Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:48 PM EDT

PDB ID	:	1FQ8
Title	:	X-RAY STRUCTURE OF DIFLUOROSTATINE INHIBITOR CP81,198 BOUND TO SACCHAROPEPSIN
Authors	:	Cronin, N.B.; Badasso, M.O.; Tickle, I.J.; Dreyer, T.; Hoover, D.J.; Rosati, R.L.; Humblet, C.C.; Lunney, E.A.; Cooper, J.B.
Deposited on	:	2000-09-04
Resolution	:	2.80 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 (1)) were used in the production of this report:

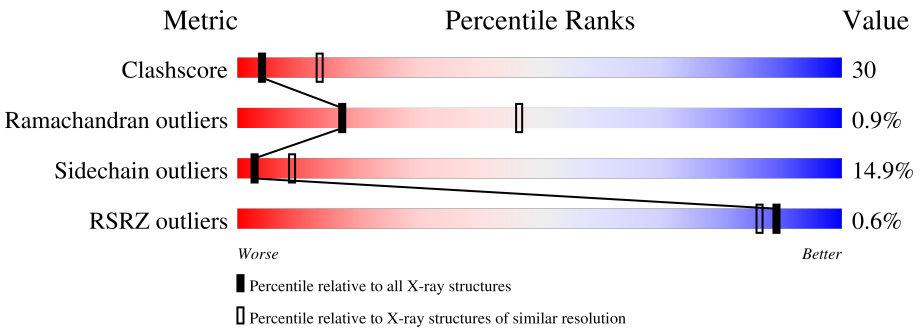
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	329	% 48% 35% 15% .
2	B	5	40% 40% 20%

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
2	NAG	B	2	X	-	-	-
2	MAN	B	3	X	-	-	-
2	MAN	B	4	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2812 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.

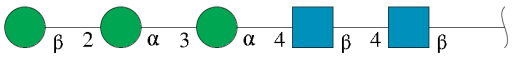
- Molecule 1 is a protein called SACCHAROPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2528	1618	396	508	6	0	0	0

There is a discrepancy between the modelled and reference sequences:

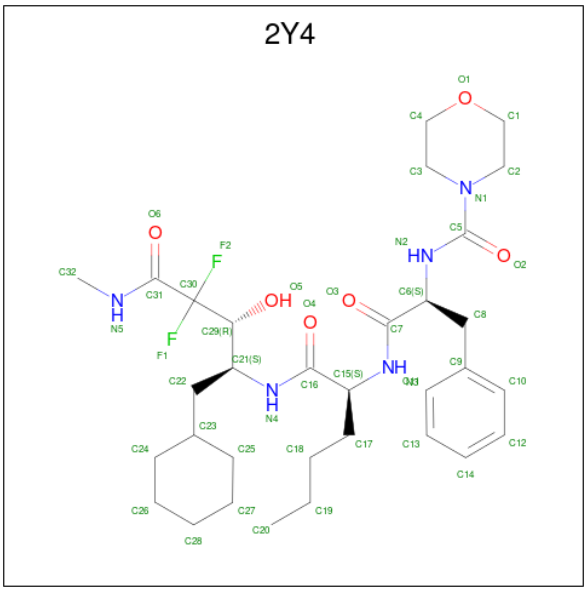
Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ILE	LEU	conflict	UNP P07267

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



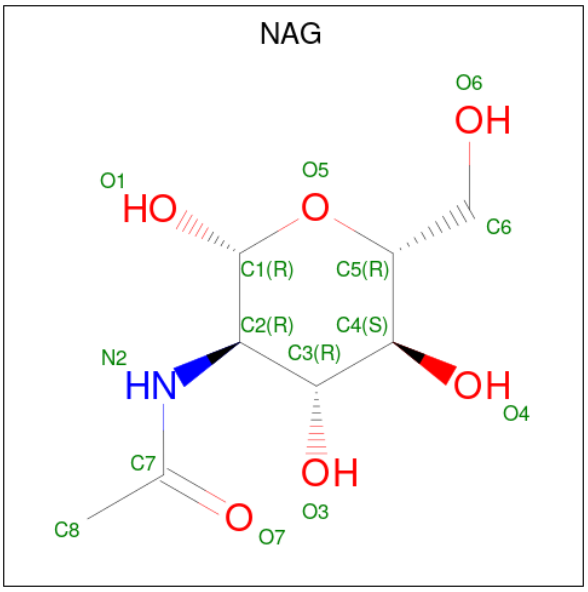
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	61	34	2	25	0	0	0

- Molecule 3 is N-[(2S)-1-[[(2S)-1-[[(2S,3R)-1-cyclohexyl-4,4-difluoro-3-hydroxy-5-(methylamino)-5-oxo-pentan-2-yl]amino]-1-oxo-hexan-2 -yl]amino]-1-oxo-3-phenyl-propan-2-yl]morpholine-4-carboxamide (three-letter code: 2Y4) (formula: $C_{32}H_{49}F_2N_5O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	45	32	2	5	6	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is water.

