



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:48 PM GMT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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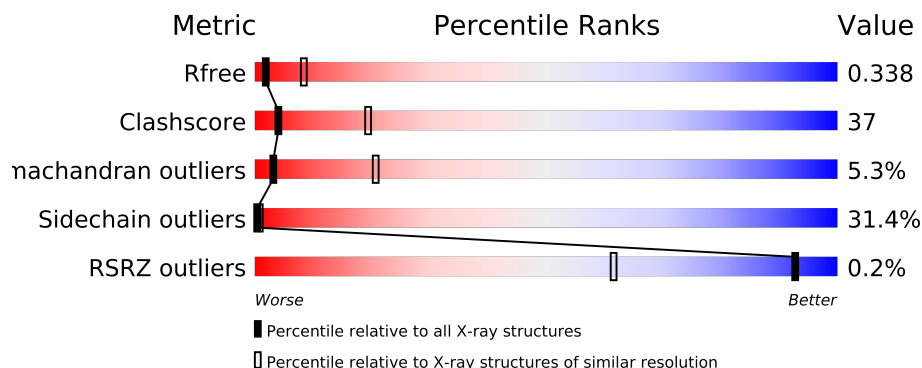
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	254	
2	B	266	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	PT1	A	321	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4123 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

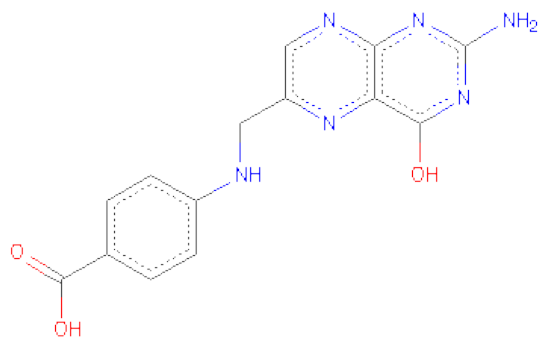
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	3	Total	C	N	O	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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.23Å 74.23Å 190.98Å 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 3.05Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.219 , 0.317 0.237 , 0.338	Depositor DCC
$R_{free}$ test set	563 reflections (5.25%)	DCC
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 , 27.2	EDS
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 11960 reflections	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	B	23	0	21	3	0
4	B	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 37.

