:LEU:HD13	2.01	0.43
1:N:464:ILE:O	1:N:464:ILE:CG2	2.66	0.43
1:N:94:ILE:HD12	1:N:359:ASN:ND2	2.33	0.43
1:N:463:LYS:C	1:N:465:GLU:N	2.72	0.43
2:L:119:PRO:HG3	3:H:226:ARG:NH2	2.34	0.43
3:H:124:LEU:HD21	3:H:143:LEU:HB2	2.00	0.43
1:N:192:ILE:HG12	1:N:205:ILE:HG23	2.00	0.42
1:N:246:ALA:HA	1:N:274:HIS:HE2	1.84	0.42
1:N:425:GLU:OE1	1:N:427:ILE:HD11	2.19	0.42
1:N:453:LEU:HD23	1:N:453:LEU:N	2.34	0.42
2:L:21:ILE:O	2:L:72:THR:HA	2.19	0.42
2:L:12:SER:HA	2:L:105:GLU:O	2.19	0.42
4:A:4:MAN:O3	4:A:5:MAN:C1	2.67	0.42
1:N:130:ARG:HH21	1:N:160:SER:HB2	1.84	0.42
1:N:87:LEU:HD13	1:N:282:GLY:HA3	2.02	0.42
1:N:276:GLU:HB3	1:N:292:ARG:HB3	2.01	0.42
3:H:4:LEU:HD23	3:H:24:ALA:HA	2.01	0.42
1:N:419:ARG:HD2	1:N:448:SER:O	2.20	0.42
1:N:300:ARG:O	1:N:317:ILE:HG12	2.20	0.42
1:N:458:TRP:HA	1:N:459:PRO:HD2	1.80	0.42
1:N:176:ILE:HG22	1:N:177:GLY:N	2.36	0.41
1:N:330:ASP:HA	1:N:331:PRO:HD2	1.94	0.41
2:L:115:VAL:HG13	2:L:136:LEU:HG	2.02	0.41
1:N:368:ARG:NH1	2:L:55:HIS:CD2	2.86	0.41
1:N:451:GLU:HB2	1:N:453:LEU:CD2	2.49	0.41
3:H:184:LEU:HD22	3:H:184:LEU:N	2.30	0.41
1:N:430:ARG:HG3	1:N:434:ASP:HA	2.01	0.41
3:H:139:THR:O	3:H:140:LEU:HD23	2.21	0.41
3:H:224:GLU:O	3:H:226:ARG:HG2	2.20	0.41
1:N:373:GLY:CA	1:N:398:VAL:HG13	2.47	0.41
2:L:80:ALA:HB1	2:L:168:SER:O	2.20	0.41
1:N:183:CYS:HB3	1:N:230:CYS:O	2.21	0.41
3:H:87:THR:O	3:H:87:THR:HG23	2.21	0.41
2:L:33:VAL:HG21	2:L:71:TYR:CD2	2.56	0.41
2:L:35:TRP:O	2:L:47:LEU:HB2	2.21	0.41
1:N:161:TRP:CE2	1:N:167:PRO:HD3	2.55	0.40
1:N:216:ASN:HD21	1:N:220:ARG:HH21	1.68	0.40
1:N:242:THR:HA	1:N:252:THR:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:274:HIS:HE1	1:N:294:ASN:HB3	1.86	0.40
2:L:143:ASP:O	2:L:198:HIS:CD2	2.75	0.40
2:L:159:VAL:HA	2:L:178:THR:O	2.22	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	N	387/389 (100%)	336 (87%)	48 (12%)	3 (1%)	19 35
2	L	212/214 (99%)	187 (88%)	19 (9%)	6 (3%)	5 7
3	H	219/221 (99%)	180 (82%)	30 (14%)	9 (4%)	3 3
All	All	818/824 (99%)	703 (86%)	97 (12%)	18 (2%)	6 10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	154	GLU
2	L	158	GLY
3	H	16	GLU
3	H	87	THR
3	H	162	ASN
2	L	51	ALA
3	H	102	TYR
3	H	134	THR
3	H	226	ARG
1	N	346	ASN
2	L	60	ASP
2	L	78	VAL
1	N	295	TRP
3	H	52(A)	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	222	ILE
3	H	180	SER
3	H	57	PRO
2	L	68	GLY