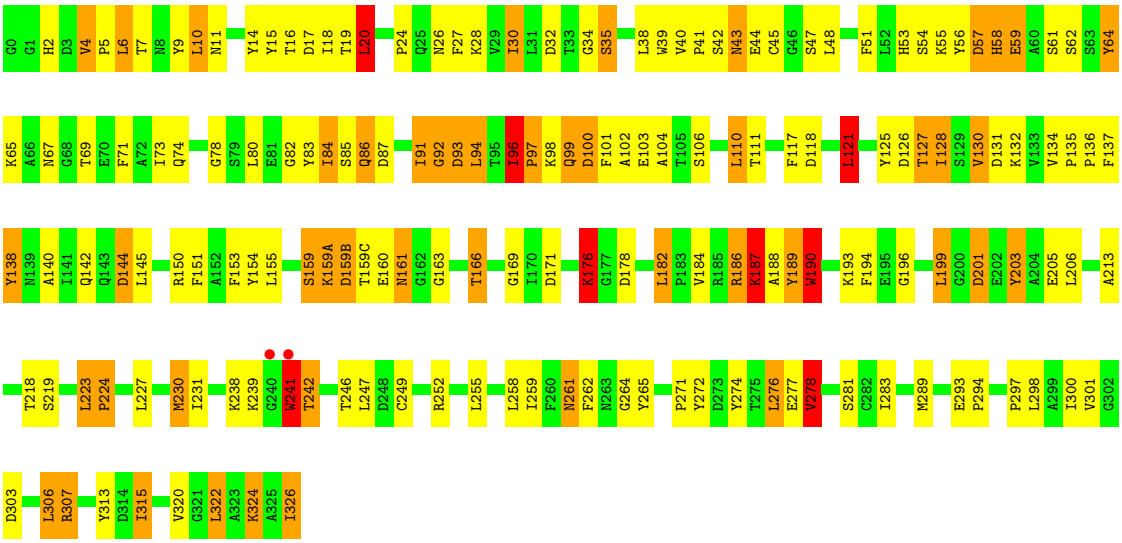
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	164	164	164	0	0

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: SACCHAROPEPSIN

Chain A:



• Molecule 2: beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-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 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.82Å 86.82Å 110.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.40 – 2.80 15.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.40-2.80) 99.5 (15.41-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.48 (at 2.81Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.190 , 0.270 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2812	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 2Y4, MAN

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	0.78	0/2592	1.89	86/3526 (2.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	6	0

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ASP	CB-CG-OD1	-11.98	107.51	118.30
1	A	130	VAL	CA-CB-CG1	9.93	125.80	110.90
1	A	189	TYR	CA-CB-CG	9.78	131.98	113.40
1	A	150	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	278	VAL	CA-CB-CG1	9.57	125.26	110.90
1	A	150	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	186	ARG	CG-CD-NE	8.92	130.54	111.80
1	A	324	LYS	CA-CB-CG	8.85	132.87	113.40
1	A	239	LYS	CD-CE-NZ	8.54	131.35	111.70
1	A	289	MET	CG-SD-CE	8.50	113.80	100.20
1	A	230	MET	CG-SD-CE	-8.48	86.63	100.20
1	A	203	TYR	CB-CG-CD1	8.14	125.89	121.00
1	A	178	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	186	ARG	CA-CB-CG	7.90	130.79	113.40
1	A	4	VAL	CA-CB-CG1	7.82	122.63	110.90
1	A	301	VAL	CA-CB-CG1	7.76	122.54	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	TYR	CB-CG-CD1	-7.75	116.35	121.00
1	A	153	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	A	96	ILE	C-N-CD	7.60	144.37	128.40
1	A	132	LYS	CD-CE-NZ	7.50	128.94	111.70
1	A	34	GLY	C-N-CA	7.49	140.41	121.70
1	A	62	SER	C-N-CA	7.37	140.12	121.70
1	A	166	THR	CA-CB-CG2	7.35	122.68	112.40
1	A	153	PHE	CG-CD2-CE2	-7.33	112.74	120.80
1	A	298	LEU	CA-CB-CG	7.33	132.15	115.30
1	A	138	TYR	CB-CG-CD1	7.32	125.39	121.00
1	A	201	ASP	CB-CG-OD1	7.26	124.84	118.30
1	A	131	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	100	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	92	GLY	C-N-CA	7.16	139.59	121.70
1	A	171	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	176	LYS	CD-CE-NZ	7.12	128.07	111.70
1	A	94	LEU	CA-CB-CG	7.04	131.50	115.30
1	A	57	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	320	VAL	CG1-CB-CG2	6.88	121.91	110.90
1	A	154	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	94	LEU	CB-CG-CD2	-6.80	99.44	111.00
1	A	322	LEU	CB-CG-CD2	6.78	122.52	111.00
1	A	307	ARG	CG-CD-NE	-6.75	97.62	111.80
1	A	150	ARG	CD-NE-CZ	6.70	132.98	123.60
1	A	138	TYR	CA-CB-CG	6.69	126.11	113.40
1	A	186	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	A	6	LEU	CB-CG-CD1	6.57	122.17	111.00
1	A	189	TYR	CA-C-N	6.48	131.46	117.20
1	A	252	ARG	CG-CD-NE	6.46	125.36	111.80
1	A	126	ASP	C-N-CA	6.41	137.72	121.70
1	A	20	LEU	C-N-CA	-6.25	109.17	122.30
1	A	96	ILE	CA-CB-CG2	6.25	123.40	110.90
1	A	199	LEU	CA-CB-CG	6.13	129.41	115.30
1	A	94	LEU	CB-CG-CD1	-6.13	100.58	111.00
1	A	187	LYS	CD-CE-NZ	-6.10	97.67	111.70
1	A	186	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	A	306	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	201	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	258	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	194	PHE	CB-CG-CD1	5.94	124.96	120.80
1	A	184	VAL	CA-CB-CG2	-5.93	102.00	110.90
1	A	315	ILE	CA-CB-CG1	5.81	122.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	97	PRO	N-CD-CG	-5.77	94.55	103.20
1	A	272	TYR	C-N-CA	5.71	135.98	121.70
1	A	93	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	86	GLN	N-CA-CB	5.67	120.82	110.60
1	A	86	GLN	CB-CA-C	5.65	121.70	110.40
1	A	144	ASP	C-N-CA	5.63	135.78	121.70
1	A	252	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	150	ARG	CB-CG-CD	-5.56	97.14	111.60
1	A	182	LEU	CB-CG-CD1	5.56	120.45	111.00
1	A	190	TRP	CA-C-O	5.52	131.68	120.10
1	A	47	SER	O-C-N	5.50	131.50	122.70
1	A	20	LEU	O-C-N	-5.47	113.91	123.20
1	A	306	LEU	N-CA-CB	5.44	121.29	110.40
1	A	189	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	93	ASP	CA-CB-CG	-5.38	101.57	113.40
1	A	78	GLY	C-N-CA	5.32	135.01	121.70
1	A	97	PRO	CA-N-CD	-5.25	104.14	111.50
1	A	203	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	99	GLN	C-N-CA	-5.22	108.66	121.70
1	A	134	VAL	CA-CB-CG1	5.17	118.65	110.90
1	A	189	TYR	O-C-N	-5.16	114.44	122.70
1	A	84	ILE	N-CA-CB	5.12	122.58	110.80
1	A	227	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	121	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	155	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	223	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	255	LEU	CB-CG-CD2	-5.01	102.49	111.00

