



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:49 pm GMT

PDB ID : 1HWN  
Title : EBULIN COMPLEXED WITH GALACTOSE, 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 : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

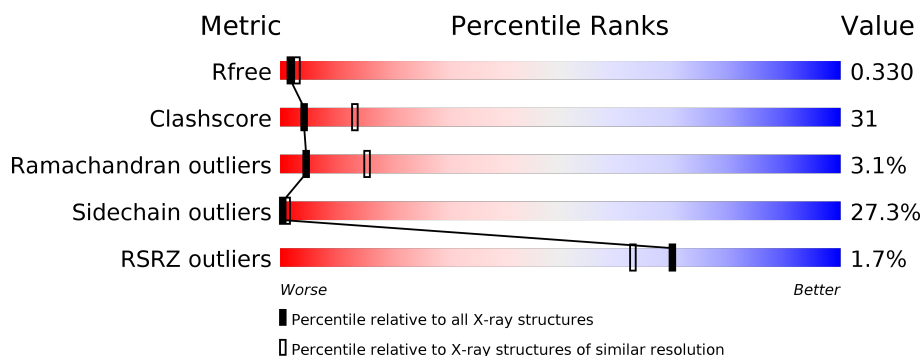
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>36%</div> <div>50%</div> <div>14%</div> </div> </div>
2	B	266	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>49%</div> <div>16%</div> </div> </div>

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
4	GAL	B	280	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4133 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.

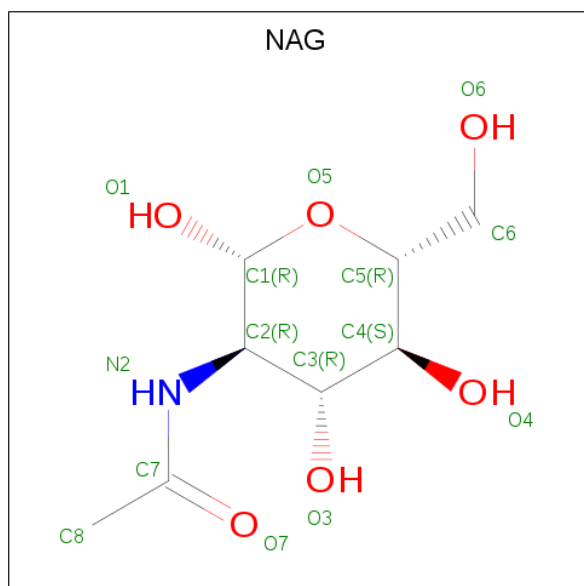
- Molecule 1 is a protein called EBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2007	1267	344	391	5			

- Molecule 2 is a protein called EBULIN.

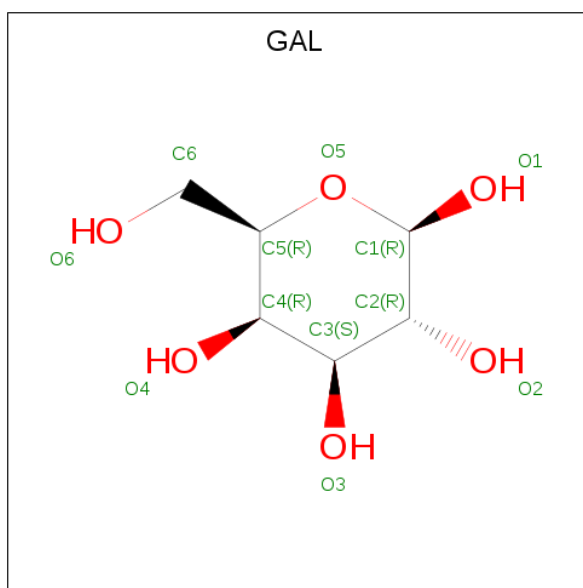
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			2028	1253	359	400	16			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	27	Total	O	0	0
			27	27		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.60Å 73.60Å 190.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 36.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 92.1 (36.13-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.264 , 0.328 0.282 , 0.330	Depositor DCC
$R_{free}$ test set	853 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/2044	0.42	0/2777
2	B	0.24	0/2065	0.44	0/2813
All	All	0.25	0/4109	0.43	0/5590

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2007	0	1982	125	0
2	B	2028	0	1959	137	0
3	B	28	0	25	1	0
4	B	24	0	24	3	0
5	A	19	0	0	0	0
5	B	27	0	0	0	0
All	All	4133	0	3990	251	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 31.

