WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:36 PM EDT

PDB ID	:	1FQ6
Title	:	X-RAY STRUCTURE OF GLYCOL INHIBITOR PD-133,450 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	:	2000-09-03
Resolution	:	2.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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 ⓘ

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

The reported resolution of this entry is 2.70 Å.

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

Metric	Percentile Ranks	Value
Clashscore		24
Ramachandran outliers		0.3%
Sidechain outliers		19.0%
RSRZ outliers		1.5%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
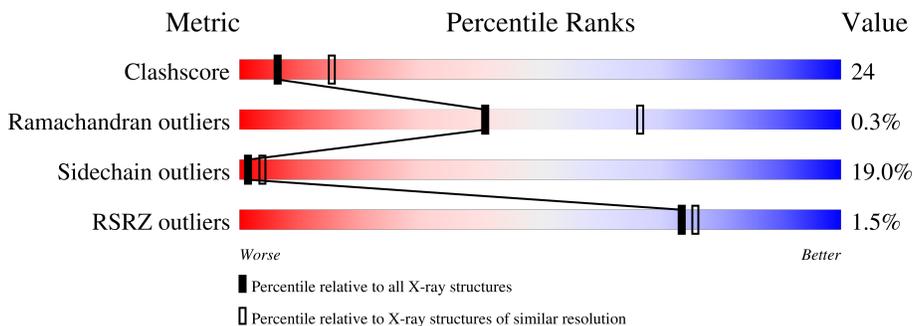
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	2% — 54% / 36% / 9% •
2	B	5	60% / 40%

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	GUP	B	5	X	-	-	-
4	NAG	A	337	X	-	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 2749 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
1	A	329	Total 2528	C 1618	N 396	O 508	S 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 alpha-L-gulopyranose-(1-2)-beta-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.
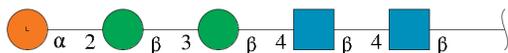
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 3 is N-[(1S)-2-{[(2S,3R,4S)-1-cyclohexyl-3,4-dihydroxy-6-methylheptan-2-yl]amino}-1-(ethylsulfanyl)-2-oxoethyl]-Nalpha-(morpholin-4-ylsulfonyl)-L-phenylalaninamide (three-letter code: 0QF) (formula: $C_{31}H_{52}N_4O_7S_2$).
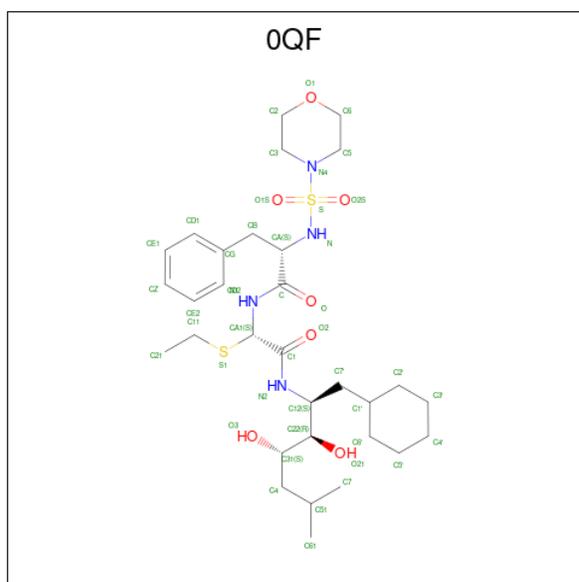
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			44	31	4	7	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
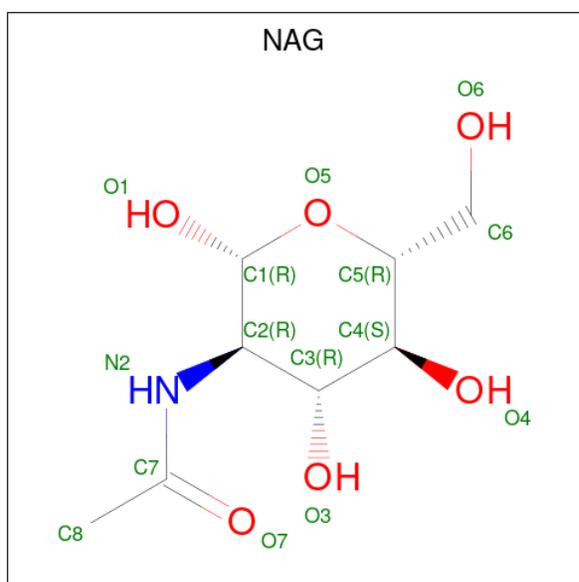
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total 102	O 102	0	0