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	16	THR	CB
1	A	63	SER	CA
1	A	96	ILE	CB
1	A	166	THR	CB
1	A	241	TRP	CA
1	A	315	ILE	CB

There are no planarity outliers.

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	2528	0	2401	146	5
2	B	61	0	50	9	1
3	A	45	0	49	3	0
4	A	14	0	13	0	0
5	A	164	0	0	26	6
All	All	2812	0	2513	155	8

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 30.

All (155) 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:A:69:THR:HB	1:A:84:ILE:HD13	1.21	1.10
1:A:242:THR:CG2	1:A:242:THR:O	2.02	1.07
1:A:242:THR:O	1:A:242:THR:HG22	1.37	1.06
1:A:189:TYR:O	1:A:190:TRP:HB2	1.59	1.01
1:A:261:ASN:HD22	1:A:261:ASN:C	1.66	0.98
1:A:97:PRO:HD3	5:A:515:HOH:O	1.65	0.97
1:A:261:ASN:HD21	1:A:264:GLY:H	1.19	0.90
1:A:97:PRO:O	1:A:98:LYS:HB2	1.69	0.90
1:A:69:THR:HB	1:A:84:ILE:CD1	2.02	0.89
1:A:159(B):ASP:HB3	5:A:635:HOH:O	1.73	0.88
1:A:128:ILE:O	1:A:128:ILE:HG12	1.73	0.87
1:A:58:HIS:HB2	1:A:64:TYR:CD2	2.10	0.87
2:B:4:MAN:C2	2:B:5:BMA:C1	2.61	0.78
1:A:161:ASN:HA	5:A:661:HOH:O	1.84	0.77
1:A:121:LEU:C	1:A:121:LEU:HD12	2.05	0.77
1:A:176:LYS:HG2	1:A:326:ILE:HD12	1.68	0.75
1:A:201:ASP:HB2	5:A:638:HOH:O	1.86	0.75
1:A:84:ILE:HG22	1:A:85:SER:N	1.99	0.75
1:A:159:SER:HA	5:A:654:HOH:O	1.87	0.75
1:A:32:ASP:OD2	1:A:35:SER:HB2	1.87	0.74
1:A:84:ILE:CG2	1:A:85:SER:N	2.51	0.74
1:A:159(C):THR:OG1	1:A:160:GLU:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:HB3	1:A:118:ASP:OD1	1.88	0.72
1:A:84:ILE:CG2	1:A:85:SER:H	2.01	0.72
1:A:38:LEU:HD13	1:A:121:LEU:HB2	1.73	0.71
1:A:182:LEU:CD1	1:A:322:LEU:HD12	2.20	0.71
2:B:4:MAN:C2	2:B:4:MAN:O2	2.38	0.70
1:A:84:ILE:H	1:A:84:ILE:HD12	1.55	0.70
1:A:57:ASP:OD1	1:A:59:GLU:HG3	1.91	0.70
1:A:159(C):THR:HA	5:A:640:HOH:O	1.93	0.69
1:A:4:VAL:HG23	1:A:16:THR:HG21	1.73	0.69
1:A:86:GLN:O	1:A:87:ASP:HB2	1.91	0.69
2:B:3:MAN:C1	2:B:3:MAN:O2	2.40	0.69
1:A:16:THR:HG22	1:A:17:ASP:H	1.57	0.69
1:A:137:PHE:HE2	1:A:315:ILE:CG2	2.04	0.69
1:A:65:LYS:HE3	5:A:649:HOH:O	1.92	0.68
1:A:58:HIS:HB2	1:A:64:TYR:CG	2.28	0.68
1:A:64:TYR:CD1	1:A:65:LYS:N	2.62	0.68
1:A:48:LEU:HD12	1:A:48:LEU:O	1.92	0.68
2:B:3:MAN:O2	2:B:3:MAN:H3	1.93	0.68
1:A:313:TYR:N	1:A:313:TYR:CD1	2.62	0.67
2:B:3:MAN:O2	2:B:3:MAN:C2	2.43	0.67
1:A:261:ASN:HD21	1:A:264:GLY:N	1.92	0.66
2:B:4:MAN:O2	2:B:4:MAN:C1	2.44	0.66
1:A:261:ASN:HD22	1:A:262:PHE:N	1.93	0.65
1:A:303:ASP:O	1:A:307:ARG:HG3	1.96	0.65
1:A:96:ILE:HA	5:A:515:HOH:O	1.96	0.65
1:A:189:TYR:O	1:A:190:TRP:CB	2.31	0.65
1:A:182:LEU:HD11	1:A:322:LEU:HD12	1.79	0.64
1:A:261:ASN:C	1:A:261:ASN:ND2	2.42	0.64
1:A:161:ASN:C	1:A:161:ASN:HD22	2.00	0.63
1:A:51:PHE:HB3	5:A:555:HOH:O	1.99	0.62
1:A:16:THR:HG22	1:A:17:ASP:N	2.15	0.62
1:A:261:ASN:ND2	1:A:264:GLY:H	1.95	0.61
1:A:86:GLN:NE2	1:A:98:LYS:HA	2.16	0.61
1:A:30:ILE:HD12	1:A:117:PHE:CD2	2.36	0.60
1:A:84:ILE:HD12	1:A:84:ILE:N	2.16	0.60
2:B:3:MAN:O2	2:B:3:MAN:C3	2.49	0.60
1:A:86:GLN:HE21	1:A:98:LYS:HA	1.66	0.60
1:A:196:GLY:HA3	1:A:203:TYR:OH	2.03	0.59
2:B:4:MAN:O2	2:B:4:MAN:C3	2.50	0.59
1:A:6:LEU:HB2	1:A:163:GLY:CA	2.33	0.58
1:A:277:GLU:HG2	5:A:557:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD13	5:A:501:HOH:O	2.03	0.58
1:A:205:GLU:O	1:A:206:LEU:HD23	2.04	0.57
1:A:213:ALA:HB3	1:A:300:ILE:HG12	1.87	0.57
1:A:166:THR:HG22	1:A:169:GLY:O	2.05	0.56
1:A:84:ILE:CG2	1:A:100:ASP:HB3	2.36	0.56
1:A:110:LEU:HD12	5:A:642:HOH:O	2.04	0.56
1:A:65:LYS:HB3	1:A:86:GLN:HG2	1.87	0.56
1:A:145:LEU:HD22	5:A:524:HOH:O	2.04	0.56
1:A:246:THR:HG22	1:A:283:ILE:HG22	1.89	0.56
1:A:271:PRO:HA	1:A:274:TYR:CE2	2.41	0.56
1:A:9:TYR:CZ	1:A:10:LEU:HD22	2.42	0.55
1:A:97:PRO:O	1:A:98:LYS:CB	2.45	0.55
1:A:4:VAL:CG2	1:A:16:THR:HG21	2.37	0.55
1:A:151:PHE:HA	1:A:166:THR:O	2.08	0.54