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	N	342/342 (100%)	300 (88%)	42 (12%)	4 9
2	L	190/190 (100%)	153 (80%)	37 (20%)	1 2
3	H	187/187 (100%)	161 (86%)	26 (14%)	3 6
All	All	719/719 (100%)	614 (85%)	105 (15%)	3 5

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	82	ARG
1	N	89	LYS
1	N	97	TRP
1	N	99	ILE
1	N	118	ARG
1	N	125	ASP
1	N	134	LEU
1	N	141	ARG
1	N	154	GLN
1	N	156	ARG
1	N	160	SER
1	N	170	ASN
1	N	174	GLU
1	N	202	SER
1	N	212	VAL
1	N	220	ARG
1	N	222	ILE
1	N	247	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	254	ILE
1	N	261	LYS
1	N	263	LEU
1	N	276	GLU
1	N	283	GLU
1	N	302	VAL
1	N	311	THR
1	N	313	THR
1	N	329	ASN
1	N	336	LYS
1	N	342	PRO
1	N	346	ASN
1	N	358	VAL
1	N	364	ARG
1	N	384	THR
1	N	387	LYS
1	N	388	SER
1	N	391	THR
1	N	395	GLN
1	N	396	THR
1	N	419	ARG
1	N	435	LYS
1	N	448	SER
1	N	453	LEU
2	L	4	MET
2	L	5	THR
2	L	7	SER
2	L	11	MET
2	L	13	THR
2	L	20	THR
2	L	21	ILE
2	L	26	SER
2	L	30	SER
2	L	31	THR
2	L	42	GLN
2	L	43	SER
2	L	45	LYS
2	L	47	LEU
2	L	52	SER
2	L	56	ILE
2	L	58	VAL
2	L	61	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	67	SER
2	L	70	ASP
2	L	76	SER
2	L	81	GLU
2	L	83	LEU
2	L	90	GLN
2	L	116	SER
2	L	122	SER
2	L	137	ASN
2	L	141	PRO
2	L	142	LYS
2	L	151	ASP
2	L	156	GLN
2	L	160	LEU
2	L	175	MET
2	L	179	LEU
2	L	209	PHE
2	L	212	ASN
2	L	213	GLU
3	H	13	LYS
3	H	21	SER
3	H	28	THR
3	H	61	GLU
3	H	70	SER
3	H	71	LEU
3	H	73	THR
3	H	74	SER
3	H	80	LEU
3	H	92	CYS
3	H	109	VAL
3	H	113	SER
3	H	117	THR
3	H	120	SER
3	H	124	LEU
3	H	150	GLU
3	H	156	THR
3	H	184	LEU
3	H	190	SER
3	H	193	VAL
3	H	196	SER
3	H	198	THR
3	H	202	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	217	THR
3	H	218	LYS
3	H	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	95	ASN
1	N	170	ASN
1	N	208	ASN
1	N	216	ASN
1	N	359	ASN
1	N	392	GLN
1	N	395	GLN
1	N	455	GLN
2	L	161	ASN
3	H	6	GLN
3	H	53	ASN
3	H	82(B)	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 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	A	1	4,1	14,14,15	0.61	0	17,19,21	1.69	5 (29%)
4	NAG	A	2	4	14,14,15	0.80	0	17,19,21	2.01	3 (17%)
4	BMA	A	3	4	11,11,12	1.82	2 (18%)	15,15,17	1.80	5 (33%)
4	MAN	A	4	4	11,11,12	1.17	1 (9%)	15,15,17	3.28	8 (53%)
4	MAN	A	5	4	11,11,12	1.21	2 (18%)	15,15,17	3.06	6 (40%)
4	MAN	A	6	4	11,11,12	1.68	4 (36%)	15,15,17	1.98	1 (6%)