3 Residue-property plots ⓘ

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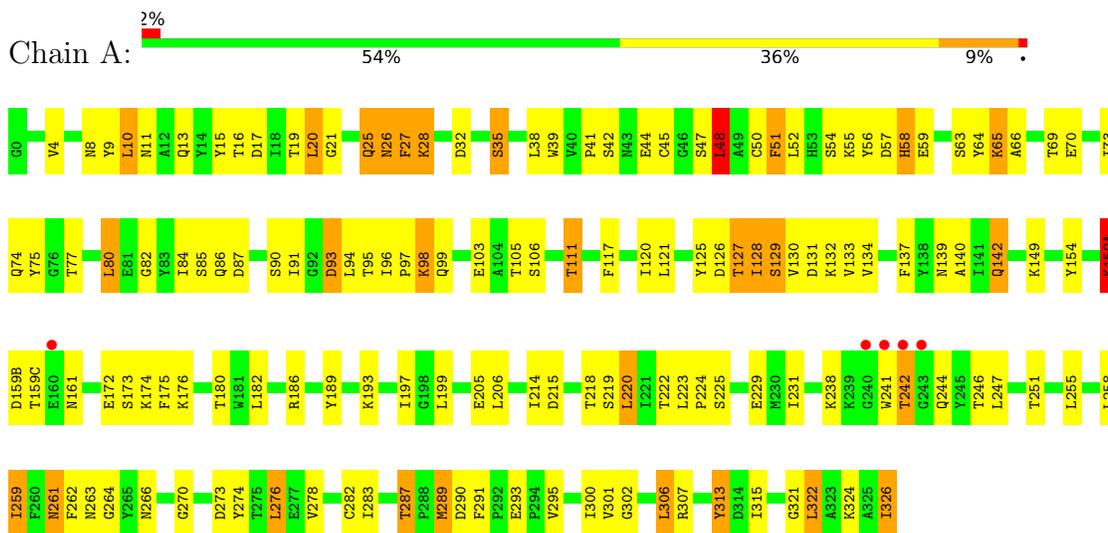
• Molecule 2: alpha-L-gulopyranose-(1-2)-beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.91Å 86.91Å 110.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.60 – 2.70 15.63 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.60-2.70) 99.2 (15.63-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.73Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.180 , 0.270 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 100.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2749	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 0QF, GUP, 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	A	0.55	0/2592	1.17	14/3526 (0.4%)

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	3	0

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	TRP	CA-CB-CG	12.84	138.10	113.70
1	A	4	VAL	CA-CB-CG1	7.70	122.45	110.90
1	A	93	ASP	CB-CG-OD1	-7.46	111.59	118.30
1	A	48	LEU	CA-CB-CG	7.04	131.49	115.30
1	A	220	LEU	CB-CG-CD2	6.78	122.52	111.00
1	A	186	ARG	CA-CB-CG	6.76	128.27	113.40
1	A	295	VAL	CG1-CB-CG2	6.73	121.66	110.90
1	A	241	TRP	N-CA-CB	6.59	122.46	110.60
1	A	63	SER	N-CA-CB	6.37	120.06	110.50
1	A	159(A)	LYS	CD-CE-NZ	-6.22	97.38	111.70
1	A	295	VAL	CA-CB-CG1	6.07	120.01	110.90
1	A	278	VAL	CA-CB-CG2	6.04	119.97	110.90
1	A	242	THR	CA-C-N	5.25	126.70	116.20
1	A	301	VAL	CG1-CB-CG2	5.21	119.23	110.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63	SER	CA
1	A	86	GLN	CA
1	A	241	TRP	CA

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	A	2528	0	2400	122	0
2	B	61	0	49	3	0
3	A	44	0	52	10	0
4	A	14	0	13	3	0
5	A	102	0	0	3	0
All	All	2749	0	2514	125	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 24.