1:A:84:ILE:HG21	1:A:100:ASP:HB3	1.88	0.54
1:A:67:ASN:C	1:A:67:ASN:OD1	2.46	0.54
1:A:140:ALA:O	1:A:145:LEU:HB2	2.08	0.54
1:A:48:LEU:HA	5:A:555:HOH:O	2.08	0.54
1:A:219:SER:HB2	3:A:400:2Y4:H3	1.89	0.54
1:A:6:LEU:HB2	1:A:163:GLY:HA3	1.90	0.54
1:A:188:ALA:HB3	5:A:566:HOH:O	2.07	0.53
1:A:276:LEU:HD23	1:A:283:ILE:HD11	1.91	0.53
1:A:223:LEU:HB3	1:A:224:PRO:HD2	1.91	0.53
1:A:15:TYR:CE2	1:A:28:LYS:HD3	2.44	0.53
1:A:315:ILE:HD12	5:A:532:HOH:O	2.08	0.53
1:A:249:CYS:HB3	5:A:550:HOH:O	2.08	0.53
1:A:86:GLN:O	1:A:87:ASP:CB	2.53	0.52
1:A:42:SER:O	1:A:55:LYS:HG2	2.10	0.52
1:A:69:THR:CB	1:A:84:ILE:HD13	2.15	0.52
1:A:38:LEU:HD12	1:A:39:TRP:H	1.76	0.50
1:A:6:LEU:HB2	1:A:163:GLY:C	2.31	0.50
1:A:84:ILE:HG23	1:A:85:SER:H	1.75	0.50
1:A:18:ILE:O	1:A:18:ILE:HG13	2.09	0.50
1:A:30:ILE:CD1	1:A:117:PHE:CD2	2.95	0.49
1:A:48:LEU:HD12	1:A:48:LEU:C	2.32	0.49
1:A:30:ILE:HD12	1:A:117:PHE:CG	2.47	0.49
1:A:218:THR:HG23	3:A:400:2Y4:H15	1.93	0.49
1:A:17:ASP:OD2	1:A:28:LYS:HE2	2.13	0.49
1:A:91:ILE:O	1:A:92:GLY:C	2.50	0.49
1:A:2:HIS:HD2	1:A:93:ASP:OD2	1.96	0.48
1:A:2:HIS:HE1	5:A:632:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG22	1:A:127:THR:O	2.13	0.48
1:A:324:LYS:HD3	5:A:634:HOH:O	2.13	0.48
1:A:83:TYR:HD1	1:A:84:ILE:O	1.97	0.47
1:A:121:LEU:C	1:A:121:LEU:CD1	2.79	0.47
1:A:11:ASN:HB3	1:A:307:ARG:NH1	2.29	0.47
1:A:121:LEU:HD12	1:A:121:LEU:O	2.15	0.47
1:A:187:LYS:HZ3	1:A:187:LYS:HG3	1.27	0.46
1:A:278:VAL:O	1:A:278:VAL:HG12	2.16	0.46
1:A:41:PRO:HA	1:A:104:ALA:HB3	1.98	0.46
1:A:39:TRP:HE3	1:A:40:VAL:N	2.14	0.46
1:A:58:HIS:HB2	1:A:64:TYR:CE2	2.50	0.45
1:A:9:TYR:CE1	1:A:10:LEU:HD22	2.51	0.45
1:A:137:PHE:HE2	1:A:315:ILE:HG21	1.80	0.45
1:A:41:PRO:HG2	1:A:54:SER:O	2.17	0.45
1:A:51:PHE:CB	5:A:555:HOH:O	2.61	0.45
1:A:86:GLN:HG3	1:A:87:ASP:N	2.33	0.44
1:A:99:GLN:OE1	1:A:136:PRO:HA	2.17	0.44
1:A:176:LYS:HE3	1:A:176:LYS:HB2	1.59	0.44
1:A:84:ILE:HG23	1:A:101:PHE:O	2.17	0.44
1:A:159(A):LYS:HB2	1:A:159(A):LYS:HE2	1.82	0.44
1:A:28:LYS:HD2	5:A:546:HOH:O	2.17	0.44
1:A:326:ILE:OXT	1:A:326:ILE:HG22	2.17	0.43
1:A:5:PRO:O	1:A:16:THR:HG23	2.18	0.43
1:A:94:LEU:HD23	5:A:524:HOH:O	2.18	0.43
1:A:56:TYR:HD2	1:A:103:GLU:OE1	2.02	0.43
1:A:71:PHE:CE1	1:A:130:VAL:CG1	3.02	0.43
1:A:135:PRO:HG2	1:A:138:TYR:CD1	2.53	0.43
1:A:219:SER:CB	3:A:400:2Y4:H3	2.48	0.43
1:A:84:ILE:HG22	1:A:85:SER:H	1.68	0.43
1:A:128:ILE:HD12	1:A:128:ILE:HG21	1.64	0.43
1:A:7:THR:O	1:A:14:TYR:HA	2.19	0.43
2:B:4:MAN:C3	2:B:5:BMA:C1	2.96	0.42
1:A:294:PRO:HG2	5:A:664:HOH:O	2.18	0.42
1:A:145:LEU:HD11	5:A:515:HOH:O	2.19	0.42
1:A:137:PHE:HE2	1:A:315:ILE:HG23	1.80	0.42
1:A:19:THR:HB	1:A:24:PRO:HB3	2.00	0.42
1:A:73:ILE:CG2	1:A:80:LEU:HD21	2.49	0.42
1:A:259:ILE:HG21	1:A:259:ILE:HD13	1.79	0.42
1:A:261:ASN:HA	1:A:265:TYR:O	2.19	0.42
1:A:186:ARG:HH11	1:A:186:ARG:HD2	1.58	0.42
1:A:297:PRO:HD2	5:A:628:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:CD1	1:A:64:TYR:C	2.89	0.41
1:A:125:TYR:CD2	1:A:187:LYS:HB3	2.55	0.41
1:A:28:LYS:HE3	5:A:546:HOH:O	2.19	0.41
1:A:61:SER:HB3	1:A:64:TYR:HB2	2.03	0.41
1:A:73:ILE:CG2	1:A:80:LEU:CD2	2.98	0.41
1:A:82:GLY:HA3	1:A:103:GLU:O	2.20	0.41
1:A:101:PHE:HD1	1:A:102:ALA:N	2.19	0.40
1:A:20:LEU:HA	1:A:20:LEU:HD12	1.36	0.40
1:A:223:LEU:O	1:A:224:PRO:C	2.59	0.40
1:A:127:THR:O	1:A:127:THR:CG2	2.70	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MET:CB	5:A:633:HOH:O[5_675]	1.17	1.03
1:A:230:MET:CG	5:A:633:HOH:O[5_675]	1.19	1.01
5:A:622:HOH:O	5:A:623:HOH:O[3_565]	1.89	0.31
2:B:5:BMA:O3	5:A:654:HOH:O[3_565]	1.93	0.27
1:A:230:MET:SD	5:A:633:HOH:O[5_675]	1.95	0.25
1:A:43:ASN:O	1:A:241:TRP:CZ2[6_555]	1.99	0.21
5:A:654:HOH:O	5:A:655:HOH:O[2_664]	1.99	0.21
1:A:45:CYS:O	1:A:241:TRP:CZ3[6_555]	2.07	0.13