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	A	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
4	MAN	A	4	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5	4	-	2/2/19/22	1/1/1/1
4	MAN	A	6	4	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	BMA	C6-C5	3.83	1.64	1.51
4	A	6	MAN	C1-C2	2.90	1.58	1.52
4	A	6	MAN	C6-C5	2.64	1.60	1.51
4	A	3	BMA	C4-C5	2.63	1.58	1.53
4	A	5	MAN	C4-C3	2.50	1.58	1.52
4	A	6	MAN	O5-C5	2.37	1.48	1.43
4	A	4	MAN	C6-C5	2.15	1.59	1.51
4	A	6	MAN	O5-C1	2.06	1.47	1.43
4	A	5	MAN	O5-C5	2.06	1.47	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5	MAN	C1-O5-C5	8.27	123.40	112.19
4	A	4	MAN	C1-O5-C5	7.01	121.69	112.19
4	A	6	MAN	C1-O5-C5	6.74	121.33	112.19
4	A	4	MAN	C1-C2-C3	6.69	117.89	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2	NAG	C8-C7-N2	5.86	126.02	116.10
4	A	5	MAN	O5-C1-C2	4.99	118.48	110.77
4	A	4	MAN	O2-C2-C3	-4.18	101.76	110.14
4	A	4	MAN	O4-C4-C3	4.04	119.70	110.35
4	A	1	NAG	C1-C2-N2	-3.78	104.03	110.49
4	A	2	NAG	O7-C7-C8	-3.65	115.28	122.06
4	A	5	MAN	C1-C2-C3	-3.12	105.83	109.67
4	A	3	BMA	O5-C5-C4	-3.06	103.39	110.83
4	A	3	BMA	C6-C5-C4	2.92	119.85	113.00
4	A	4	MAN	C6-C5-C4	-2.91	106.18	113.00
4	A	3	BMA	O5-C5-C6	2.90	111.74	107.20
4	A	1	NAG	C6-C5-C4	2.88	119.76	113.00
4	A	3	BMA	C1-O5-C5	2.82	116.01	112.19
4	A	2	NAG	C1-O5-C5	2.78	115.96	112.19
4	A	4	MAN	O5-C1-C2	2.78	115.06	110.77
4	A	5	MAN	O2-C2-C1	2.73	114.75	109.15
4	A	5	MAN	C2-C3-C4	2.68	115.53	110.89
4	A	1	NAG	C4-C3-C2	-2.59	107.23	111.02
4	A	1	NAG	C8-C7-N2	2.58	120.47	116.10
4	A	5	MAN	C3-C4-C5	2.57	114.82	110.24
4	A	4	MAN	O3-C3-C2	-2.42	105.35	109.99
4	A	4	MAN	O2-C2-C1	-2.36	104.32	109.15
4	A	3	BMA	O6-C6-C5	2.32	119.24	111.29
4	A	1	NAG	O3-C3-C2	2.07	113.75	109.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	6	MAN	O5-C5-C6-O6
4	A	3	BMA	C4-C5-C6-O6
4	A	6	MAN	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6
4	A	5	MAN	C4-C5-C6-O6
4	A	5	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