All (125) 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:242:THR:O	1:A:242:THR:HG22	1.44	1.14
1:A:261:ASN:HD22	1:A:261:ASN:C	1.50	1.12
1:A:242:THR:O	1:A:242:THR:CG2	1.98	1.06
1:A:69:THR:HB	1:A:84:ILE:HD13	1.48	0.96
1:A:13:GLN:HE21	3:A:400:0QF:HE2	1.34	0.91
1:A:261:ASN:C	1:A:261:ASN:ND2	2.29	0.86
1:A:39:TRP:CE2	1:A:80:LEU:HD21	2.14	0.82
1:A:86:GLN:HE21	1:A:98:LYS:HA	1.46	0.80
1:A:38:LEU:HD13	1:A:121:LEU:HG	1.63	0.79
1:A:84:ILE:HG22	1:A:85:SER:N	1.99	0.77
1:A:19:THR:OG1	1:A:90:SER:HB3	1.84	0.76
1:A:261:ASN:HD22	1:A:262:PHE:N	1.83	0.75
1:A:84:ILE:CG2	1:A:85:SER:N	2.50	0.75
1:A:261:ASN:HD21	1:A:264:GLY:H	1.31	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:OD1	1:A:59:GLU:HG2	1.87	0.74
1:A:39:TRP:CZ2	1:A:80:LEU:HD21	2.22	0.74
1:A:41:PRO:HG2	1:A:54:SER:O	1.87	0.74
1:A:246:THR:HG22	1:A:283:ILE:HG22	1.68	0.74
1:A:137:PHE:HE2	1:A:315:ILE:HG21	1.52	0.73
1:A:154:TYR:CG	1:A:174:LYS:HD3	2.24	0.73
1:A:132:LYS:HD2	5:A:639:HOH:O	1.90	0.71
1:A:11:ASN:HB3	1:A:307:ARG:NH1	2.06	0.71
1:A:13:GLN:NE2	3:A:400:0QF:HE2	2.05	0.71
1:A:128:ILE:O	1:A:128:ILE:HG12	1.92	0.70
1:A:86:GLN:CG	1:A:87:ASP:H	2.04	0.69
1:A:73:ILE:HG22	1:A:80:LEU:CD1	2.23	0.69
1:A:84:ILE:CG2	1:A:85:SER:H	2.06	0.69
1:A:159(A):LYS:HG2	1:A:159(B):ASP:N	2.09	0.67
1:A:225:SER:O	1:A:229:GLU:HG3	1.94	0.67
1:A:9:TYR:CE2	1:A:10:LEU:HD22	2.29	0.67
1:A:9:TYR:CZ	1:A:10:LEU:HD22	2.31	0.65
1:A:291:PHE:CZ	1:A:300:ILE:HD11	2.32	0.65
1:A:86:GLN:CG	1:A:87:ASP:N	2.57	0.64
1:A:189:TYR:CE1	3:A:400:0QF:H73	2.32	0.64
1:A:32:ASP:OD2	1:A:35:SER:HB2	1.98	0.64
1:A:48:LEU:HD12	1:A:52:LEU:CD1	2.27	0.64
1:A:58:HIS:HB2	1:A:64:TYR:CD2	2.34	0.63
1:A:48:LEU:HD12	1:A:52:LEU:HD12	1.82	0.62
1:A:58:HIS:HB2	1:A:64:TYR:CG	2.36	0.61
1:A:51:PHE:C	1:A:51:PHE:CD1	2.74	0.60
1:A:15:TYR:CE1	1:A:28:LYS:HD3	2.37	0.60
1:A:205:GLU:O	1:A:206:LEU:HD23	2.02	0.60
1:A:86:GLN:O	1:A:87:ASP:HB2	2.02	0.60
1:A:84:ILE:HD11	1:A:131:ASP:OD2	2.03	0.59
1:A:326:ILE:O	1:A:326:ILE:HG23	2.04	0.57
1:A:313:TYR:N	1:A:313:TYR:CD1	2.73	0.57
1:A:127:THR:HG22	1:A:127:THR:O	2.04	0.57
1:A:86:GLN:HG3	1:A:87:ASP:H	1.71	0.55
1:A:111:THR:HG22	3:A:400:0QF:HE1	1.87	0.55
1:A:242:THR:O	1:A:242:THR:HG23	1.99	0.54
1:A:126:ASP:O	1:A:129:SER:HB3	2.08	0.54
1:A:225:SER:HB3	1:A:290:ASP:OD2	2.07	0.54
2:B:3:BMA:O2	2:B:4:BMA:C1	2.55	0.54
1:A:218:THR:HG23	3:A:400:0QF:HA1	1.89	0.53
1:A:161:ASN:HD21	1:A:174:LYS:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:HE2	1:A:315:ILE:CG2	2.22	0.52
1:A:35:SER:OG	1:A:75:TYR:HE1	1.93	0.52
1:A:20:LEU:O	1:A:25:GLN:HG3	2.09	0.52
1:A:42:SER:O	1:A:55:LYS:HG2	2.09	0.52
1:A:86:GLN:HE21	1:A:98:LYS:CA	2.19	0.52
1:A:161:ASN:HD21	1:A:174:LYS:CE	2.23	0.52
1:A:84:ILE:HG23	1:A:85:SER:H	1.74	0.51
1:A:259:ILE:HD12	4:A:337:NAG:H5	1.92	0.51