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	327/329 (99%)	293 (90%)	31 (10%)	3 (1%)	17 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	TRP
1	A	127	THR
1	A	190	TRP

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	268/268 (100%)	228 (85%)	40 (15%)	3 9

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

Mol	Chain	Res	Type
1	A	10	LEU
1	A	20	LEU
1	A	26	ASN
1	A	27	PHE
1	A	30	ILE
1	A	35	SER
1	A	43	ASN
1	A	44	GLU
1	A	58	HIS
1	A	59	GLU
1	A	74	GLN
1	A	91	ILE
1	A	96	ILE
1	A	106	SER
1	A	110	LEU
1	A	111	THR
1	A	121	LEU
1	A	128	ILE
1	A	142	GLN
1	A	144	ASP
1	A	159	SER
1	A	159(A)	LYS
1	A	159(B)	ASP
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	176	LYS
1	A	187	LYS
1	A	193	LYS
1	A	199	LEU
1	A	224	PRO
1	A	231	ILE
1	A	238	LYS
1	A	241	TRP
1	A	242	THR
1	A	247	LEU
1	A	261	ASN
1	A	278	VAL
1	A	281	SER
1	A	293	GLU
1	A	306	LEU
1	A	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	43	ASN
1	A	86	GLN
1	A	161	ASN
1	A	232	ASN
1	A	261	ASN
1	A	317	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)