All (251) 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:263:VAL:HB	2:B:264:PRO:HD2	1.44	0.98
2:B:37:GLN:HB3	2:B:117:THR:HA	1.44	0.94
2:B:44:GLN:HG3	2:B:47:GLN:HG3	1.49	0.93
2:B:132:THR:HB	2:B:179:ASP:HB3	1.53	0.87
2:B:177:LEU:HD11	2:B:261:THR:HG21	1.57	0.86
2:B:45:ARG:HA	2:B:48:GLN:HE21	1.38	0.86
2:B:23:VAL:HG22	2:B:36:ILE:HD12	1.60	0.84
2:B:58:ARG:HB3	2:B:63:CYS:HA	1.58	0.84
1:A:127:ARG:HH12	1:A:195:ASN:HD21	1.25	0.82
1:A:134:PRO:HG3	1:A:178:LEU:HA	1.61	0.81
1:A:213:PRO:HG3	2:B:133:VAL:HG11	1.67	0.76
2:B:263:VAL:HB	2:B:264:PRO:CD	2.17	0.74
1:A:67:VAL:HG12	1:A:83:ALA:HB2	1.70	0.73
2:B:127:ALA:HB3	2:B:211:GLY:HA2	1.70	0.72
2:B:204:ILE:HD12	2:B:246:VAL:HG12	1.70	0.72
2:B:226:VAL:HG12	2:B:233:VAL:HG13	1.71	0.72
2:B:37:GLN:HA	2:B:118:LEU:HD23	1.71	0.72
2:B:235:ASP:HB3	2:B:257:GLN:HG2	1.73	0.71
2:B:200:SER:O	2:B:201:LYS:HB2	1.91	0.71
2:B:263:VAL:CB	2:B:264:PRO:HD2	2.18	0.70
2:B:124:ILE:H	2:B:129:GLN:HE22	1.41	0.69
1:A:218:VAL:HB	1:A:230:VAL:HG13	1.73	0.69
1:A:202:LEU:O	1:A:206:LEU:HB2	1.92	0.68
2:B:150:MET:HB2	2:B:163:MET:HG2	1.74	0.68
2:B:74:TYR:HA	2:B:119:LEU:HA	1.75	0.68
2:B:85:GLU:HG3	2:B:89:LYS:HE3	1.74	0.68
1:A:45:GLU:HA	1:A:48:VAL:HG12	1.74	0.68
2:B:209:CYS:HA	2:B:215:GLN:HE22	1.57	0.68
1:A:29:VAL:HG12	1:A:73:VAL:HG23	1.77	0.67
1:A:232:ASN:OD1	1:A:235:GLU:HB2	1.96	0.65
2:B:203:LEU:HA	2:B:247:ILE:HG22	1.77	0.64
1:A:191:LEU:O	1:A:194:GLU:HG2	1.98	0.64
2:B:126:ALA:HA	2:B:213:ALA:HA	1.78	0.64
1:A:61:ASN:OD1	1:A:65:ASP:HB2	1.98	0.63
1:A:161:VAL:HB	1:A:162:PRO:HD3	1.79	0.63
1:A:202:LEU:HD12	1:A:203:GLU:N	2.14	0.63
2:B:108:THR:HG23	2:B:129:GLN:HG2	1.78	0.63
2:B:183:ILE:O	2:B:193:VAL:HG23	1.98	0.63
1:A:115:ASN:OD1	1:A:118:ASN:HB2	1.98	0.63
2:B:256:ASN:HD21	4:B:290:GAL:H2	1.65	0.62
2:B:148:ASN:HB3	2:B:150:MET:HG3	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ILE:HB	2:B:23:VAL:HG12	1.80	0.62
1:A:161:VAL:HB	1:A:162:PRO:CD	2.30	0.62
2:B:232:ARG:HB3	2:B:248:ILE:HB	1.81	0.61
2:B:154:ALA:HB2	2:B:175:TRP:CH2	2.36	0.61
1:A:154:LEU:HA	1:A:157:LEU:HD12	1.83	0.61
1:A:202:LEU:HD23	1:A:248:ARG:NH1	2.15	0.60
2:B:142:THR:HB	2:B:263:VAL:HA	1.83	0.60
1:A:45:GLU:HA	1:A:48:VAL:CG1	2.31	0.60
2:B:36:ILE:HG22	2:B:118:LEU:HB2	1.83	0.60