1:A:26:ASN:HD22	1:A:27:PHE:N	2.08	0.51
1:A:261:ASN:HD21	1:A:264:GLY:N	2.05	0.51
1:A:65:LYS:HE3	1:A:66:ALA:O	2.11	0.50
1:A:8:ASN:OD1	1:A:8:ASN:C	2.50	0.50
1:A:50:CYS:O	1:A:55:LYS:HE3	2.12	0.49
1:A:127:THR:O	1:A:127:THR:CG2	2.60	0.49
1:A:223:LEU:O	1:A:224:PRO:C	2.49	0.49
1:A:20:LEU:HB2	1:A:27:PHE:CE1	2.48	0.49
1:A:96:ILE:HG12	1:A:140:ALA:HB2	1.94	0.49
1:A:77:THR:HG1	3:A:400:0QF:H5'1	1.78	0.48
1:A:266:ASN:ND2	4:A:337:NAG:H82	2.28	0.48
1:A:48:LEU:HD12	1:A:52:LEU:HD11	1.96	0.48
1:A:16:THR:O	1:A:28:LYS:HA	2.14	0.47
1:A:65:LYS:O	1:A:86:GLN:HA	2.13	0.47
1:A:73:ILE:CG2	1:A:80:LEU:CD1	2.92	0.47
1:A:125:TYR:O	1:A:128:ILE:HG22	2.15	0.47
1:A:45:CYS:HB2	1:A:105:THR:O	2.14	0.47
1:A:270:GLY:O	1:A:273:ASP:HB2	2.15	0.47
1:A:8:ASN:OD1	1:A:9:TYR:N	2.48	0.47
1:A:270:GLY:HA3	5:A:529:HOH:O	2.13	0.46
3:A:400:0QF:HB2	3:A:400:0QF:H3'2	1.96	0.46
1:A:133:VAL:HG12	1:A:134:VAL:N	2.31	0.46
1:A:159(A):LYS:CG	1:A:159(B):ASP:N	2.76	0.46
1:A:180:THR:O	1:A:321:GLY:HA2	2.16	0.46
1:A:95:THR:O	1:A:97:PRO:HD3	2.15	0.46
1:A:149:LYS:HB3	1:A:315:ILE:HG23	1.98	0.46
1:A:20:LEU:HB2	1:A:27:PHE:HE1	1.81	0.45
1:A:38:LEU:HD12	1:A:120:ILE:O	2.16	0.45
1:A:222:THR:HA	1:A:287:THR:O	2.16	0.45
1:A:276:LEU:O	1:A:282:CYS:HA	2.17	0.45
3:A:400:0QF:C61	3:A:400:0QF:H211	2.46	0.45
1:A:218:THR:HG23	3:A:400:0QF:O	2.17	0.45
1:A:266:ASN:ND2	4:A:337:NAG:C7	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:O	1:A:10:LEU:HB2	2.18	0.44
1:A:291:PHE:CZ	1:A:300:ILE:CD1	3.00	0.44
1:A:215:ASP:O	1:A:302:GLY:HA2	2.18	0.44
1:A:86:GLN:O	1:A:87:ASP:CB	2.65	0.44
1:A:142:GLN:OE1	2:B:4:BMA:H62	2.17	0.44
1:A:9:TYR:CZ	1:A:10:LEU:CD2	2.98	0.43
1:A:27:PHE:CZ	1:A:56:TYR:HB2	2.53	0.43
1:A:48:LEU:CD1	1:A:52:LEU:HD11	2.47	0.43
1:A:86:GLN:HG2	1:A:87:ASP:N	2.30	0.43
1:A:21:GLY:HA2	1:A:87:ASP:OD1	2.19	0.42
1:A:130:VAL:O	1:A:131:ASP:HB2	2.18	0.42
1:A:84:ILE:H	1:A:84:ILE:HD12	1.84	0.42
1:A:142:GLN:CD	2:B:4:BMA:H62	2.40	0.42
1:A:283:ILE:O	1:A:283:ILE:HG13	2.19	0.42
1:A:300:ILE:HD13	3:A:400:0QF:H211	2.00	0.42
1:A:121:LEU:C	1:A:121:LEU:HD23	2.39	0.42
1:A:291:PHE:CE2	1:A:300:ILE:HD11	2.55	0.42
1:A:82:GLY:HA3	1:A:103:GLU:O	2.20	0.42
1:A:172:GLU:HA	1:A:175:PHE:CE1	2.54	0.41
1:A:182:LEU:HD12	1:A:322:LEU:HD22	2.02	0.41
1:A:251:THR:O	1:A:255:LEU:HG	2.19	0.41
1:A:258:LEU:HB2	1:A:274:TYR:CD2	2.55	0.41
1:A:220:LEU:HB2	5:A:667:HOH:O	2.19	0.41
1:A:261:ASN:ND2	1:A:262:PHE:N	2.60	0.41
1:A:182:LEU:HD22	1:A:263:ASN:HB3	2.02	0.41
1:A:117:PHE:CD1	1:A:117:PHE:O	2.74	0.40
1:A:289:MET:HE3	1:A:289:MET:HB2	1.82	0.40
1:A:38:LEU:HD13	1:A:121:LEU:CG	2.43	0.40
1:A:214:ILE:HG23	1:A:306:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	304 (93%)	22 (7%)	1 (0%)	41	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	THR