All (300) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:B:123:ASN:HA	2:B:129:GLN:HE22	1.43	0.83
1:A:29:VAL:HA	1:A:73:VAL:HG13	1.61	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	Distance(Å)	Clash(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:72:ASP:HB3	1:A:75:ASN:OD1	1.96	0.65
1:A:231:ASP:OD2	2:B:134:SER:HB2	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:36:ILE:HD11	2:B:64:MET:HG3	1.81	0.62
2:B:196:ASN:HA	2:B:207:ARG:HH22	1.64	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:29:VAL:HG21	1:A:76:LEU:HD21	1.82	0.61
1:A:172:GLN:HE21	1:A:172:GLN:HA	1.66	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
2:B:160:ASN:HA	2:B:205:VAL:HG12	1.83	0.59
1:A:161:VAL:HB	1:A:162:PRO:CD	2.31	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
2:B:224:SER:HB2	2:B:233:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:234:MET:HG3	2:B:234:MET:O	2.04	0.57
2:B:108:THR:HG23	2:B:129:GLN:HG2	1.85	0.56
1:A:152:ARG:O	1:A:156:VAL:HG23	2.05	0.56
2:B:234:MET:HA	2:B:247:ILE:O	2.06	0.56
2:B:69:LEU:HD11	2:B:103:SER:HB3	1.85	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
2:B:159:ASN:O	2:B:206:ILE:HG13	2.07	0.55
1:A:40:PRO:HG2	1:A:244:ILE:HD13	1.87	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
2:B:54:ASP:O	2:B:55:LYS:CB	2.55	0.55
1:A:93:ALA:HA	1:A:97:GLN:OE1	2.07	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:216:ARG:HD3	2:B:228:LEU:CD1	2.38	0.54
2:B:192:CYS:N	2:B:209:CYS:SG	2.81	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
2:B:198:TYR:HD2	2:B:230:SER:HB3	1.72	0.54
2:B:157:GLU:O	2:B:158:ASN:HB2	2.08	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
2:B:74:TYR:HA	2:B:119:LEU:CB	2.37	0.54
1:A:207:SER:O	1:A:211:VAL:HG21	2.08	0.54
2:B:71:SER:N	2:B:105:LEU:HD21	2.23	0.54
1:A:39:LEU:HB2	1:A:245:LEU:HD11	1.90	0.54
1:A:250:VAL:HG13	2:B:3:GLU:O	2.08	0.54
1:A:19:ARG:HB2	1:A:175:ARG:HH21	1.73	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:249:PHE:CG	2:B:250:PRO:HD2	2.45	0.52
1:A:192:SER:CB	1:A:221:GLN:HG3	2.39	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
2:B:124:ILE:O	2:B:125:HIS:HB2	2.11	0.51
1:A:24:ASN:O	1:A:28:ARG:HG2	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: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:130:ILE:O	1:A:130:ILE:HG22	2.11	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
2:B:126:ALA:HB1	2:B:211:GLY:O	2.13	0.49
1:A:75:ASN:OD1	1:A:77:TYR:HB2	2.13	0.49
1:A:44:ARG:H	1:A:47:GLU:HG3	1.77	0.49
2:B:22:CYS:SG	2:B:137:VAL:HG11	2.53	0.49
2:B:27:ASN:HA	3:B:281: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:203:LEU:HA	2:B:247:ILE:HG22	1.93	0.48
2:B:200:SER:HB3	2:B:249:PHE:CD1	2.48	0.48
2:B:105:LEU:HB2	2:B:120:LEU:HD12	1.96	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:LYS:N	1:A:14:LYS:HE3	2.27	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
2:B:200:SER:O	2:B:201:LYS:HB2	2.14	0.48
1:A:35:GLU:HB3	1:A:40:PRO:HA	1.95	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
2:B:49:TRP:CZ3	2:B:64:MET:HB2	2.49	0.47
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:70:ASN:O	2:B:71:SER:C	2.52	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: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
2:B:28:GLY:HA2	2:B:46:ASN:HB3	1.96	0.47
1:A:50:VAL:HG12	1:A:96:LEU:HD11	1.97	0.47
1:A:51:LYS:HD3	1:A:52:ASN:HD21	1.79	0.47
2:B:35:PRO:HA	2:B:76:MET:HB2	1.97	0.47
1:A:19:ARG:HB2	1:A:175:ARG:HD3	1.96	0.47
2:B:160:ASN:HD21	2:B:203:LEU:HD21	1.80	0.46
1:A:72:ASP:HB2	1:A:79:VAL:HG22	1.96	0.46