1:A:252:THR:HG22	2:B:5:CYS:H	1.67	0.59
1:A:94:THR:O	1:A:97:GLN:HG2	2.02	0.59
2:B:18:ARG:HG2	2:B:112:GLY:HA2	1.85	0.59
2:B:36:ILE:HD11	2:B:49:TRP:HZ2	1.66	0.59
2:B:154:ALA:HB1	2:B:206:ILE:HD13	1.85	0.58
1:A:134:PRO:HG3	1:A:178:LEU:HD23	1.86	0.58
1:A:218:VAL:HB	1:A:230:VAL:CG1	2.33	0.58
1:A:224:ASP:OD1	1:A:226:THR:HB	2.04	0.57
1:A:26:ARG:HG3	1:A:165:ALA:HB1	1.86	0.57
1:A:90:PHE:HB3	1:A:113:THR:HA	1.86	0.57
2:B:201:LYS:HA	2:B:247:ILE:HD13	1.86	0.57
2:B:45:ARG:HA	2:B:48:GLN:NE2	2.15	0.57
1:A:213:PRO:HG3	2:B:133:VAL:CG1	2.33	0.57
1:A:8:PHE:HB2	1:A:21:PHE:CD1	2.39	0.57
1:A:57:VAL:O	1:A:68:THR:HA	2.05	0.57
2:B:161:VAL:HG22	2:B:204:ILE:O	2.05	0.57
1:A:235:GLU:HG2	2:B:140:ILE:HD11	1.87	0.56
1:A:18:TYR:HD2	1:A:175:ARG:HG2	1.71	0.56
1:A:249:CYS:SG	1:A:250:VAL:N	2.78	0.56
1:A:123:ALA:HB2	1:A:151:ALA:HB3	1.87	0.56
2:B:226:VAL:HG12	2:B:233:VAL:HG22	1.86	0.56
1:A:19:ARG:HB2	1:A:175:ARG:CZ	2.36	0.56
1:A:26:ARG:HH21	1:A:165:ALA:HA	1.69	0.56
1:A:10:LEU:HD11	1:A:137:LEU:HD13	1.87	0.56
2:B:125:HIS:HB3	2:B:228:LEU:HB3	1.88	0.55
2:B:49:TRP:HB3	2:B:57:ILE:HG22	1.88	0.55
2:B:166:CYS:HA	2:B:173:GLN:HE22	1.71	0.55
2:B:24:ASP:O	2:B:36:ILE:HD13	2.05	0.55
2:B:224:SER:HB2	2:B:233:VAL:HG11	1.89	0.55
1:A:1:ILE:HG12	1:A:100:ASN:HB2	1.88	0.55
1:A:177:SER:HB2	1:A:182:THR:O	2.07	0.55
2:B:23:VAL:HG13	2:B:23:VAL:O	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:LEU:O	2:B:261:THR:HA	2.07	0.54
1:A:199:SER:O	1:A:202:LEU:HG	2.08	0.54
1:A:59:LEU:HD11	1:A:161:VAL:HG21	1.89	0.54
2:B:44:GLN:CG	2:B:47:GLN:HG3	2.33	0.54
1:A:39:LEU:HB2	1:A:245:LEU:HD23	1.90	0.54
2:B:45:ARG:NE	2:B:60:MET:HG3	2.23	0.53
1:A:156:VAL:O	1:A:160:MET:HB2	2.08	0.53
2:B:54:ASP:O	2:B:89:LYS:HD2	2.09	0.52
1:A:97:GLN:O	1:A:101:LEU:HB2	2.09	0.52
1:A:54:PHE:CZ	1:A:97:GLN:HB3	2.44	0.52
1:A:201:SER:HA	1:A:245:LEU:HD12	1.91	0.52
1:A:6:VAL:HG21	1:A:25:LEU:HA	1.92	0.52
2:B:142:THR:HB	2:B:263:VAL:CA	2.39	0.52
1:A:241:GLY:HA3	2:B:260:ARG:HH21	1.74	0.52
2:B:178:PHE:HB3	2:B:180:ASP:OD1	2.09	0.52
1:A:205:GLN:HE22	1:A:248:ARG:H	1.57	0.51
1:A:9:ASN:O	1:A:13:ALA:HB2	2.10	0.51
2:B:17:GLY:O	2:B:18:ARG:HB2	2.10	0.51
1:A:97:GLN:HB2	1:A:101:LEU:HD12	1.92	0.51
2:B:91:GLU:HB3	2:B:99:ILE:HG22	1.93	0.51
1:A:172:GLN:HB3	2:B:262:GLN:HE21	1.76	0.51