5.3.2 Protein sidechains ⓘ

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%)	217 (81%)	51 (19%)	1	4

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	17	ASP
1	A	20	LEU
1	A	25	GLN
1	A	26	ASN
1	A	27	PHE
1	A	28	LYS
1	A	35	SER
1	A	44	GLU
1	A	47	SER
1	A	48	LEU
1	A	51	PHE
1	A	58	HIS
1	A	65	LYS
1	A	70	GLU
1	A	74	GLN
1	A	80	LEU
1	A	91	ILE
1	A	93	ASP
1	A	94	LEU

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Mol	Chain	Res	Type
1	A	98	LYS
1	A	99	GLN
1	A	106	SER
1	A	111	THR
1	A	128	ILE
1	A	129	SER
1	A	139	ASN
1	A	142	GLN
1	A	159(A)	LYS
1	A	159(C)	THR
1	A	173	SER
1	A	176	LYS
1	A	193	LYS
1	A	197	ILE
1	A	199	LEU
1	A	219	SER
1	A	231	ILE
1	A	238	LYS
1	A	244	GLN
1	A	247	LEU
1	A	259	ILE
1	A	261	ASN
1	A	276	LEU
1	A	287	THR
1	A	289	MET
1	A	293	GLU
1	A	306	LEU
1	A	313	TYR
1	A	322	LEU
1	A	324	LYS
1	A	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	13	GLN
1	A	26	ASN
1	A	58	HIS
1	A	86	GLN
1	A	142	GLN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	232	ASN
1	A	261	ASN
1	A	317	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	2,1	14,14,15	1.16	2 (14%)	17,19,21	1.64	5 (29%)
2	NAG	B	2	2	14,14,15	1.04	1 (7%)	17,19,21	1.86	4 (23%)
2	BMA	B	3	2	11,11,12	1.20	0	15,15,17	3.01	5 (33%)
2	BMA	B	4	2	11,11,12	1.20	2 (18%)	15,15,17	2.73	3 (20%)
2	GUP	B	5	2	11,11,12	1.56	2 (18%)	15,15,17	3.47	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	-	2/2/19/22	0/1/1/1
2	GUP	B	5	2	1/1/4/5	1/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GUP	C2-C3	-3.08	1.48	1.52
2	B	4	BMA	O5-C1	2.49	1.47	1.43
2	B	1	NAG	O4-C4	2.21	1.48	1.43
2	B	1	NAG	C2-N2	2.21	1.50	1.46
2	B	4	BMA	O4-C4	2.19	1.48	1.43
2	B	5	GUP	C1-C2	-2.14	1.47	1.52
2	B	2	NAG	O4-C4	2.05	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	GUP	C1-C2-C3	10.29	122.31	109.67
2	B	4	BMA	O5-C5-C4	8.83	132.31	110.83
2	B	3	BMA	O5-C5-C4	-8.82	89.36	110.83
2	B	3	BMA	C1-O5-C5	5.33	119.41	112.19
2	B	2	NAG	C1-O5-C5	5.30	119.37	112.19
2	B	5	GUP	C2-C3-C4	4.49	118.67	110.89
2	B	5	GUP	O5-C5-C4	4.34	121.40	110.83
2	B	5	GUP	C6-C5-C4	3.99	122.34	113.00
2	B	4	BMA	O5-C1-C2	-3.67	105.11	110.77
2	B	1	NAG	O5-C5-C4	3.14	118.47	110.83
2	B	1	NAG	C2-N2-C7	-3.12	118.45	122.90
2	B	5	GUP	O2-C2-C3	2.56	115.26	110.14
2	B	1	NAG	C1-O5-C5	2.46	115.52	112.19
2	B	2	NAG	C8-C7-N2	-2.33	112.16	116.10
2	B	3	BMA	C3-C4-C5	-2.30	106.14	110.24
2	B	3	BMA	O5-C1-C2	-2.16	107.44	110.77
2	B	2	NAG	C3-C4-C5	-2.15	106.40	110.24
2	B	1	NAG	O3-C3-C4	-2.13	105.44	110.35
2	B	4	BMA	O2-C2-C3	2.04	114.22	110.14
2	B	1	NAG	O5-C5-C6	-2.01	104.05	107.20
2	B	2	NAG	O3-C3-C4	-2.01	105.69	110.35
2	B	3	BMA	O2-C2-C1	-2.01	105.04	109.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	5	GUP	C1

All (9) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	BMA	1	0
2	B	4	BMA	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 oligosaccharide.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings
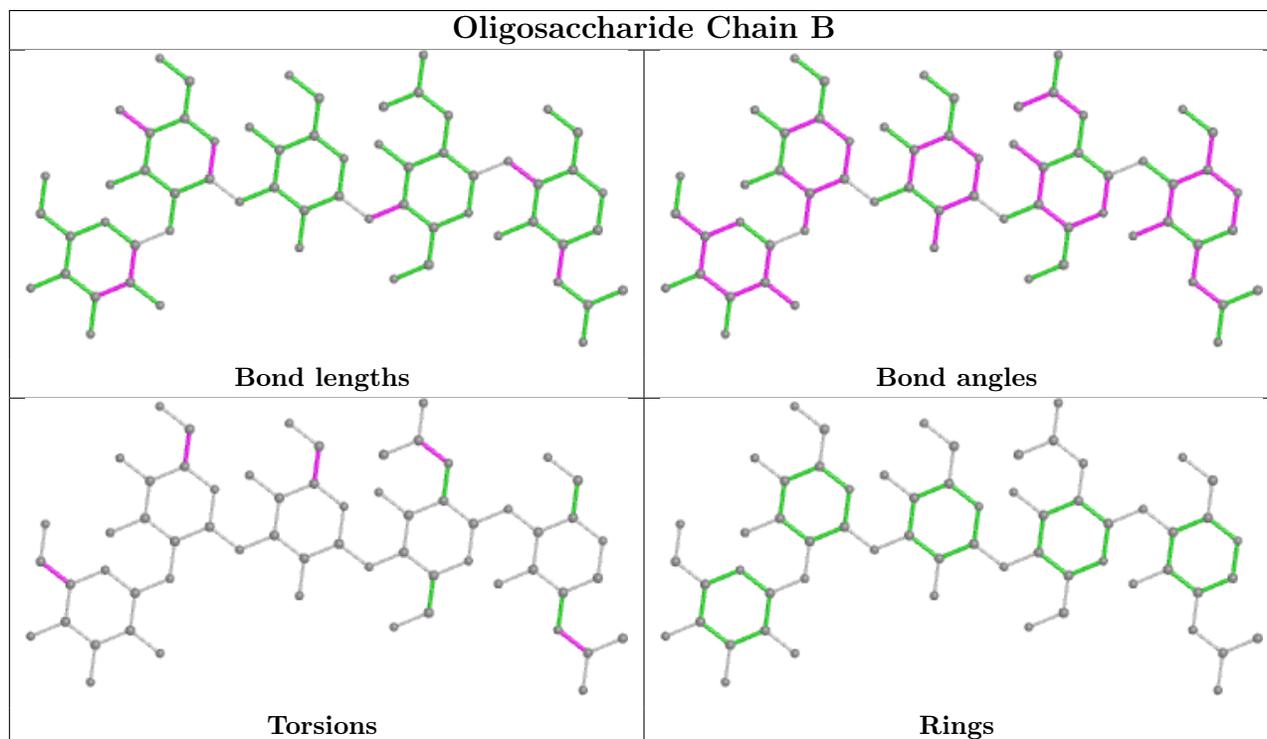
5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
4	NAG	A	337	1	14,14,15	1.00	1 (7%)	17,19,21	1.52	3 (17%)
3	0QF	A	400	-	43,46,46	0.86	3 (6%)	51,62,62	4.52	13 (25%)

