



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:53 PM BST

PDB ID : 1HWP  
Title : EBULIN COMPLEXED WITH PTEROIC ACID, TRIGONAL CRYSTAL FORM  
Authors : Pascal, J.M.; Day, P.J.; Monzingo, A.F.; Ernst, S.R.; Robertus, J.D.  
Deposited on : 2001-01-09  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.13.1  
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) : 2.13.1

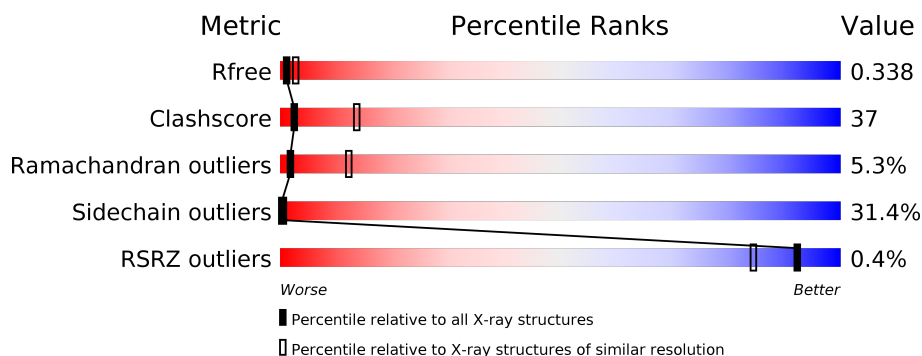
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	254	
2	B	266	
3	C	2	
4	D	3	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BGC	C	1	-	-	-	X
3	GAL	C	2	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4123 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 EBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1990	1257	341	387	5			

- Molecule 2 is a protein called EBULIN.

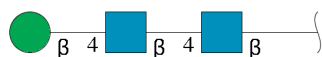
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			2028	1253	359	400	16			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



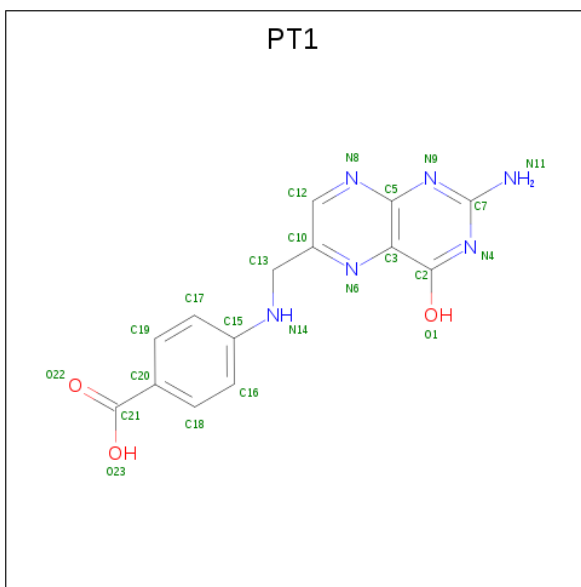
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is an oligosaccharide called 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is PTEROIC ACID (three-letter code: PT1) (formula: C<sub>14</sub>H<sub>12</sub>N<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	14	6	3		

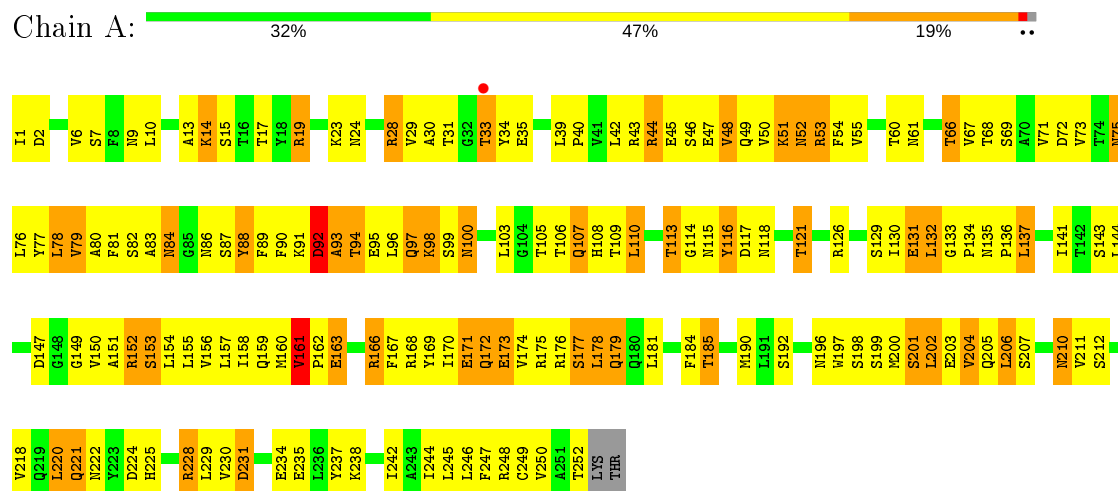
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	12	Total	O	0	0
			12	12		

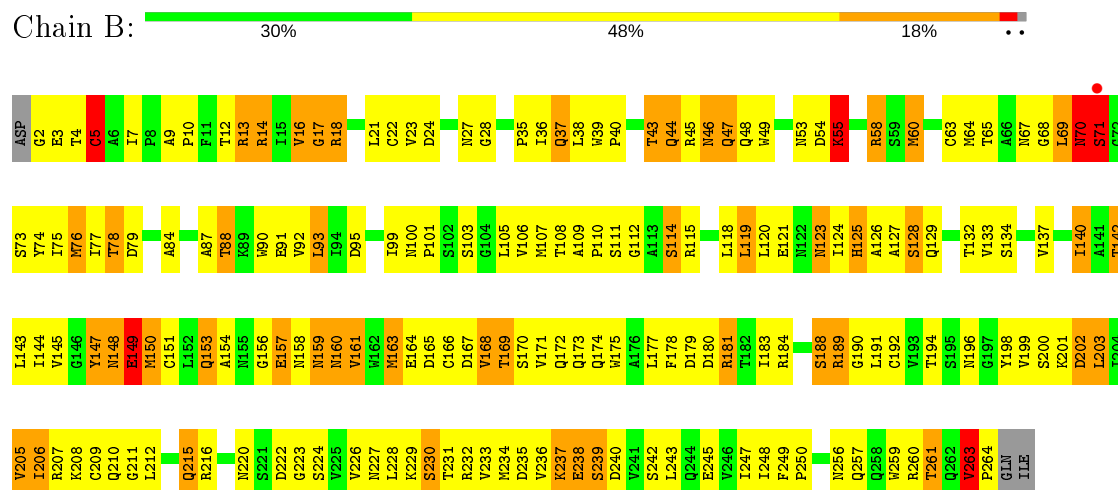
### 3 Residue-property plots

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: EBULIN



#### • Molecule 2: EBULIN



#### • Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



B0C1  
GAL2

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

Chain D:

100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.23 Å 74.23 Å 190.98 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 29.30 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.10) 92.4 (29.30-3.05)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.05 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.219 , 0.317 0.233 , 0.338	Depositor DCC
$R_{free}$ test set	596 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: PT1, GAL, BGC, 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	0.26	0/2027	0.47	0/2756
2	B	0.24	0/2065	0.50	0/2813
All	All	0.25	0/4092	0.48	0/5569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1990	0	1962	149	0
2	B	2028	0	1959	167	0
3	C	23	0	21	3	0
4	D	39	0	34	0	0
5	A	23	0	10	1	0
6	A	8	0	0	1	0
6	B	12	0	0	0	0
All	All	4123	0	3986	300	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 37.