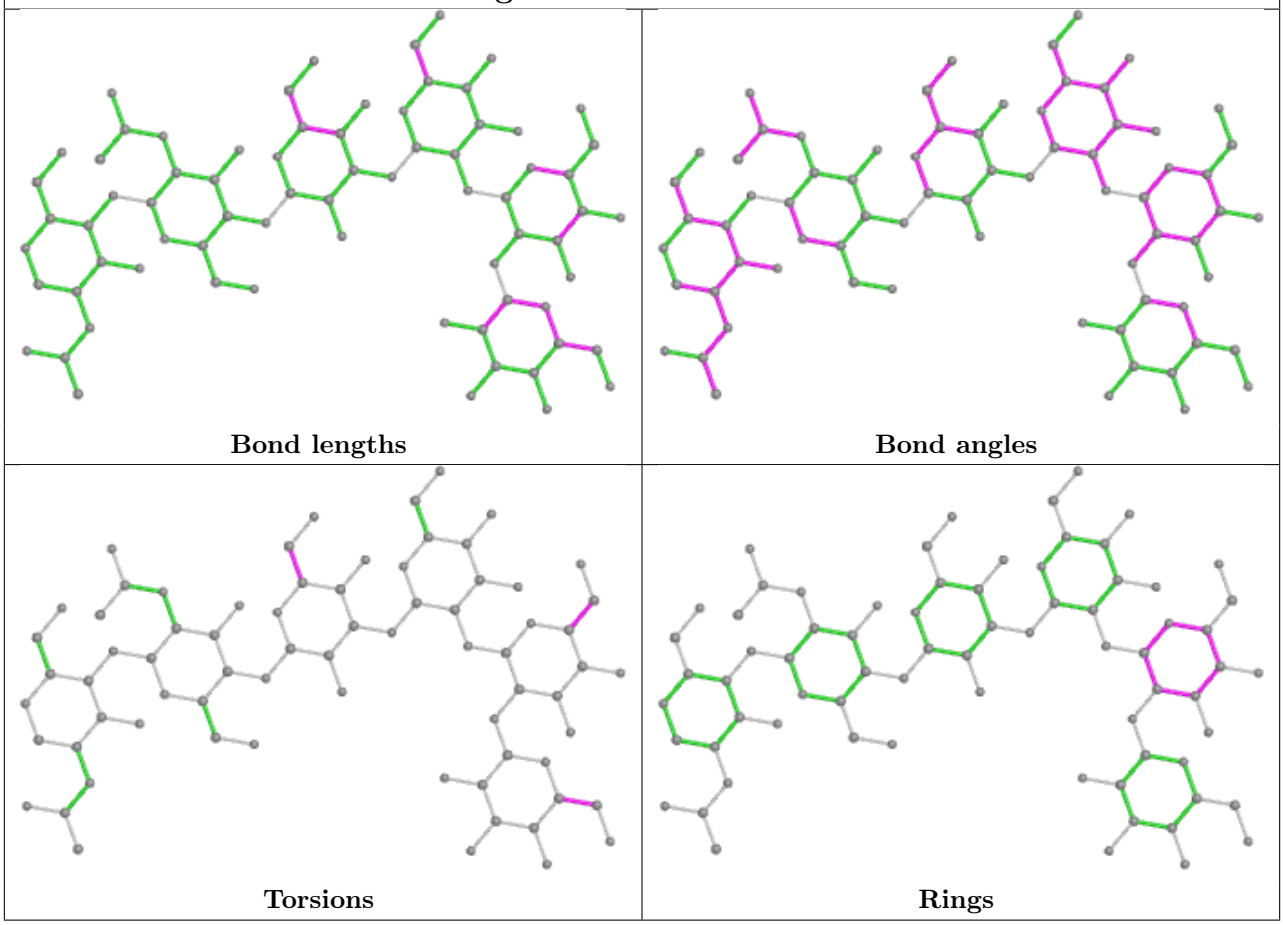
Mol	Chain	Res	Type	Atoms
4	A	5	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4	MAN	1	0
4	A	5	MAN	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.

Oligosaccharide Chain A



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	N	475(A)	1	14,14,15	1.45	2 (14%)	17,19,21	1.78	5 (29%)
5	NAG	N	476(A)	1	14,14,15	0.88	1 (7%)	17,19,21	1.74	6 (35%)