1:A:234:GLU:O	1:A:238:LYS:HG3	2.15	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:55:VAL:HB	1:A:71:VAL:CG2	2.45	0.46
1:A:133:GLY:C	1:A:136:PRO:HD2	2.35	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
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:169:TYR:HE1	2:B:263:VAL:HG22	1.81	0.45
1:A:44:ARG:O	1:A:48:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:68:GLY:O	2:B:73:SER:HB2	2.17	0.45
2:B:235:ASP:OD1	2:B:235:ASP:C	2.55	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
2:B:163:MET:HE1	2:B:259:TRP:CH2	2.52	0.44
1:A:96:LEU:O	1:A:100:ASN:HB2	2.17	0.44
1:A:250:VAL:CG2	2:B:4:THR:HA	2.41	0.44
2:B:154:ALA:O	2:B:172:GLN:HG2	2.17	0.44
1:A:78:LEU:O	1:A:90:PHE:HE2	2.01	0.44
2:B:181:ARG:HD3	2:B:181:ARG:HA	1.39	0.44
1:A:15:SER:HA	1:A:178:LEU:CD1	2.47	0.44
2:B:99:ILE:HA	2:B:106:VAL:HG12	1.99	0.44
2:B:105:LEU:HB3	2:B:120:LEU:HB3	1.99	0.44
1:A:173:GLU:HA	1:A:173:GLU:OE1	2.17	0.44
2:B:14:ARG:HG3	2:B:14:ARG:NH1	2.33	0.43
2:B:263:VAL:O	2:B:264:PRO:C	2.57	0.43
1:A:150:VAL:HG12	1:A:153:SER:OG	2.18	0.43
2:B:78:THR:CG2	2:B:79:ASP:N	2.81	0.43
1:A:175:ARG:O	1:A:179:GLN:HB2	2.18	0.43
2:B:230:SER:C	2:B:232:ARG:H	2.22	0.43
2:B:188:SER:C	2:B:190:GLY:H	2.21	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
2:B:158:ASN:HD22	2:B:158:ASN:N	2.16	0.43
1:A:53:ARG:HG2	6:A:311:HOH:O	2.17	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:29:VAL:HG21	1:A:76:LEU:CD2	2.47	0.43
1:A:218:VAL:CG1	1:A:220:LEU:HD13	2.48	0.43
1:A:129:SER:HA	1:A:185:THR:HG21	2.01	0.43
2:B:90:TRP:CH2	2:B:120:LEU:HD21	2.36	0.42
2:B:114:SER:O	2:B:115:ARG:HB2	2.18	0.42
1:A:35:GLU:CB	1:A:40:PRO:HA	2.50	0.42
2:B:127:ALA:HB3	2:B:211:GLY:CA	2.23	0.42
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.34	0.42
1:A:1:ILE:HD12	1:A:100:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:91:GLU:HB3	2:B:99:ILE:CG2	2.49	0.42
2:B:121:GLU:HA	2:B:121:GLU:OE2	2.19	0.42
1:A:133:GLY:O	1:A:137:LEU:HB2	2.19	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:74:TYR:HA	2:B:119:LEU:CA	2.49	0.42
1:A:175:ARG:HA	1:A:178:LEU:CD1	2.50	0.42
2:B:147:TYR:CD1	2:B:256:ASN:HA	2.54	0.42
2:B:46:ASN:ND2	3:B:280:GAL:H2	2.35	0.42
2:B:45:ARG:HD2	2:B:60:MET:HA	2.01	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:135:ASN:N	1:A:136:PRO:CD	2.84	0.41
1:A:115:ASN:O	1:A:118:ASN:HB2	2.21	0.41
1:A:172:GLN:HE22	1:A:175:ARG:NH1	2.19	0.41
2:B:39:TRP:CG	2:B:40:PRO:HD2	2.56	0.41
2:B:27:ASN:HA	3:B:281:BGC:H4	2.01	0.41
2:B:205:VAL:HB	2:B:206:ILE:H	1.63	0.41
1:A:89:PHE:HE1	1:A:107:GLN:HG3	1.85	0.41
1:A:247:PHE:CE1	1:A:250:VAL:HG12	2.55	0.41
1:A:132:LEU:HD12	1:A:184:PHE:CZ	2.56	0.41
2:B:237:LYS:C	2:B:239:SER:H	2.23	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
1:A:116:TYR:HA	1:A:116:TYR:HD2	1.77	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
2:B:167:ASP:OD1	2:B:169:THR:HG23	2.21	0.41
1:A:154:LEU:HA	1:A:154:LEU:HD12	1.84	0.41
2:B:35:PRO:HB3	2:B:74:TYR:HE1	1.86	0.41
2:B:28:GLY:CA	2:B:46:ASN:HD22	2.34	0.41
1:A:80:ALA:HB1	1:A:88:TYR:O	2.21	0.41
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:109:ALA:O	2:B:110:PRO:C	2.59	0.40
1:A:114:GLY:HA3	5:A:321:PT1:H111	1.86	0.40
2:B:179:ASP:C	2:B:181:ARG:H	2.24	0.40
2:B:150:MET:HE2	2:B:163:MET:O	2.22	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:44:GLN:O	2:B:48:GLN:HG3	2.22	0.40
1:A:60:THR:HA	1:A:66:THR:HB	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	250/254 (98%)	208 (83%)	31 (12%)	11 (4%)	4	25
2	B	261/266 (98%)	209 (80%)	36 (14%)	16 (6%)	2	16
All	All	511/520 (98%)	417 (82%)	67 (13%)	27 (5%)	3	21