1:A:116:TYR:CD2	1:A:127:ARG:HD3	2.46	0.51
1:A:91:LYS:HB3	1:A:113:THR:HG22	1.92	0.51
2:B:17:GLY:C	2:B:180:ASP:HB3	2.31	0.51
2:B:38:LEU:HD13	2:B:118:LEU:HD21	1.92	0.51
2:B:95:ASP:HB3	2:B:228:LEU:HD11	1.91	0.51
1:A:144:LEU:CD2	1:A:149:GLY:HA2	2.41	0.51
1:A:137:LEU:HB2	1:A:160:MET:HE1	1.94	0.50
2:B:52:TYR:HB2	2:B:54:ASP:OD1	2.10	0.50
2:B:210:GLN:HB2	2:B:212:LEU:HD13	1.92	0.50
2:B:233:VAL:O	2:B:248:ILE:HA	2.11	0.50
2:B:262:GLN:O	2:B:263:VAL:O	2.30	0.50
1:A:206:LEU:HD12	2:B:5:CYS:SG	2.51	0.50
1:A:53:ARG:HH11	1:A:53:ARG:HG3	1.77	0.50
2:B:167:ASP:H	2:B:173:GLN:NE2	2.10	0.50
2:B:142:THR:HA	2:B:263:VAL:O	2.12	0.49
2:B:194:THR:HB	2:B:207:ARG:HG2	1.93	0.49
2:B:200:SER:O	2:B:201:LYS:CB	2.59	0.49
2:B:209:CYS:C	2:B:210:GLN:HG2	2.31	0.49
2:B:34:THR:O	2:B:76:MET:HB2	2.13	0.49
1:A:201:SER:HA	1:A:245:LEU:CD1	2.43	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:VAL:HG13	1:A:48:VAL:O	2.12	0.49
2:B:202:ASP:HB2	2:B:248:ILE:HD11	1.93	0.49
1:A:212:SER:HB2	1:A:234:GLU:OE2	2.12	0.49
1:A:53:ARG:NH1	1:A:96:LEU:HD21	2.28	0.49
2:B:127:ALA:HB3	2:B:211:GLY:CA	2.41	0.49
1:A:135:ASN:HB2	1:A:136:PRO:HD3	1.95	0.49
1:A:67:VAL:HG22	1:A:141:ILE:HG23	1.95	0.49
2:B:226:VAL:CG1	2:B:233:VAL:HG22	2.43	0.49
1:A:232:ASN:N	1:A:232:ASN:HD22	2.11	0.48
1:A:170:ILE:O	1:A:174:VAL:HG23	2.12	0.48
2:B:237:LYS:HG2	2:B:238:GLU:HG2	1.95	0.48
2:B:24:ASP:HB2	2:B:47:GLN:NE2	2.28	0.48
1:A:126:ARG:O	1:A:130:ILE:HD12	2.14	0.48
2:B:12:THR:C	2:B:13:ARG:HG2	2.33	0.48
1:A:110:LEU:HD13	1:A:112:PHE:CZ	2.47	0.48
1:A:100:ASN:HA	1:A:103:LEU:HG	1.95	0.48
1:A:202:LEU:HD23	1:A:248:ARG:CZ	2.44	0.48
1:A:180:GLN:HB2	1:A:182:THR:HG22	1.95	0.48
2:B:30:ASP:HB3	2:B:60:MET:HG2	1.96	0.48
1:A:249:CYS:SG	2:B:5:CYS:N	2.87	0.48
1:A:5:SER:HB3	1:A:56:LEU:HB2	1.95	0.47
1:A:172:GLN:HA	1:A:175:ARG:HB2	1.95	0.47
2:B:180:ASP:O	2:B:181:ARG:HB2	2.13	0.47
1:A:60:THR:HG23	1:A:64:GLY:O	2.15	0.47
2:B:153:GLN:HG2	2:B:164:GLU:HB2	1.97	0.47
3:B:268:NAG:O7	3:B:268:NAG:O5	2.33	0.47
2:B:171:VAL:HA	2:B:174:GLN:HG3	1.95	0.47
1:A:53:ARG:HH12	1:A:96:LEU:HD21	1.80	0.47
2:B:41:CYS:HB3	2:B:137:VAL:HG11	1.97	0.47
1:A:252:THR:CG2	2:B:5:CYS:HB2	2.45	0.47
1:A:151:ALA:O	1:A:152:ARG:C	2.54	0.46
1:A:188:ALA:HB3	1:A:222:ASN:O	2.15	0.46
1:A:60:THR:OG1	1:A:66:THR:HB	2.15	0.46