All (300) 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)
2:B:127:ALA:HB3	2:B:211:GLY:HA2	1.31	1.13
2:B:13:ARG:HH11	2:B:13:ARG:HG3	1.20	1.03
2:B:263:VAL:HB	2:B:264:PRO:HD2	1.46	0.97
2:B:150:MET:HB3	2:B:163:MET:HG3	1.46	0.97
2:B:226:VAL:HG22	2:B:233:VAL:HG22	1.49	0.94
2:B:201:LYS:HA	2:B:247:ILE:HD12	1.52	0.92
2:B:58:ARG:HB3	2:B:63:CYS:HA	1.55	0.88
1:A:89:PHE:HB2	1:A:109:THR:HG22	1.56	0.85
2:B:36:ILE:HG22	2:B:118:LEU:HD23	1.59	0.84
1:A:29:VAL:HA	1:A:73:VAL:HG13	1.61	0.83
2:B:123:ASN:HA	2:B:129:GLN:HE22	1.43	0.83
2:B:90:TRP:HH2	2:B:120:LEU:HD21	1.43	0.81
2:B:13:ARG:HH11	2:B:13:ARG:CG	1.92	0.81
1:A:161:VAL:HB	1:A:162:PRO:HD3	1.62	0.79
1:A:10:LEU:HD11	1:A:137:LEU:HB3	1.64	0.78
1:A:224:ASP:O	1:A:225:HIS:HB2	1.83	0.78
1:A:159:GLN:HA	1:A:163:GLU:HB2	1.65	0.78
1:A:144:LEU:HA	1:A:149:GLY:HA2	1.62	0.78
1:A:202:LEU:HD12	1:A:203:GLU:N	1.99	0.77
1:A:55:VAL:HG23	1:A:73:VAL:HG22	1.65	0.77
2:B:263:VAL:CB	2:B:264:PRO:HD2	2.14	0.77
2:B:196:ASN:HA	2:B:207:ARG:NH2	1.99	0.76
2:B:238:GLU:O	2:B:239:SER:HB2	1.85	0.75
1:A:249:CYS:HB2	2:B:5:CYS:HA	1.68	0.74
1:A:44:ARG:HH12	2:B:2:GLY:HA2	1.51	0.74
1:A:250:VAL:HG22	2:B:4:THR:HA	1.69	0.73
1:A:71:VAL:HA	1:A:77:TYR:O	1.89	0.73
2:B:54:ASP:O	2:B:55:LYS:HB2	1.88	0.73
1:A:93:ALA:HB1	1:A:98:LYS:HD2	1.69	0.72
2:B:263:VAL:HB	2:B:264:PRO:CD	2.19	0.72
2:B:9:ALA:HB1	2:B:10:PRO:HD2	1.71	0.72
2:B:171:VAL:HA	2:B:174:GLN:HG3	1.72	0.71
2:B:18:ARG:NH1	2:B:128:SER:HB3	2.06	0.71
1:A:115:ASN:HB2	1:A:118:ASN:HD22	1.56	0.71
2:B:13:ARG:HG3	2:B:13:ARG:NH1	1.92	0.70
2:B:74:TYR:HA	2:B:119:LEU:HB3	1.74	0.69
1:A:156:VAL:O	1:A:160:MET:HG3	1.91	0.69
1:A:197:TRP:O	1:A:201:SER:HB2	1.93	0.68
1:A:158:ILE:O	1:A:162:PRO:HD2	1.94	0.68
2:B:132:THR:HB	2:B:179:ASP:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLN:HB2	2:B:46:ASN:OD1	1.93	0.68
2:B:161:VAL:HG13	2:B:206:ILE:HG12	1.76	0.68
1:A:192:SER:HB2	1:A:221:GLN:HG3	1.76	0.67
1:A:231:ASP:OD2	2:B:134:SER:HB2	1.96	0.65
1:A:72:ASP:HB3	1:A:75:ASN:OD1	1.96	0.65
1:A:175:ARG:HB3	2:B:149:GLU:OE2	1.96	0.65
2:B:142:THR:HG21	2:B:261:THR:OG1	1.95	0.65
2:B:153:GLN:HG2	2:B:173:GLN:HG2	1.78	0.65
1:A:197:TRP:HZ2	1:A:244:ILE:HG22	1.63	0.64
1:A:197:TRP:CH2	1:A:246:LEU:HB2	2.32	0.64
2:B:166:CYS:HA	2:B:173:GLN:HE22	1.62	0.64
2:B:69:LEU:O	2:B:70:ASN:HB2	1.96	0.63
2:B:154:ALA:HB2	2:B:175:TRP:CH2	2.33	0.63
2:B:216:ARG:HD3	2:B:228:LEU:HD12	1.79	0.63
1:A:150:VAL:HG22	1:A:151:ALA:H	1.64	0.63
2:B:196:ASN:HA	2:B:207:ARG:HH22	1.64	0.62
2:B:36:ILE:HD11	2:B:64:MET:HG3	1.81	0.62
1:A:210:ASN:O	2:B:93:LEU:HA	1.99	0.62
1:A:42:LEU:HD21	1:A:244:ILE:HD12	1.82	0.61
2:B:240:ASP:HB3	2:B:243:LEU:HG	1.80	0.61
1:A:9:ASN:O	1:A:13:ALA:HB2	2.00	0.61
1:A:172:GLN:HE21	1:A:172:GLN:HA	1.66	0.61
1:A:29:VAL:HG21	1:A:76:LEU:HD21	1.82	0.61
2:B:148:ASN:ND2	2:B:150:MET:HB2	2.17	0.60
1:A:174:VAL:O	1:A:178:LEU:HG	2.01	0.60
1:A:87:SER:HB3	1:A:105:THR:OG1	2.00	0.60
1:A:44:ARG:HG2	1:A:47:GLU:HG2	1.83	0.60
2:B:67:ASN:HD22	2:B:68:GLY:H	1.50	0.60
1:A:161:VAL:HB	1:A:162:PRO:CD	2.31	0.59
2:B:160:ASN:HA	2:B:205:VAL:HG12	1.83	0.59
1:A:30:ALA:HB2	1:A:244:ILE:HD11	1.84	0.59
2:B:167:ASP:H	2:B:173:GLN:NE2	2.00	0.59
1:A:201:SER:O	1:A:204:VAL:HG12	2.02	0.59
1:A:202:LEU:HA	1:A:205:GLN:HG3	1.83	0.59
2:B:230:SER:OG	2:B:232:ARG:HD3	2.02	0.59
2:B:144:ILE:HG12	2:B:175:TRP:CD1	2.39	0.58
2:B:24:ASP:HB3	2:B:47:GLN:HG3	1.84	0.58
2:B:76:MET:HG2	2:B:77:ILE:N	2.18	0.58
1:A:144:LEU:HD23	1:A:149:GLY:HA2	1.84	0.58
1:A:83:ALA:O	1:A:86:ASN:HB2	2.04	0.58
2:B:153:GLN:HG3	2:B:173:GLN:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:SER:HB2	2:B:233:VAL:HG11	1.87	0.57
2:B:234:MET:HG3	2:B:234:MET:O	2.04	0.57
1:A:152:ARG:O	1:A:156:VAL:HG23	2.05	0.56
2:B:108:THR:HG23	2:B:129:GLN:HG2	1.85	0.56
2:B:69:LEU:HD11	2:B:103:SER:HB3	1.85	0.56
2:B:234:MET:HA	2:B:247:ILE:O	2.06	0.56
2:B:147:TYR:HB2	2:B:236:VAL:HG21	1.88	0.56
2:B:145:VAL:HG22	2:B:151:CYS:SG	2.46	0.56
2:B:203:LEU:HD21	2:B:245:GLU:HB2	1.88	0.55
1:A:40:PRO:HG2	1:A:244:ILE:HD13	1.87	0.55
2:B:159:ASN:O	2:B:206:ILE:HG13	2.07	0.55
1:A:118:ASN:O	1:A:121:THR:HG22	2.07	0.55
1:A:134:PRO:HD3	1:A:177:SER:OG	2.06	0.55
2:B:177:LEU:HD23	2:B:183:ILE:HG23	1.89	0.55
1:A:93:ALA:HA	1:A:97:GLN:OE1	2.07	0.55
2:B:54:ASP:O	2:B:55:LYS:CB	2.55	0.55
1:A:135:ASN:HB2	1:A:136:PRO:HD3	1.88	0.55
1:A:172:GLN:HE22	1:A:175:ARG:CZ	2.20	0.55
1:A:228:ARG:NH2	2:B:140:ILE:HG23	2.22	0.55