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	337	1	1/1/5/7	5/6/23/26	0/1/1/1
3	0QF	A	400	-	-	8/45/66/66	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	0QF	O2S-S	3.29	1.46	1.43
3	A	400	0QF	O1S-S	3.16	1.46	1.43
4	A	337	NAG	O4-C4	2.19	1.48	1.43
3	A	400	0QF	C5-N4	-2.06	1.45	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	0QF	C6-C5-N4	21.53	120.86	108.18
3	A	400	0QF	C2-C3-N4	19.07	119.41	108.18
3	A	400	0QF	C5-N4-C3	-6.96	104.46	112.17
3	A	400	0QF	O2S-S-O1S	-5.45	111.73	119.72
3	A	400	0QF	O1-C2-C3	-5.36	99.98	111.80
3	A	400	0QF	C51-C4-C31	-4.69	108.30	114.82
3	A	400	0QF	O1-C6-C5	-4.53	101.82	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	0QF	O3-C31-C22	4.38	119.75	109.10
4	A	337	NAG	O5-C5-C4	3.47	119.27	110.83
4	A	337	NAG	C1-O5-C5	3.19	116.51	112.19
3	A	400	0QF	C4'-C3'-C2'	2.37	116.25	111.42
3	A	400	0QF	C5'-C4'-C3'	2.34	118.39	111.18
3	A	400	0QF	CA1-N1-C	2.34	126.66	121.99
4	A	337	NAG	O3-C3-C4	-2.13	105.42	110.35
3	A	400	0QF	CA-N-S	-2.11	116.24	120.36
3	A	400	0QF	N-S-N4	2.10	115.74	108.39

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	337	NAG	C1

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	0QF	C3-N4-S-O1S
3	A	400	0QF	O2-C1-CA1-N1
3	A	400	0QF	N2-C1-CA1-N1
3	A	400	0QF	C21-C11-S1-CA1
4	A	337	NAG	C8-C7-N2-C2
4	A	337	NAG	O7-C7-N2-C2
4	A	337	NAG	C1-C2-N2-C7
3	A	400	0QF	O21-C22-C31-C4
3	A	400	0QF	C3-N4-S-O2S
3	A	400	0QF	O3-C31-C4-C51
4	A	337	NAG	C3-C2-N2-C7
4	A	337	NAG	O5-C5-C6-O6
3	A	400	0QF	C5-N4-S-O2S