2:B:144:ILE:HG22	2:B:259:TRP:HE3	1.79	0.46
2:B:17:GLY:HA3	2:B:130:GLY:O	2.15	0.46
1:A:114:GLY:O	1:A:115:ASN:HB3	2.15	0.46
1:A:133:GLY:O	1:A:137:LEU:HB2	2.16	0.46
2:B:15:ILE:O	2:B:22:CYS:HA	2.16	0.46
1:A:163:GLU:OE1	1:A:194:GLU:HB2	2.16	0.46
1:A:53:ARG:HH11	1:A:96:LEU:HD11	1.81	0.46
2:B:90:TRP:HH2	2:B:120:LEU:HD21	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ASN:C	2:B:55:LYS:H	2.20	0.45
1:A:158:ILE:O	1:A:162:PRO:HG2	2.16	0.45
1:A:101:LEU:HA	1:A:101:LEU:HD23	1.85	0.45
2:B:178:PHE:HB2	2:B:182:THR:O	2.17	0.45
2:B:118:LEU:HD11	2:B:131:TRP:CZ2	2.51	0.45
2:B:124:ILE:HG13	2:B:129:GLN:HE22	1.81	0.45
2:B:58:ARG:HB3	2:B:63:CYS:CA	2.40	0.45
2:B:49:TRP:HB3	2:B:57:ILE:CG2	2.47	0.44
1:A:195:ASN:HD22	1:A:195:ASN:N	2.15	0.44
2:B:140:ILE:HG22	2:B:142:THR:HG22	1.99	0.44
1:A:10:LEU:HB2	1:A:60:THR:O	2.18	0.44
2:B:99:ILE:HG13	2:B:106:VAL:HG12	1.98	0.44
1:A:238:LYS:HG2	2:B:177:LEU:CD1	2.48	0.44
2:B:226:VAL:CG1	2:B:233:VAL:HG13	2.46	0.44
1:A:144:LEU:HD22	1:A:149:GLY:HA2	2.00	0.44
2:B:188:SER:C	2:B:190:GLY:H	2.20	0.44
1:A:232:ASN:ND2	1:A:232:ASN:N	2.66	0.44
1:A:230:VAL:HG21	1:A:236:LEU:HB2	1.99	0.44
2:B:257:GLN:HG3	4:B:290:GAL:O2	2.18	0.44
2:B:220:ASN:HB3	2:B:222:ASP:OD1	2.18	0.43
1:A:98:LYS:H	1:A:98:LYS:HG3	1.64	0.43
1:A:172:GLN:HB3	2:B:262:GLN:NE2	2.32	0.43
2:B:41:CYS:CB	2:B:137:VAL:HG11	2.48	0.43
1:A:166:ARG:HD2	1:A:197:TRP:CE2	2.53	0.43
2:B:144:ILE:HD12	2:B:152:LEU:HD23	2.01	0.43
2:B:260:ARG:NH1	2:B:261:THR:O	2.51	0.43
1:A:229:LEU:HD12	1:A:229:LEU:H	1.83	0.43
2:B:160:ASN:H	2:B:160:ASN:HD22	1.66	0.43
1:A:120:GLU:OE2	1:A:127:ARG:HG3	2.19	0.43
1:A:137:LEU:HD21	1:A:157:LEU:HD23	2.00	0.43
2:B:108:THR:O	2:B:118:LEU:HD13	2.18	0.43
1:A:97:GLN:HE21	1:A:97:GLN:HB3	1.57	0.43
1:A:94:THR:OG1	1:A:96:LEU:HD23	2.19	0.42
1:A:197:TRP:HZ2	1:A:244:ILE:HG22	1.84	0.42
1:A:67:VAL:CG2	1:A:141:ILE:HG23	2.49	0.42
1:A:159:GLN:HA	1:A:163:GLU:HB3	2.01	0.42
2:B:216:ARG:O	2:B:227:ASN:HA	2.19	0.42
2:B:260:ARG:HD3	2:B:262:GLN:HE21	1.84	0.42
1:A:44:ARG:H	1:A:44:ARG:HG3	1.66	0.42
2:B:181:ARG:HD3	2:B:181:ARG:HA	1.78	0.42
1:A:197:TRP:CH2	1:A:246:LEU:HB2	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:O	1:A:109:THR:HA	2.19	0.42
2:B:235:ASP:CB	2:B:257:GLN:HG2	2.48	0.42