1:A:168:ARG:HA	1:A:171:GLU:HB3	1.89	0.54
2:B:199:VAL:HG12	2:B:202:ASP:OD2	2.06	0.54
2:B:194:THR:OG1	2:B:207:ARG:HB2	2.07	0.54
2:B:192:CYS:N	2:B:209:CYS:SG	2.81	0.54
2:B:216:ARG:HD3	2:B:228:LEU:CD1	2.38	0.54
2:B:157:GLU:O	2:B:158:ASN:HB2	2.08	0.54
2:B:198:TYR:HD2	2:B:230:SER:HB3	1.72	0.54
2:B:36:ILE:CD1	2:B:64:MET:HG3	2.37	0.54
2:B:69:LEU:HD11	2:B:103:SER:CB	2.38	0.54
1:A:161:VAL:CB	1:A:162:PRO:HD3	2.35	0.54
2:B:17:GLY:O	2:B:18:ARG:HB2	2.07	0.54
2:B:90:TRP:CZ3	2:B:100:ASN:HB2	2.43	0.54
1:A:207:SER:O	1:A:211:VAL:HG21	2.08	0.54
2:B:74:TYR:HA	2:B:119:LEU:CB	2.37	0.54
1:A:19:ARG:HB2	1:A:175:ARG:HH21	1.73	0.54
1:A:250:VAL:HG13	2:B:3:GLU:O	2.08	0.54
1:A:39:LEU:HB2	1:A:245:LEU:HD11	1.90	0.54
2:B:71:SER:N	2:B:105:LEU:HD21	2.23	0.54
1:A:95:GLU:O	1:A:99:SER:HB2	2.08	0.53
1:A:144:LEU:HA	1:A:149:GLY:CA	2.34	0.53
2:B:220:ASN:HB3	2:B:222:ASP:OD1	2.09	0.53
1:A:157:LEU:O	1:A:161:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASN:HD21	1:A:228:ARG:HD2	1.74	0.53
2:B:74:TYR:HA	2:B:119:LEU:HA	1.90	0.53
2:B:199:VAL:O	2:B:202:ASP:HB2	2.07	0.53
2:B:14:ARG:HB2	2:B:134:SER:O	2.08	0.53
2:B:58:ARG:HB3	2:B:63:CYS:CA	2.34	0.52
1:A:90:PHE:HB3	1:A:113:THR:HA	1.91	0.52
1:A:197:TRP:CZ3	1:A:246:LEU:HB2	2.44	0.52
2:B:18:ARG:HG2	2:B:112:GLY:CA	2.40	0.52
1:A:192:SER:CB	1:A:221:GLN:HG3	2.39	0.52
2:B:249:PHE:CG	2:B:250:PRO:HD2	2.45	0.52
1:A:238:LYS:HD3	2:B:177:LEU:HD13	1.90	0.52
1:A:50:VAL:HA	1:A:53:ARG:HB2	1.92	0.52
1:A:24:ASN:O	1:A:28:ARG:HG2	2.11	0.51
2:B:124:ILE:O	2:B:125:HIS:HB2	2.11	0.51
1:A:137:LEU:HD22	1:A:141:ILE:HD11	1.92	0.51
2:B:43:THR:C	2:B:44:GLN:HE21	2.14	0.51
1:A:172:GLN:NE2	1:A:172:GLN:HA	2.26	0.51
1:A:206:LEU:HD13	2:B:5:CYS:SG	2.50	0.51
1:A:155:LEU:O	1:A:159:GLN:HG3	2.11	0.51
1:A:202:LEU:HD23	1:A:248:ARG:CZ	2.42	0.50
1:A:172:GLN:CA	1:A:172:GLN:HE21	2.21	0.50
2:B:16:VAL:HG12	2:B:21:LEU:O	2.11	0.50
1:A:130:ILE:HG22	1:A:130:ILE:O	2.11	0.50
1:A:94:THR:O	1:A:97:GLN:HG2	2.12	0.50
2:B:142:THR:HG21	2:B:261:THR:CB	2.41	0.50
1:A:202:LEU:HD23	1:A:248:ARG:NH2	2.26	0.50
1:A:162:PRO:O	1:A:166:ARG:HG2	2.12	0.50
2:B:18:ARG:HG2	2:B:112:GLY:HA3	1.92	0.50
1:A:137:LEU:HG	1:A:160:MET:SD	2.52	0.50
2:B:114:SER:O	2:B:115:ARG:CB	2.60	0.50
1:A:196:ASN:O	1:A:200:MET:HG2	2.12	0.49
1:A:44:ARG:H	1:A:47:GLU:HG3	1.77	0.49
1:A:75:ASN:OD1	1:A:77:TYR:HB2	2.13	0.49
2:B:126:ALA:HB1	2:B:211:GLY:O	2.13	0.49
2:B:22:CYS:SG	2:B:137:VAL:HG11	2.53	0.49
2:B:27:ASN:HA	3:C:1:BGC:O4	2.13	0.49
1:A:100:ASN:HA	1:A:103:LEU:HD11	1.95	0.49
1:A:92:ASP:OD1	1:A:113:THR:HB	2.12	0.49
1:A:54:PHE:CD2	1:A:79:VAL:HG21	2.48	0.48
2:B:105:LEU:HB2	2:B:120:LEU:HD12	1.96	0.48
2:B:200:SER:HB3	2:B:249:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:LEU:HA	2:B:247:ILE:HG22	1.93	0.48
1:A:14:LYS:HE3	1:A:14:LYS:N	2.27	0.48
1:A:44:ARG:HG2	1:A:47:GLU:CG	2.43	0.48
1:A:88:TYR:N	1:A:88:TYR:CD1	2.81	0.48
1:A:170:ILE:HG12	1:A:190:MET:HG3	1.96	0.48
2:B:237:LYS:HG2	2:B:245:GLU:OE1	2.13	0.48
2:B:209:CYS:HA	2:B:215:GLN:OE1	2.13	0.48
1:A:35:GLU:HB3	1:A:40:PRO:HA	1.95	0.48
2:B:200:SER:O	2:B:201:LYS:HB2	2.14	0.48
1:A:33:THR:O	1:A:35:GLU:HG2	2.14	0.48
2:B:235:ASP:HB3	2:B:257:GLN:HG2	1.95	0.48
1:A:144:LEU:CD2	1:A:149:GLY:HA2	2.44	0.47
1:A:167:PHE:HB2	1:A:170:ILE:HD12	1.97	0.47
2:B:49:TRP:CZ3	2:B:64:MET:HB2	2.49	0.47
1:A:144:LEU:CD2	1:A:153:SER:HB2	2.44	0.47
1:A:51:LYS:O	1:A:51:LYS:HG2	2.15	0.47
2:B:70:ASN:O	2:B:71:SER:C	2.52	0.47
2:B:156:GLY:O	2:B:159:ASN:HB2	2.14	0.47
1:A:144:LEU:HD21	1:A:153:SER:HB2	1.96	0.47
1:A:51:LYS:HD3	1:A:52:ASN:HD21	1.79	0.47
1:A:50:VAL:HG12	1:A:96:LEU:HD11	1.97	0.47
2:B:28:GLY:HA2	2:B:46:ASN:HB3	1.96	0.47
1:A:19:ARG:HB2	1:A:175:ARG:HD3	1.96	0.47
2:B:35:PRO:HA	2:B:76:MET:HB2	1.97	0.47
1:A:234:GLU:O	1:A:238:LYS:HG3	2.15	0.46
1:A:72:ASP:HB2	1:A:79:VAL:HG22	1.96	0.46
2:B:160:ASN:HD21	2:B:203:LEU:HD21	1.80	0.46
2:B:84:ALA:O	2:B:88:THR:HG22	2.15	0.46
1:A:54:PHE:CE2	1:A:79:VAL:HG21	2.50	0.46
1:A:53:ARG:HA	1:A:53:ARG:HD2	1.55	0.46
1:A:133:GLY:C	1:A:136:PRO:HD2	2.35	0.46
1:A:55:VAL:HB	1:A:71:VAL:CG2	2.45	0.46
2:B:9:ALA:HB1	2:B:10:PRO:CD	2.44	0.46
1:A:19:ARG:HG3	1:A:175:ARG:NH2	2.31	0.46
1:A:35:GLU:HB2	1:A:39:LEU:O	2.16	0.46
1:A:19:ARG:HB2	1:A:175:ARG:NH2	2.31	0.46
2:B:260:ARG:NH2	2:B:261:THR:HG23	2.31	0.46
2:B:18:ARG:HH11	2:B:128:SER:HB3	1.80	0.45
2:B:35:PRO:HB3	2:B:74:TYR:CE1	2.50	0.45
2:B:156:GLY:O	2:B:206:ILE:HD12	2.16	0.45