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
5	NAG	N	475(A)	1	-	0/6/23/26	0/1/1/1
5	NAG	N	476(A)	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	475(A)	NAG	C2-N2	-3.86	1.39	1.46
5	N	475(A)	NAG	O5-C1	2.23	1.47	1.43
5	N	476(A)	NAG	C4-C3	2.03	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	476(A)	NAG	C4-C3-C2	-3.54	105.83	111.02
5	N	475(A)	NAG	C8-C7-N2	3.40	121.86	116.10
5	N	475(A)	NAG	C6-C5-C4	3.10	120.27	113.00
5	N	476(A)	NAG	C8-C7-N2	2.74	120.74	116.10
5	N	475(A)	NAG	O5-C5-C6	-2.52	103.26	107.20
5	N	475(A)	NAG	O3-C3-C4	2.42	115.94	110.35
5	N	475(A)	NAG	O4-C4-C5	2.37	115.19	109.30
5	N	476(A)	NAG	C1-C2-N2	2.24	114.32	110.49
5	N	476(A)	NAG	O7-C7-C8	-2.13	118.10	122.06
5	N	476(A)	NAG	O5-C5-C6	2.10	110.50	107.20
5	N	476(A)	NAG	O5-C5-C4	-2.08	105.76	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	476(A)	NAG	O5-C5-C6-O6
5	N	476(A)	NAG	C1-C2-N2-C7
5	N	476(A)	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	475(A)	NAG	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	N	389/389 (100%)	-1.17	1 (0%)	94	94	2, 3, 18, 39	0
2	L	214/214 (100%)	-0.77	2 (0%)	84	86	2, 19, 38, 68	0
3	H	221/221 (100%)	-0.58	6 (2%)	54	58	2, 24, 44, 67	0
All	All	824/824 (100%)	-0.91	9 (1%)	80	82	2, 12, 37, 68	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	135	GLY	5.6
3	H	130	ASP	5.1
3	H	134	THR	4.2
2	L	214	CYS	4.0
2	L	213	GLU	3.4
3	H	133	THR	3.4
3	H	227	GLY	3.2
3	H	128	CYS	2.5
1	N	465	GLU	2.1

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)

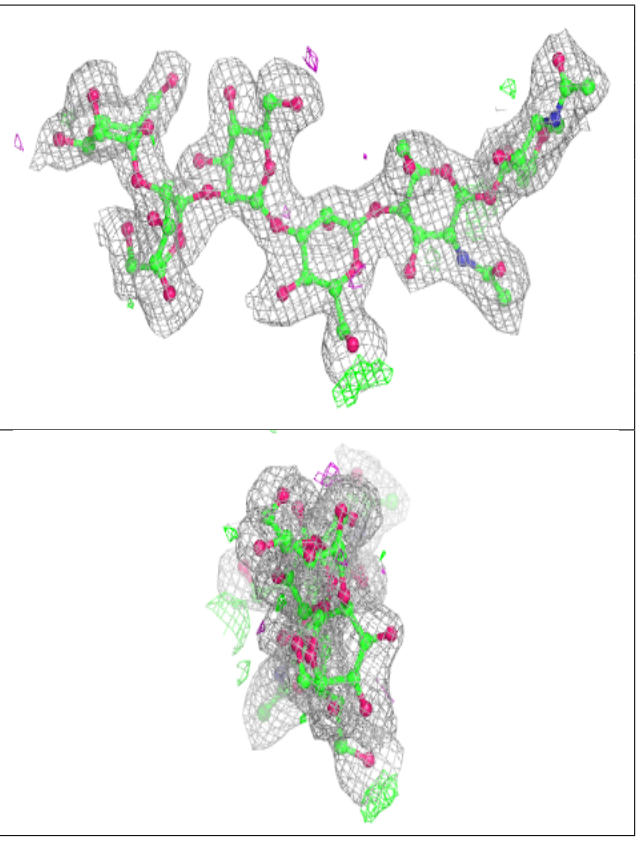
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	A	4	11/12	0.96	0.10	6,7,9,11	0
4	MAN	A	5	11/12	0.96	0.10	10,13,15,17	0
4	BMA	A	3	11/12	0.97	0.09	5,7,8,9	0
4	NAG	A	1	14/15	0.97	0.10	8,11,16,17	0
4	NAG	A	2	14/15	0.97	0.09	8,11,12,13	0
4	MAN	A	6	11/12	0.97	0.10	13,14,15,16	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 A:

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



6.4 Ligands (i)

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
5	NAG	N	476(A)	14/15	0.92	0.14	20,22,26,27	0
6	CA	N	1	1/1	0.95	0.18	44,44,44,44	0
5	NAG	N	475(A)	14/15	0.97	0.10	19,22,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.