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	337	NAG	3	0
3	A	400	0QF	10	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 0QF A 400
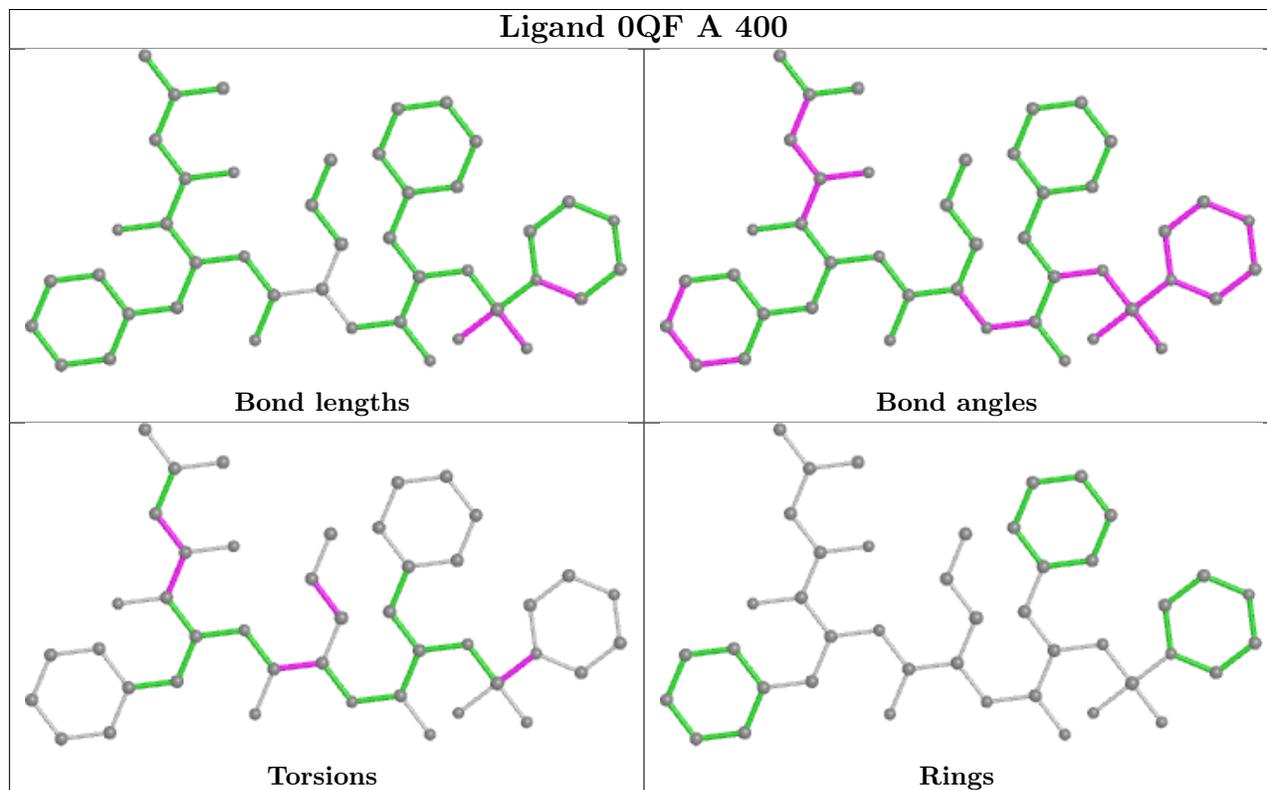
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.73	5 (1%)	73	76	4, 24, 60, 130	4 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	TRP	4.9
1	A	242	THR	4.7
1	A	240	GLY	4.3
1	A	243	GLY	2.7
1	A	160	GLU	2.6

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

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	GUP	B	5	11/12	0.61	0.31	35,45,69,157	0
2	BMA	B	3	11/12	0.89	0.24	22,33,63,67	0
2	NAG	B	1	14/15	0.92	0.16	29,42,108,121	0
2	BMA	B	4	11/12	0.93	0.22	0,31,71,73	0
2	NAG	B	2	14/15	0.97	0.10	6,37,55,134	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

WORLDWIDE
wwPDB
PROTEIN DATA BANK

charide. Each fit is shown from different orientation to approximate a three-dimensional view.
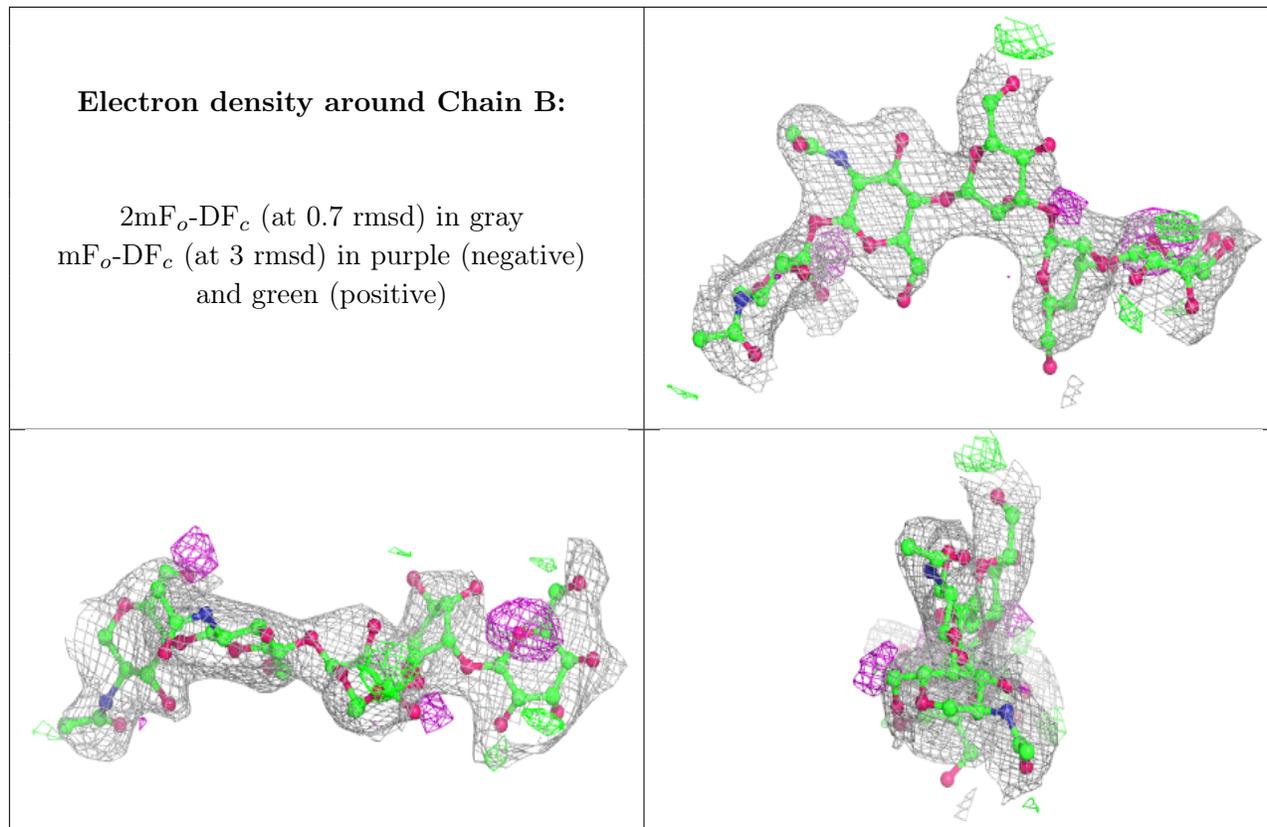
Electron density around Chain B:

$2mF_o$-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, 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	0.82	0.22	30,47,157,157	0
3	0QF	A	400	44/44	0.95	0.16	3,31,96,157	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 0QF A 400:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
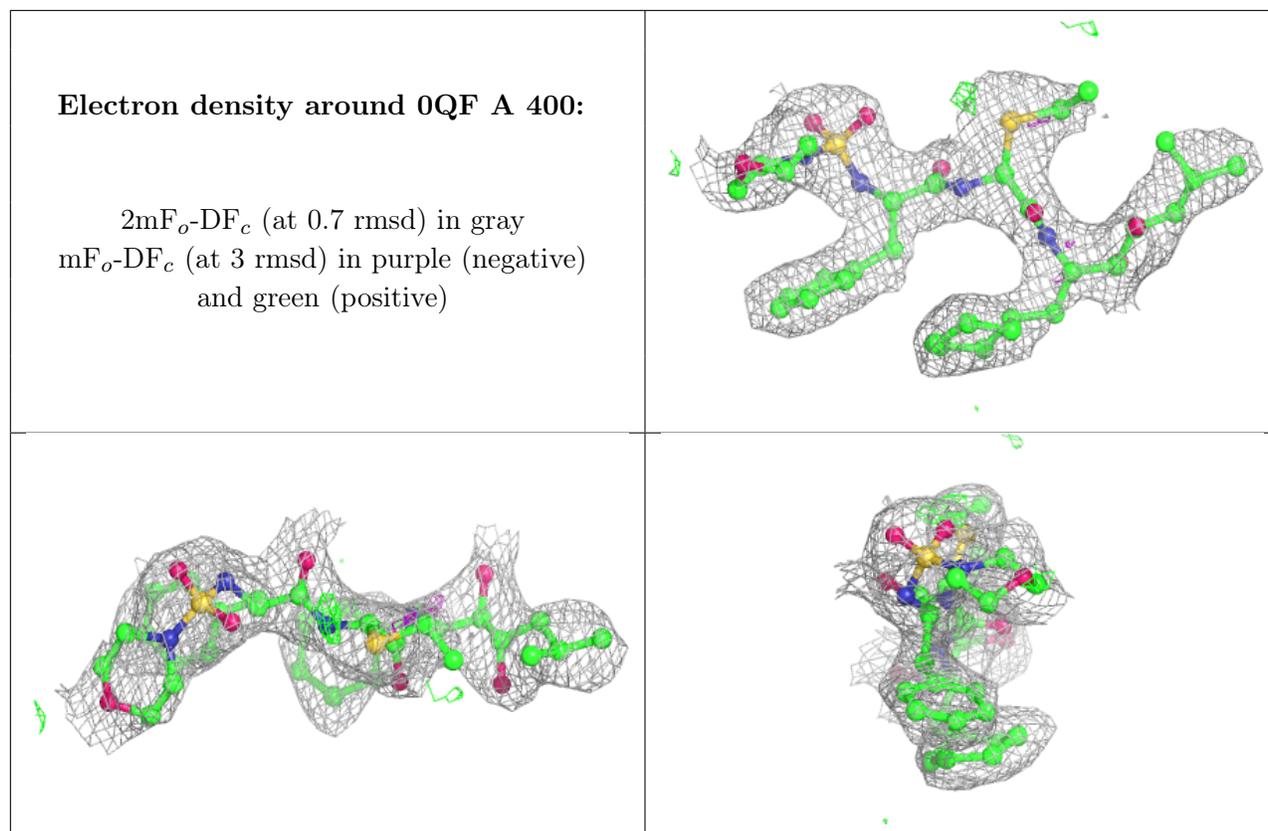
6.5 Other polymers (i)

There are no such residues in this entry.