2:B:91:GLU:HB3	2:B:99:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLN:HE22	1:A:248:ARG:H	1.63	0.45
2:B:124:ILE:O	2:B:229:LYS:HD2	2.16	0.45
1:A:44:ARG:O	1:A:48:VAL:HG12	2.17	0.45
1:A:169:TYR:HE1	2:B:263:VAL:HG22	1.81	0.45
2:B:140:ILE:H	2:B:140:ILE:HG13	1.47	0.45
1:A:197:TRP:CZ2	1:A:244:ILE:HG22	2.50	0.45
2:B:24:ASP:OD2	2:B:39:TRP:HB3	2.16	0.45
2:B:233:VAL:O	2:B:248:ILE:HA	2.16	0.45
2:B:75:ILE:HG22	2:B:76:MET:N	2.31	0.45
2:B:235:ASP:OD1	2:B:235:ASP:C	2.55	0.45
2:B:68:GLY:O	2:B:73:SER:HB2	2.17	0.45
1:A:238:LYS:CD	2:B:177:LEU:HD13	2.47	0.45
2:B:178:PHE:HB3	2:B:180:ASP:OD1	2.16	0.45
1:A:39:LEU:CD1	1:A:245:LEU:HD21	2.47	0.44
1:A:96:LEU:O	1:A:100:ASN:HB2	2.17	0.44
2:B:163:MET:HE1	2:B:259:TRP:CH2	2.52	0.44
1:A:250:VAL:CG2	2:B:4:THR:HA	2.41	0.44
1:A:78:LEU:O	1:A:90:PHE:HE2	2.01	0.44
2:B:154:ALA:O	2:B:172:GLN:HG2	2.17	0.44
1:A:15:SER:HA	1:A:178:LEU:CD1	2.47	0.44
2:B:181:ARG:HD3	2:B:181:ARG:HA	1.39	0.44
2:B:99:ILE:HA	2:B:106:VAL:HG12	1.99	0.44
1:A:173:GLU:HA	1:A:173:GLU:OE1	2.17	0.44
2:B:105:LEU:HB3	2:B:120:LEU:HB3	1.99	0.44
2:B:14:ARG:NH1	2:B:14:ARG:HG3	2.33	0.43
1:A:150:VAL:HG12	1:A:153:SER:OG	2.18	0.43
1:A:175:ARG:O	1:A:179:GLN:HB2	2.18	0.43
2:B:263:VAL:O	2:B:264:PRO:C	2.57	0.43
2:B:78:THR:CG2	2:B:79:ASP:N	2.81	0.43
2:B:188:SER:C	2:B:190:GLY:H	2.21	0.43
2:B:230:SER:C	2:B:232:ARG:H	2.22	0.43
1:A:161:VAL:CB	1:A:162:PRO:CD	2.96	0.43
2:B:153:GLN:HB2	2:B:164:GLU:HB2	2.00	0.43
1:A:53:ARG:HG2	6:A:311:HOH:O	2.17	0.43
2:B:158:ASN:HD22	2:B:158:ASN:N	2.16	0.43
1:A:60:THR:HA	1:A:66:THR:HA	2.01	0.43
1:A:248:ARG:HG3	1:A:248:ARG:HH11	1.83	0.43
1:A:129:SER:HA	1:A:185:THR:HG21	2.01	0.43
1:A:218:VAL:CG1	1:A:220:LEU:HD13	2.48	0.43
1:A:29:VAL:HG21	1:A:76:LEU:CD2	2.47	0.43
2:B:114:SER:O	2:B:115:ARG:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:TRP:CH2	2:B:120:LEU:HD21	2.36	0.42
1:A:35:GLU:CB	1:A:40:PRO:HA	2.50	0.42
1:A:1:ILE:HD12	1:A:100:ASN:OD1	2.20	0.42
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.34	0.42
2:B:127:ALA:HB3	2:B:211:GLY:CA	2.23	0.42
1:A:44:ARG:HH12	2:B:2:GLY:CA	2.27	0.42
2:B:230:SER:O	2:B:232:ARG:N	2.52	0.42
2:B:39:TRP:CD2	2:B:40:PRO:HD2	2.54	0.42
2:B:7:ILE:HD12	2:B:53:ASN:HD21	1.85	0.42
1:A:205:GLN:HE22	1:A:248:ARG:N	2.18	0.42
2:B:121:GLU:HA	2:B:121:GLU:OE2	2.19	0.42
2:B:91:GLU:HB3	2:B:99:ILE:CG2	2.49	0.42
1:A:133:GLY:O	1:A:137:LEU:HB2	2.19	0.42
1:A:175:ARG:HA	1:A:178:LEU:CD1	2.50	0.42
1:A:201:SER:O	1:A:205:GLN:HG3	2.20	0.42
1:A:205:GLN:HE21	1:A:248:ARG:HB2	1.85	0.42
2:B:147:TYR:CD1	2:B:256:ASN:HA	2.54	0.42
2:B:74:TYR:HA	2:B:119:LEU:CA	2.49	0.42
2:B:45:ARG:HD2	2:B:60:MET:HA	2.01	0.42
2:B:46:ASN:ND2	3:C:2:GAL:H2	2.35	0.42
2:B:148:ASN:HD22	2:B:150:MET:HB2	1.85	0.41
1:A:1:ILE:HG22	1:A:2:ASP:N	2.36	0.41
1:A:237:TYR:OH	2:B:223:GLY:HA2	2.20	0.41
1:A:115:ASN:O	1:A:118:ASN:HB2	2.21	0.41
1:A:135:ASN:N	1:A:136:PRO:CD	2.84	0.41
1:A:172:GLN:HE22	1:A:175:ARG:NH1	2.19	0.41
2:B:27:ASN:HA	3:C:1:BGC:H4	2.01	0.41
2:B:39:TRP:CG	2:B:40:PRO:HD2	2.56	0.41
1:A:89:PHE:HE1	1:A:107:GLN:HG3	1.85	0.41
1:A:132:LEU:HD12	1:A:184:PHE:CZ	2.56	0.41
1:A:247:PHE:CE1	1:A:250:VAL:HG12	2.55	0.41
2:B:205:VAL:HB	2:B:206:ILE:H	1.63	0.41
1:A:116:TYR:HA	1:A:116:TYR:HD2	1.77	0.41
1:A:81:PHE:HZ	1:A:149:GLY:HA3	1.85	0.41
2:B:227:ASN:O	2:B:230:SER:O	2.39	0.41
2:B:237:LYS:C	2:B:239:SER:H	2.23	0.41
2:B:226:VAL:HG22	2:B:233:VAL:CG2	2.34	0.41
1:A:67:VAL:HB	1:A:141:ILE:HG23	2.03	0.41
1:A:154:LEU:HA	1:A:154:LEU:HD12	1.84	0.41
2:B:167:ASP:OD1	2:B:169:THR:HG23	2.21	0.41
1:A:80:ALA:HB1	1:A:88:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLY:CA	2:B:46:ASN:HD22	2.34	0.41
2:B:35:PRO:HB3	2:B:74:TYR:HE1	1.86	0.41
1:A:114:GLY:HA3	5:A:321:PT1:H111	1.86	0.40
2:B:109:ALA:O	2:B:110:PRO:C	2.59	0.40
2:B:37:GLN:HA	2:B:118:LEU:HD22	2.03	0.40
1:A:250:VAL:HG22	2:B:3:GLU:O	2.21	0.40
2:B:76:MET:CE	2:B:78:THR:HB	2.52	0.40
2:B:84:ALA:HB3	2:B:87:ALA:HB3	2.03	0.40
2:B:179:ASP:C	2:B:181:ARG:H	2.24	0.40
1:A:60:THR:HA	1:A:66:THR:HB	2.03	0.40
1:A:75:ASN:O	1:A:76:LEU:HB2	2.21	0.40
2:B:74:TYR:CA	2:B:119:LEU:HB3	2.48	0.40
2:B:150:MET:HE2	2:B:163:MET:O	2.22	0.40
2:B:44:GLN:O	2:B:48:GLN:HG3	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	A	250/254 (98%)	208 (83%)	31 (12%)	11 (4%)	2	15
2	B	261/266 (98%)	209 (80%)	36 (14%)	16 (6%)	1	9
All	All	511/520 (98%)	417 (82%)	67 (13%)	27 (5%)	2	12