5 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	B	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	2.21	5 (29%)
2	NAG	B	2	2	14,14,15	1.24	2 (14%)	17,19,21	2.76	7 (41%)
2	MAN	B	3	2	11,11,12	14.31	2 (18%)	15,15,17	7.10	6 (40%)
2	MAN	B	4	2	11,11,12	13.70	3 (27%)	15,15,17	7.04	11 (73%)
2	BMA	B	5	2	11,11,12	1.30	3 (27%)	15,15,17	3.17	5 (33%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	MAN	B	3	2	2/2/4/5	1/2/19/22	0/1/1/1
2	MAN	B	4	2	1/1/4/5	2/2/19/22	0/1/1/1
2	BMA	B	5	2	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	MAN	O2-C2	47.32	2.43	1.43
2	B	4	MAN	O2-C2	45.10	2.38	1.43
2	B	4	MAN	C2-C3	-3.75	1.47	1.52
2	B	4	MAN	C4-C3	-3.09	1.44	1.52
2	B	1	NAG	C2-N2	2.64	1.50	1.46
2	B	5	BMA	O5-C1	2.59	1.47	1.43
2	B	2	NAG	O4-C4	2.52	1.48	1.43
2	B	2	NAG	C2-N2	2.44	1.50	1.46
2	B	3	MAN	O4-C4	2.33	1.48	1.43
2	B	5	BMA	C2-C3	-2.25	1.49	1.52
2	B	5	BMA	O4-C4	2.20	1.48	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	MAN	O2-C2-C1	-18.96	70.37	109.15
2	B	3	MAN	O2-C2-C3	-18.00	74.07	110.14
2	B	4	MAN	O2-C2-C1	-17.41	73.52	109.15
2	B	4	MAN	O2-C2-C3	-16.66	76.77	110.14
2	B	2	NAG	C1-O5-C5	7.45	122.28	112.19
2	B	4	MAN	C2-C3-C4	7.43	123.75	110.89
2	B	5	BMA	C1-C2-C3	7.41	118.77	109.67
2	B	5	BMA	O5-C5-C4	7.39	128.82	110.83
2	B	3	MAN	O5-C5-C4	-6.14	95.89	110.83
2	B	1	NAG	C1-O5-C5	4.93	118.87	112.19
2	B	4	MAN	O3-C3-C2	4.87	119.32	109.99
2	B	1	NAG	C2-N2-C7	-4.85	115.99	122.90
2	B	2	NAG	O5-C1-C2	4.29	118.06	111.29
2	B	4	MAN	O6-C6-C5	-4.28	96.62	111.29
2	B	4	MAN	O5-C1-C2	4.17	117.21	110.77
2	B	4	MAN	C1-C2-C3	3.88	114.44	109.67
2	B	2	NAG	O5-C5-C4	3.70	119.83	110.83
2	B	1	NAG	O5-C5-C4	3.50	119.35	110.83
2	B	3	MAN	C1-O5-C5	3.48	116.91	112.19
2	B	5	BMA	C1-O5-C5	3.45	116.87	112.19
2	B	3	MAN	O5-C5-C6	-3.01	102.49	107.20
2	B	4	MAN	C1-O5-C5	2.84	116.04	112.19
2	B	2	NAG	O7-C7-C8	2.81	127.28	122.06
2	B	2	NAG	C3-C4-C5	-2.66	105.49	110.24
2	B	4	MAN	O5-C5-C6	-2.60	103.13	107.20
2	B	5	BMA	C6-C5-C4	2.53	118.92	113.00
2	B	2	NAG	O4-C4-C5	-2.49	103.11	109.30
2	B	1	NAG	O3-C3-C4	-2.45	104.68	110.35
2	B	4	MAN	C3-C4-C5	2.40	114.52	110.24
2	B	2	NAG	C2-N2-C7	-2.38	119.51	122.90
2	B	3	MAN	O3-C3-C4	-2.36	104.89	110.35
2	B	5	BMA	C2-C3-C4	2.25	114.79	110.89
2	B	4	MAN	C6-C5-C4	-2.05	108.20	113.00
2	B	1	NAG	C1-C2-N2	-2.02	107.05	110.49

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2	NAG	C1
2	B	3	MAN	C1
2	B	3	MAN	C3
2	B	4	MAN	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	B	5	BMA	O5-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	5	BMA	C4-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6

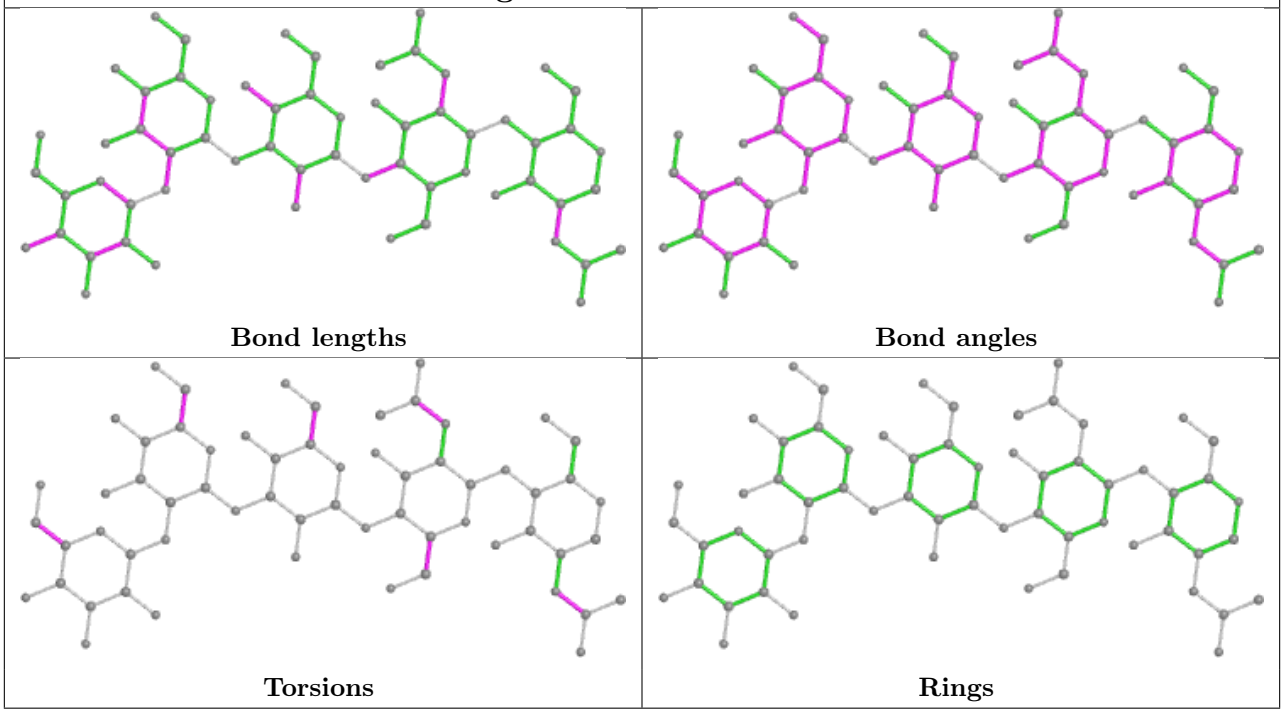
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	BMA	2	1
2	B	3	MAN	4	0
2	B	4	MAN	5	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 B