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
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

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Mol	Chain	Res	Type
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	1

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	267	2,4	12,14,15	0.54	0	15,19,21	0.73	0
4	NAG	B	268	4	12,14,15	0.66	0	15,19,21	0.60	0
4	BMA	B	269	4	10,11,12	0.40	0	11,15,17	0.25	0
3	GAL	B	280	3	10,11,12	0.45	0	11,15,17	0.90	1 (9%)
3	BGC	B	281	3	12,12,12	0.56	0	17,17,17	0.56	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
4	NAG	B	267	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	268	4	-	0/6/23/26	0/1/1/1
4	BMA	B	269	4	-	0/2/19/22	0/1/1/1
3	GAL	B	280	3	-	0/2/19/22	0/1/1/1
3	BGC	B	281	3	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	280	GAL	C3-C4-C5	-2.02	106.60	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

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	-	25,25,25	2.27	13 (52%)	35,35,35	1.68	9 (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	-	-	0/9/9/9	0/1/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	321	PT1	C12-N8	4.14	1.39	1.31
5	A	321	PT1	C16-C15	4.00	1.45	1.39
5	A	321	PT1	C18-C20	3.88	1.46	1.39
5	A	321	PT1	C10-N6	3.76	1.40	1.32
5	A	321	PT1	C18-C16	3.18	1.44	1.38
5	A	321	PT1	C19-C20	2.91	1.44	1.39
5	A	321	PT1	C19-C17	2.77	1.44	1.38
5	A	321	PT1	C12-C10	2.56	1.43	1.39
5	A	321	PT1	C3-C5	2.55	1.46	1.40
5	A	321	PT1	C17-C15	2.23	1.42	1.39
5	A	321	PT1	O1-C2	2.08	1.36	1.27
5	A	321	PT1	C20-C21	2.08	1.53	1.49
5	A	321	PT1	O22-C21	2.08	1.29	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	321	PT1	C12-N8-C5	3.95	121.29	116.85
5	A	321	PT1	C2-C3-N6	3.29	126.79	118.29
5	A	321	PT1	C13-C10-N6	3.13	122.57	116.79
5	A	321	PT1	O23-C21-O22	-2.98	116.59	123.35
5	A	321	PT1	C10-C12-N8	-2.60	120.42	123.16
5	A	321	PT1	C17-C15-N14	-2.58	115.74	121.02
5	A	321	PT1	C2-C3-C5	-2.37	113.24	116.54
5	A	321	PT1	O23-C21-C20	2.32	121.14	115.01
5	A	321	PT1	C5-C3-N6	-2.20	119.97	122.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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%)	-0.23	0 100 100	5, 23, 42, 77	0
2	B	263/266 (98%)	-0.17	0 100 100	3, 28, 47, 64	0
All	All	515/520 (99%)	-0.20	0 93 100	3, 26, 46, 77	0

There are no RSRZ outliers to report.

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	B	281	12/12	0.79	29.56	98,98,98,98	0
3	GAL	B	280	11/12	0.46	11.26	72,72,72,72	0
4	NAG	B	267	14/15	0.26	1.88	27,27,27,27	0
4	NAG	B	268	14/15	0.39	-	64,64,64,64	0
4	BMA	B	269	11/12	0.32	-	71,71,71,71	0



## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PT1	A	321	23/23	0.29	2.12	23,23,23,23	0

## 6.5 Other polymers

There are no such residues in this entry.