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
2	B	5	CYS
2	B	55	LYS
2	B	70	ASN

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Mol	Chain	Res	Type
2	B	101	PRO
2	B	263	VAL
1	A	75	ASN
1	A	84	ASN
1	A	93	ALA
1	A	131	GLU
1	A	147	ASP
1	A	161	VAL
2	B	18	ARG
2	B	160	ASN
1	A	43	ARG
1	A	92	ASP
2	B	71	SER
2	B	231	THR
1	A	100	ASN
2	B	149	GLU
2	B	205	VAL
1	A	48	VAL
2	B	125	HIS
2	B	189	ARG
2	B	107	MET
2	B	168	VAL
2	B	17	GLY

### 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	221/223 (99%)	146 (66%)	75 (34%)	0	0
2	B	228/231 (99%)	162 (71%)	66 (29%)	0	1
All	All	449/454 (99%)	308 (69%)	141 (31%)	0	0

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	SER
1	A	14	LYS
1	A	17	THR
1	A	19	ARG
1	A	23	LYS
1	A	28	ARG
1	A	31	THR
1	A	33	THR
1	A	34	TYR
1	A	44	ARG
1	A	45	GLU
1	A	46	SER
1	A	49	GLN
1	A	51	LYS
1	A	52	ASN
1	A	53	ARG
1	A	61	ASN
1	A	66	THR
1	A	68	THR
1	A	69	SER
1	A	78	LEU
1	A	79	VAL
1	A	82	SER
1	A	84	ASN
1	A	88	TYR
1	A	91	LYS
1	A	92	ASP
1	A	94	THR
1	A	97	GLN
1	A	98	LYS
1	A	106	THR
1	A	107	GLN
1	A	108	HIS
1	A	110	LEU
1	A	113	THR
1	A	116	TYR
1	A	117	ASP
1	A	121	THR
1	A	126	ARG
1	A	131	GLU
1	A	132	LEU
1	A	137	LEU

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Mol	Chain	Res	Type
1	A	143	SER
1	A	152	ARG
1	A	153	SER
1	A	161	VAL
1	A	163	GLU
1	A	166	ARG
1	A	171	GLU
1	A	172	GLN
1	A	173	GLU
1	A	176	ARG
1	A	177	SER
1	A	178	LEU
1	A	179	GLN
1	A	181	LEU
1	A	185	THR
1	A	198	SER
1	A	199	SER
1	A	201	SER
1	A	202	LEU
1	A	204	VAL
1	A	206	LEU
1	A	210	ASN
1	A	212	SER
1	A	220	LEU
1	A	221	GLN
1	A	228	ARG
1	A	229	LEU
1	A	230	VAL
1	A	231	ASP
1	A	235	GLU
1	A	242	ILE
1	A	252	THR
2	B	5	CYS
2	B	12	THR
2	B	13	ARG
2	B	14	ARG
2	B	16	VAL
2	B	23	VAL
2	B	37	GLN
2	B	38	LEU
2	B	43	THR
2	B	44	GLN

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Mol	Chain	Res	Type
2	B	46	ASN
2	B	47	GLN
2	B	55	LYS
2	B	58	ARG
2	B	60	MET
2	B	65	THR
2	B	69	LEU
2	B	70	ASN
2	B	71	SER
2	B	76	MET
2	B	78	THR
2	B	88	THR
2	B	92	VAL
2	B	93	LEU
2	B	95	ASP
2	B	111	SER
2	B	114	SER
2	B	119	LEU
2	B	123	ASN
2	B	128	SER
2	B	133	VAL
2	B	140	ILE
2	B	142	THR
2	B	143	LEU
2	B	147	TYR
2	B	148	ASN
2	B	149	GLU
2	B	150	MET
2	B	153	GLN
2	B	157	GLU
2	B	159	ASN
2	B	161	VAL
2	B	163	MET
2	B	165	ASP
2	B	168	VAL
2	B	169	THR
2	B	170	SER
2	B	181	ARG
2	B	184	ARG
2	B	188	SER
2	B	189	ARG
2	B	191	LEU