5.6 Ligand geometry (i)

2 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	2Y4	A	400	-	46,47,47	0.81	1 (2%)	52,63,63	2.06	9 (17%)
4	NAG	A	337	1	14,14,15	1.46	3 (21%)	17,19,21	3.73	9 (52%)

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	2Y4	A	400	-	-	6/52/70/70	0/3/3/3
4	NAG	A	337	1	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	337	NAG	O5-C5	2.75	1.49	1.43
4	A	337	NAG	O5-C1	2.66	1.48	1.43
4	A	337	NAG	O4-C4	2.57	1.49	1.43
3	A	400	2Y4	O6-C31	2.31	1.27	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	2Y4	O6-C31-C30	-9.79	110.50	118.32
4	A	337	NAG	O5-C1-C2	-9.01	97.06	111.29
4	A	337	NAG	C2-N2-C7	-5.73	114.75	122.90
4	A	337	NAG	O5-C5-C6	-5.33	98.85	107.20
3	A	400	2Y4	C4-C3-N1	4.91	120.30	109.84
4	A	337	NAG	O5-C5-C4	-4.71	99.36	110.83
3	A	400	2Y4	O6-C31-N5	-4.40	116.74	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	337	NAG	C8-C7-N2	-4.11	109.14	116.10
4	A	337	NAG	C1-O5-C5	-3.72	107.16	112.19
4	A	337	NAG	O6-C6-C5	-3.48	99.34	111.29
3	A	400	2Y4	C2-N1-C3	3.38	119.12	112.62
4	A	337	NAG	C4-C3-C2	3.21	115.73	111.02
3	A	400	2Y4	C21-N4-C16	3.19	128.72	123.07
4	A	337	NAG	O7-C7-C8	2.97	127.58	122.06
3	A	400	2Y4	C6-C7-N3	-2.28	111.71	116.70
3	A	400	2Y4	F2-C30-F1	-2.25	98.51	105.71
3	A	400	2Y4	C18-C17-C15	-2.18	107.18	113.92
3	A	400	2Y4	C25-C23-C24	2.17	114.62	109.33

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	2Y4	O6-C31-N5-C32
3	A	400	2Y4	F2-C30-C31-O6
4	A	337	NAG	O5-C5-C6-O6
4	A	337	NAG	C8-C7-N2-C2
4	A	337	NAG	C4-C5-C6-O6
4	A	337	NAG	O7-C7-N2-C2
3	A	400	2Y4	O5-C29-C30-F2
3	A	400	2Y4	C29-C30-C31-O6
3	A	400	2Y4	F1-C30-C31-O6
3	A	400	2Y4	N3-C15-C16-O4

There are no ring outliers.

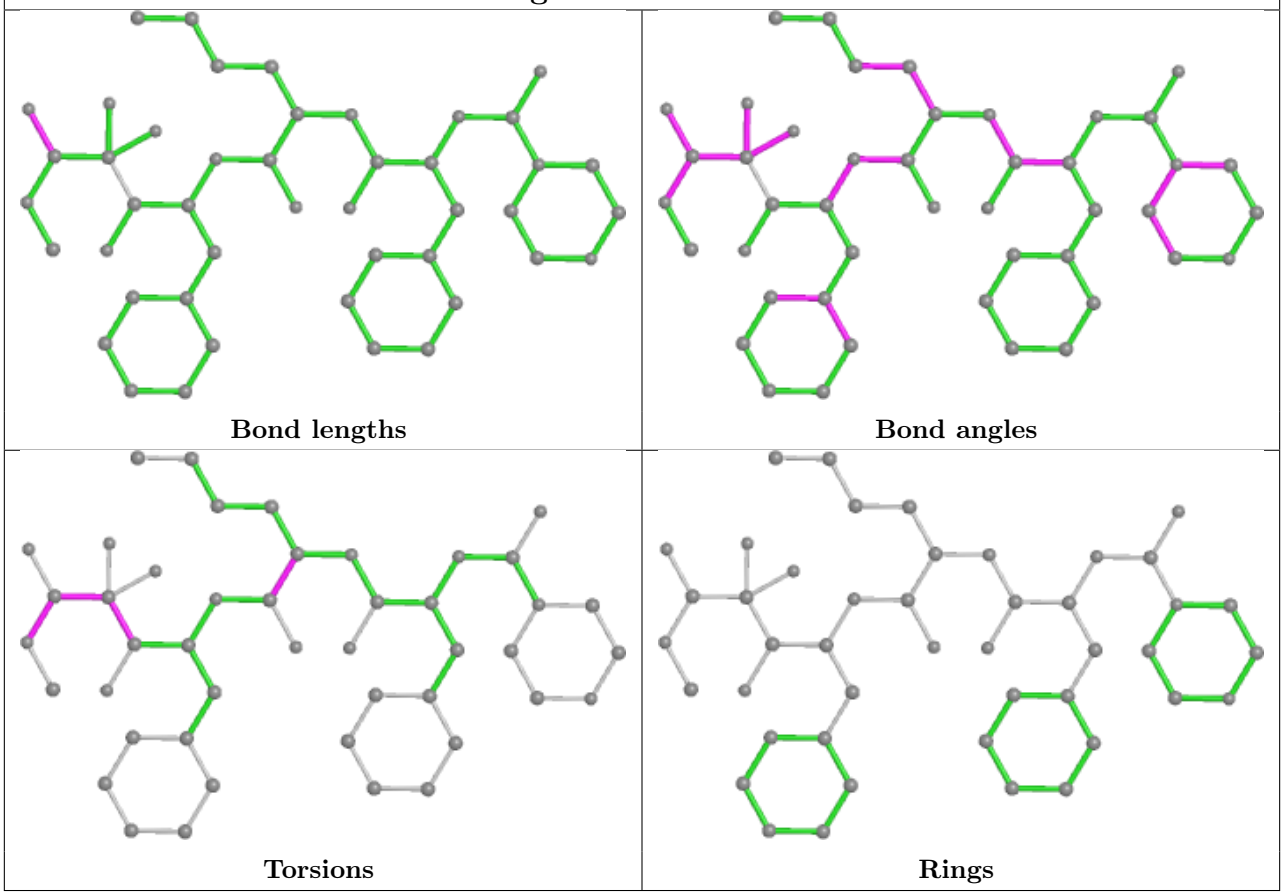
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	2Y4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 2Y4 A 400