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Mol	Chain	Res	Type
2	B	202	ASP
2	B	203	LEU
2	B	206	ILE
2	B	208	LYS
2	B	210	GLN
2	B	212	LEU
2	B	215	GLN
2	B	230	SER
2	B	237	LYS
2	B	238	GLU
2	B	239	SER
2	B	242	SER
2	B	261	THR
2	B	263	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	84	ASN
1	A	107	GLN
1	A	108	HIS
1	A	118	ASN
1	A	135	ASN
1	A	172	GLN
1	A	179	GLN
1	A	180	GLN
1	A	205	GLN
1	A	222	ASN
2	B	44	GLN
2	B	46	ASN
2	B	47	GLN
2	B	48	GLN
2	B	53	ASN
2	B	67	ASN
2	B	70	ASN
2	B	100	ASN
2	B	129	GLN
2	B	148	ASN
2	B	153	GLN
2	B	158	ASN
2	B	159	ASN

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Mol	Chain	Res	Type
2	B	173	GLN
2	B	262	GLN

### 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	$\# Z  > 2$
3	BGC	C	1	3	12,12,12	0.59	0	17,17,17	0.57	0
3	GAL	C	2	3	11,11,12	0.86	0	15,15,17	2.04	4 (26%)
4	NAG	D	1	2,4	14,14,15	0.54	0	17,19,21	0.72	0
4	NAG	D	2	4	14,14,15	0.69	0	17,19,21	0.74	0
4	BMA	D	3	4	11,11,12	0.45	0	15,15,17	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	C	1	3	-	2/2/22/22	0/1/1/1
3	GAL	C	2	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	GAL	C1-C2-C3	4.70	115.44	109.67
3	C	2	GAL	C1-O5-C5	4.48	118.26	112.19
3	C	2	GAL	O5-C1-C2	3.75	116.56	110.77
3	C	2	GAL	C3-C4-C5	-2.04	106.60	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

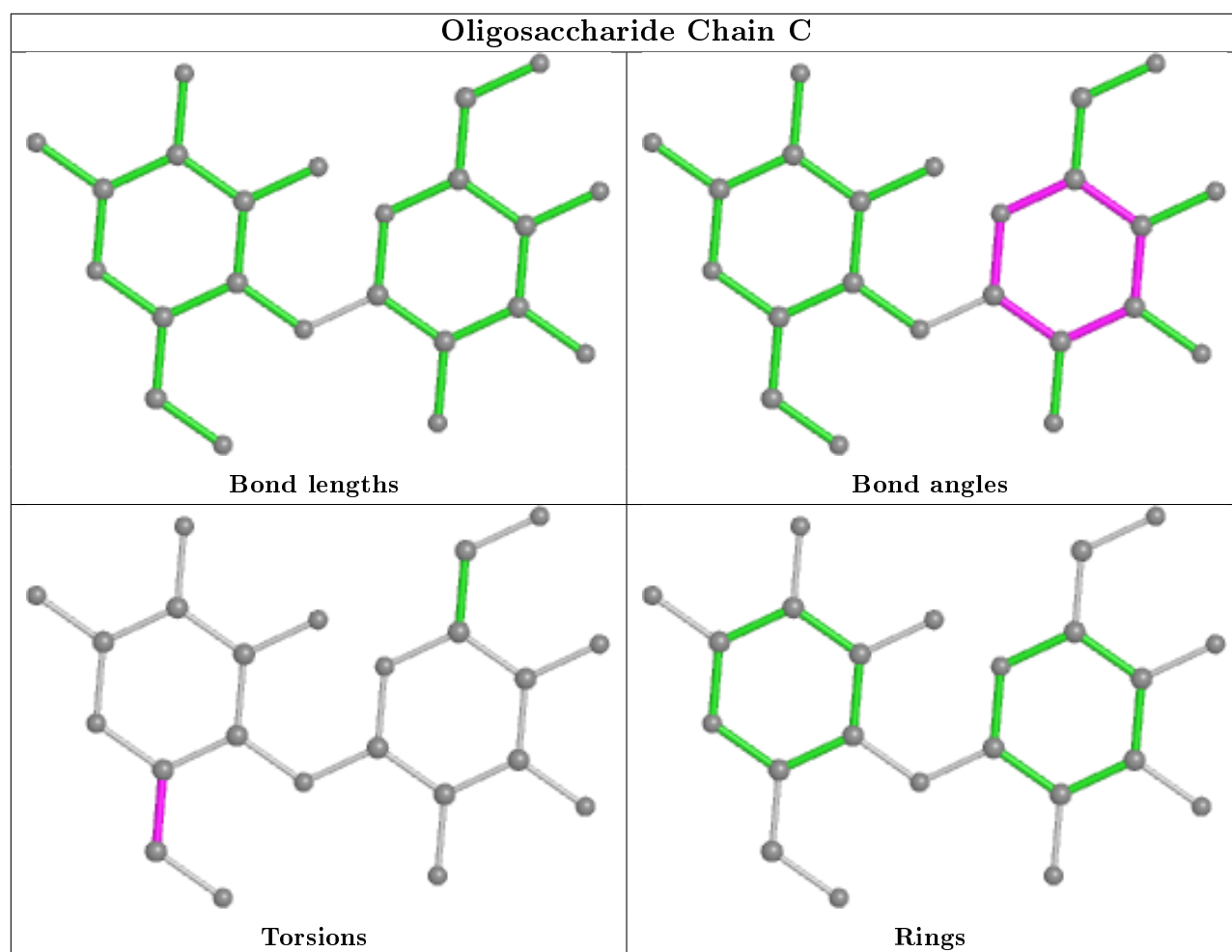
There are no ring outliers.

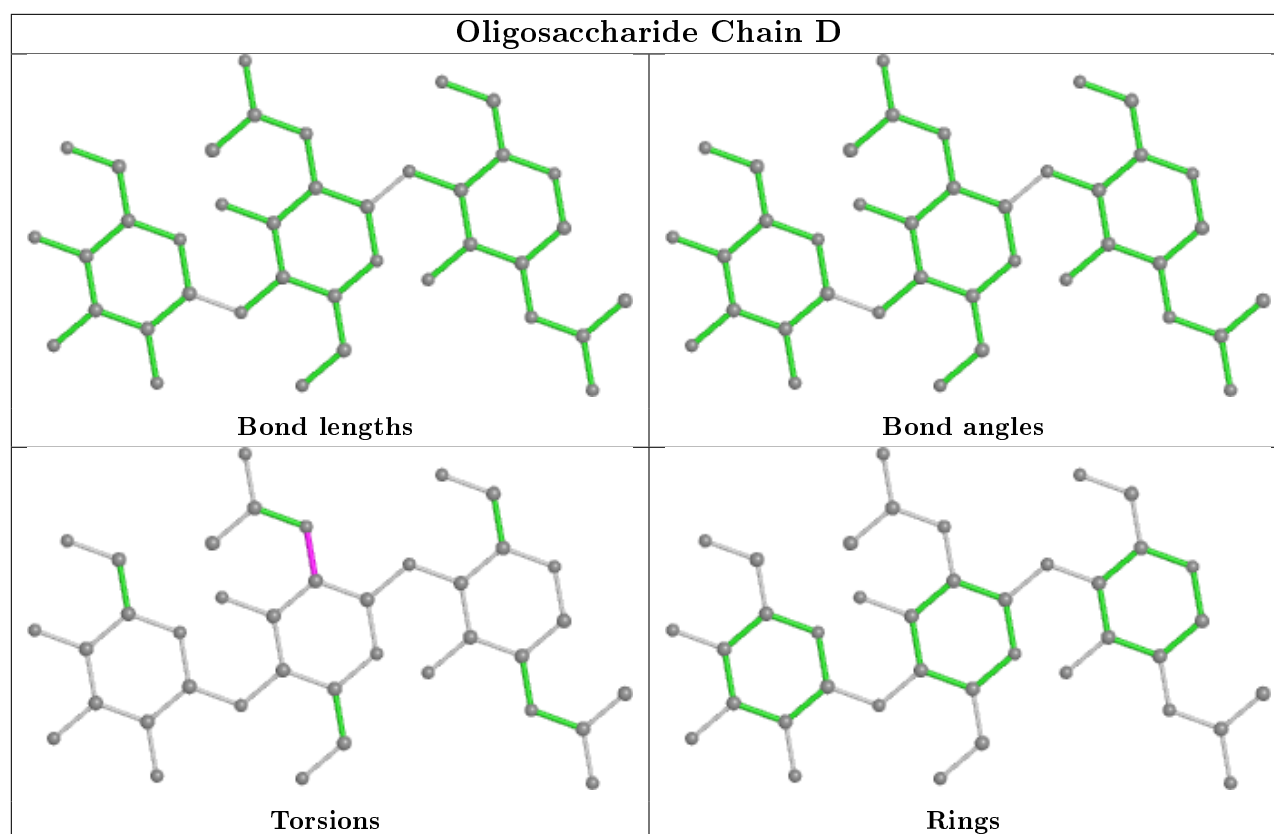
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	GAL	1	0
3	C	1	BGC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
5	PT1	A	321	-	22,25,25	2.75	11 (50%)	28,35,35	1.66	7 (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
5	PT1	A	321	-	-	2/5/9/9	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	321	PT1	C20-C21	6.26	1.53	1.47
5	A	321	PT1	C10-N6	4.62	1.40	1.32
5	A	321	PT1	C12-N8	4.57	1.39	1.31
5	A	321	PT1	C16-C15	3.96	1.45	1.39
5	A	321	PT1	C18-C16	3.35	1.44	1.38
5	A	321	PT1	C3-C5	3.22	1.46	1.40
5	A	321	PT1	C18-C20	3.14	1.46	1.39
5	A	321	PT1	C19-C17	2.92	1.44	1.38
5	A	321	PT1	C19-C20	2.35	1.44	1.39
5	A	321	PT1	C12-C10	2.20	1.43	1.39
5	A	321	PT1	C17-C15	2.19	1.42	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	321	PT1	C12-N8-C5	4.57	121.29	116.69
5	A	321	PT1	C13-C10-N6	3.33	122.57	116.66
5	A	321	PT1	C10-C12-N8	-2.76	120.42	123.13
5	A	321	PT1	C17-C15-N14	-2.52	115.74	120.97
5	A	321	PT1	C13-C10-C12	-2.09	117.91	121.55
5	A	321	PT1	C12-C10-N6	-2.03	119.52	120.85
5	A	321	PT1	C5-C3-N6	-2.02	119.97	122.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	321	PT1	C17-C15-N14-C13
5	A	321	PT1	C16-C15-N14-C13

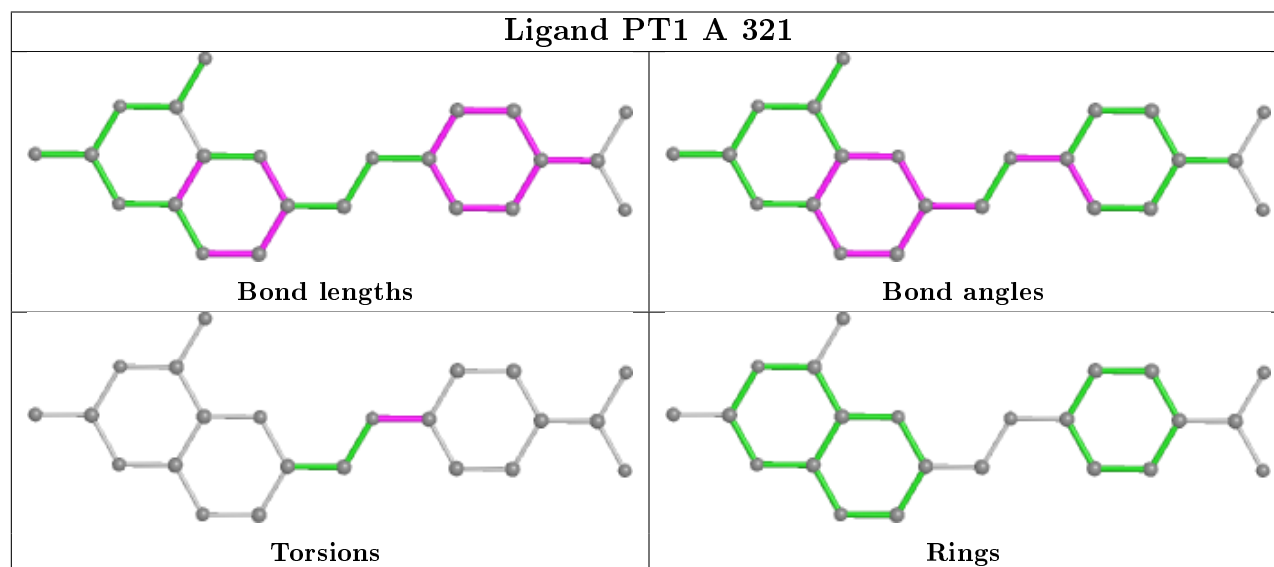
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	321	PT1	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 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 than 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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	252/254 (99%)	-0.30	1 (0%) 92 84	5, 23, 42, 77	0
2	B	263/266 (98%)	-0.17	1 (0%) 92 84	3, 28, 47, 64	0
All	All	515/520 (99%)	-0.24	2 (0%) 92 84	3, 26, 46, 77	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	THR	2.9
2	B	71	SER	2.2