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	A	329/329 (100%)	-0.87	2 (0%) 89 86	14, 26, 54, 116	4 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	TRP	3.6
1	A	240	GLY	2.9

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)

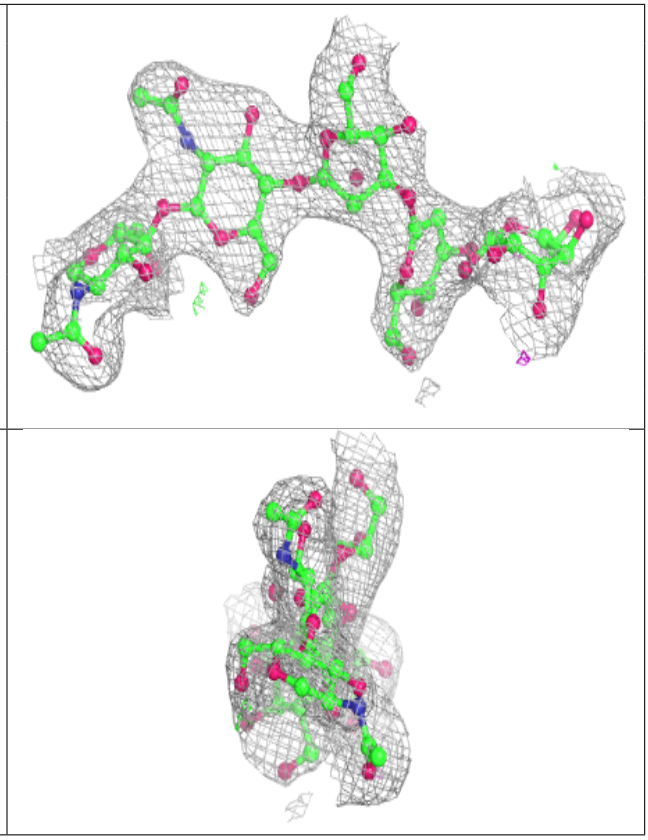
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	B	5	11/12	0.84	0.23	53,67,124,149	0
2	MAN	B	3	11/12	0.89	0.21	25,42,54,56	0
2	MAN	B	4	11/12	0.94	0.24	28,40,44,55	0
2	NAG	B	1	14/15	0.94	0.14	34,49,72,72	0
2	NAG	B	2	14/15	0.96	0.12	18,33,47,52	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 (i)

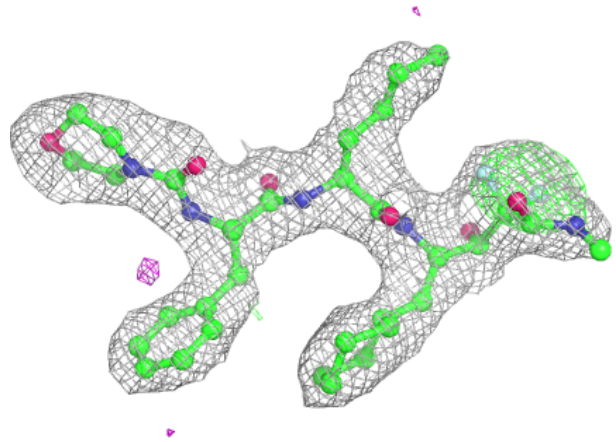
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

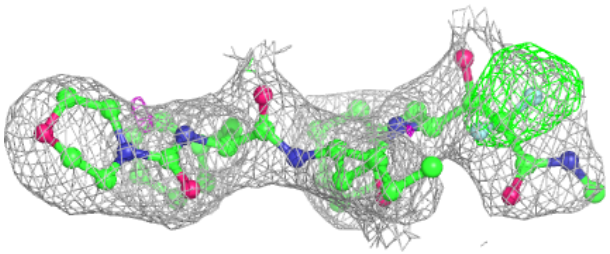
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	337	14/15	0.89	0.14	42,53,92,120	0
3	2Y4	A	400	45/45	0.91	0.15	1,24,36,44	0

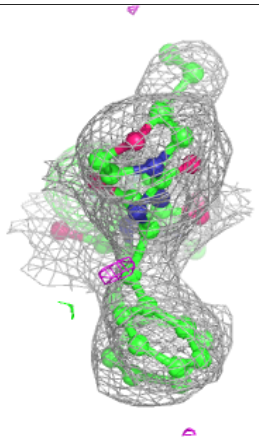
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2Y4 A 400:

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







6.5 Other polymers (i)

There are no such residues in this entry.