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

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

### 6.3 Carbohydrates [i](#)

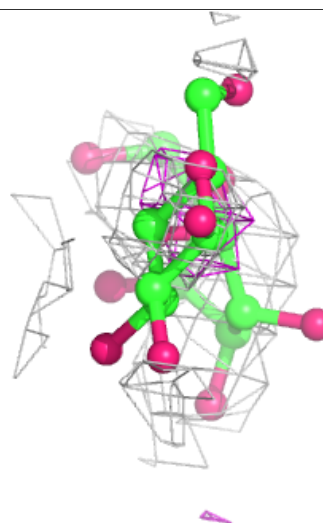
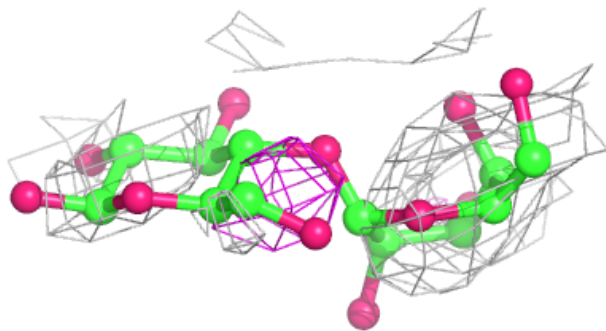
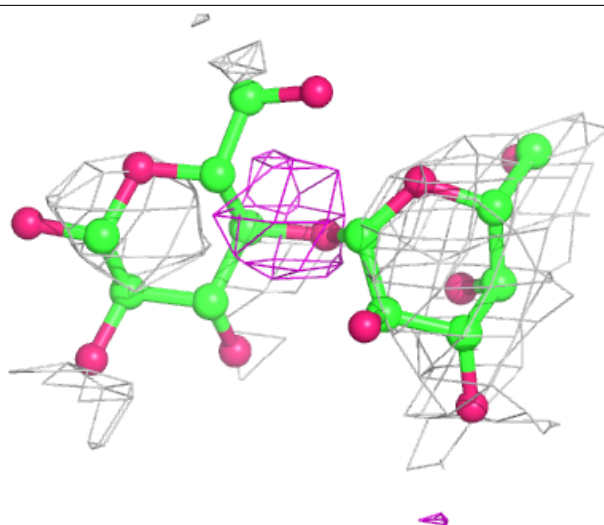
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

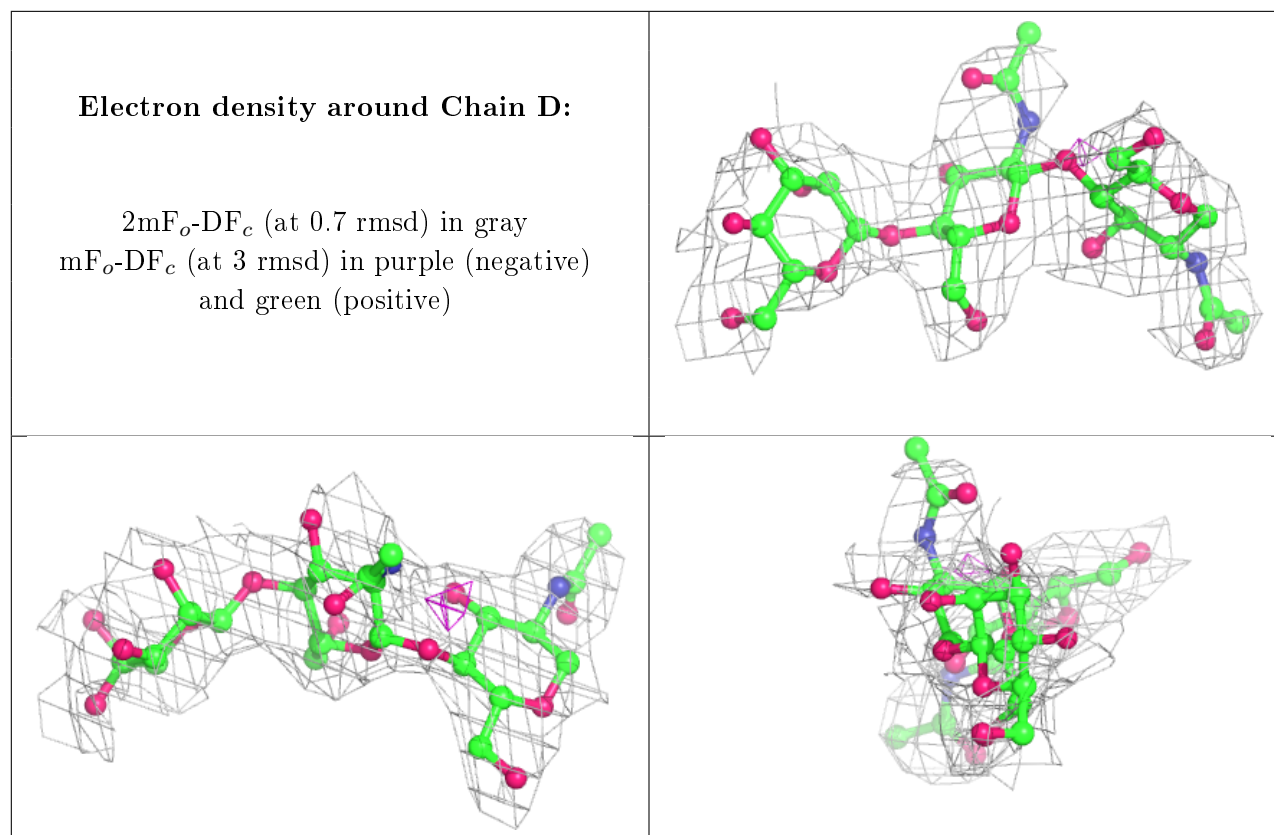
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	C	1	12/12	0.48	0.83	98,98,98,98	0
4	BMA	D	3	11/12	0.76	0.31	71,71,71,71	0
3	GAL	C	2	11/12	0.77	0.49	72,72,72,72	0
4	NAG	D	2	14/15	0.82	0.38	64,64,64,64	0
4	NAG	D	1	14/15	0.87	0.26	27,27,27,27	0

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 C:**

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





## 6.4 Ligands [i](#)

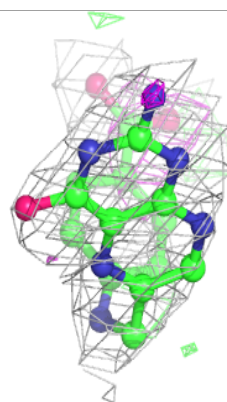
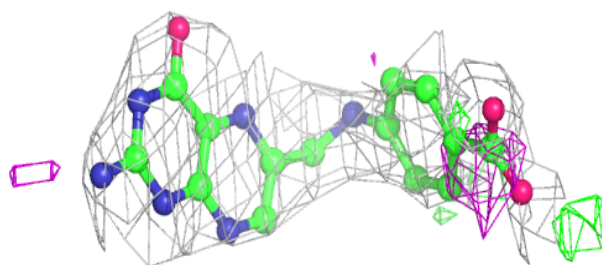
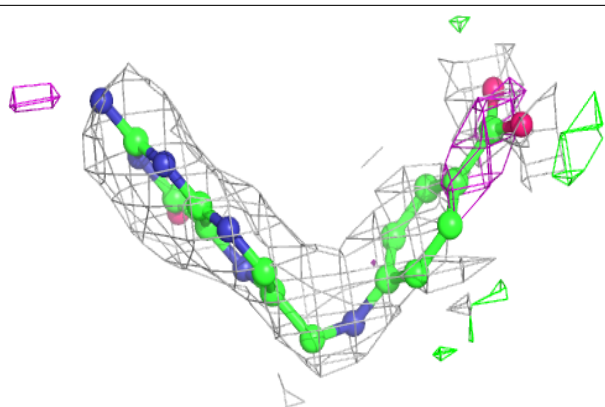
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PT1	A	321	23/23	0.83	0.28	23,23,23,23	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 PT1 A 321:**

$2mF_o-DF_c$  (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.