2:B:26:ARG:C	2:B:28:GLY:H	2.23	0.42
2:B:77:ILE:HD13	2:B:77:ILE:H	1.84	0.42
1:A:154:LEU:HA	1:A:154:LEU:HD13	1.87	0.42
1:A:72:ASP:HB3	1:A:75:ASN:OD1	2.20	0.42
2:B:27:ASN:H	4:B:280:GAL:H62	1.85	0.42
1:A:202:LEU:HD12	1:A:202:LEU:C	2.39	0.42
1:A:70:ALA:O	1:A:79:VAL:HG12	2.19	0.42
2:B:108:THR:OG1	2:B:121:GLU:HB2	2.20	0.42
2:B:85:GLU:O	2:B:89:LYS:HG2	2.19	0.42
2:B:75:ILE:CD1	2:B:118:LEU:HB3	2.50	0.42
2:B:226:VAL:HG12	2:B:233:VAL:CG1	2.46	0.42
2:B:263:VAL:O	2:B:264:PRO:C	2.58	0.42
2:B:59:SER:C	2:B:61:GLY:H	2.23	0.42
2:B:85:GLU:O	2:B:88:THR:HG22	2.19	0.42
2:B:65:THR:HA	2:B:87:ALA:O	2.20	0.41
1:A:26:ARG:CG	1:A:165:ALA:HB1	2.50	0.41
2:B:160:ASN:N	2:B:205:VAL:HG12	2.34	0.41
2:B:126:ALA:HB1	2:B:211:GLY:O	2.19	0.41
1:A:168:ARG:O	1:A:171:GLU:HB3	2.20	0.41
2:B:107:MET:CG	2:B:118:LEU:HD12	2.50	0.41
1:A:37:ASN:OD1	2:B:94:ILE:HG21	2.20	0.41
1:A:144:LEU:HD21	1:A:153:SER:HB2	2.03	0.41
1:A:170:ILE:HG23	1:A:190:MET:CE	2.50	0.41
1:A:8:PHE:HB3	1:A:59:LEU:HD23	2.02	0.41
1:A:132:LEU:HD11	1:A:186:PRO:HG3	2.03	0.41
2:B:124:ILE:HG13	2:B:129:GLN:NE2	2.35	0.41
2:B:195:SER:OG	2:B:196:ASN:N	2.54	0.41
1:A:145:TRP:HD1	1:A:146:TYR:HD2	1.69	0.41
1:A:234:GLU:O	1:A:238:LYS:HD3	2.20	0.41
1:A:8:PHE:HB2	1:A:21:PHE:CG	2.55	0.41
2:B:160:ASN:OD1	2:B:203:LEU:HD13	2.22	0.41
1:A:200:MET:HE2	1:A:200:MET:HB3	1.86	0.40
1:A:245:LEU:HA	1:A:245:LEU:HD13	1.88	0.40
1:A:81:PHE:CE2	1:A:88:TYR:HB2	2.56	0.40
2:B:126:ALA:O	2:B:216:ARG:NH2	2.54	0.40
2:B:14:ARG:O	2:B:133:VAL:HA	2.22	0.40
1:A:172:GLN:OE1	1:A:172:GLN:HA	2.21	0.40
2:B:240:ASP:OD2	2:B:243:LEU:HG	2.21	0.40
1:A:92:ASP:O	1:A:93:ALA:C	2.58	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:SER:O	2:B:105:LEU:HD22	2.21	0.40
2:B:249:PHE:CG	2:B:250:PRO:HD2	2.56	0.40
2:B:88:THR:HG23	2:B:89:LYS:HD3	2.04	0.40
1:A:3:TYR:HE1	1:A:54:PHE:H	1.69	0.40
1:A:99:SER:O	1:A:103:LEU:HD11	2.21	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	252/254 (99%)	218 (86%)	27 (11%)	7 (3%)	5	18
2	B	261/266 (98%)	212 (81%)	40 (15%)	9 (3%)	4	14
All	All	513/520 (99%)	430 (84%)	67 (13%)	16 (3%)	4	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	187	ASN
2	B	263	VAL
1	A	11	ALA
1	A	93	ALA
1	A	115	ASN
1	A	151	ALA
2	B	18	ARG
2	B	69	LEU
1	A	161	VAL
2	B	102	SER
2	B	189	ARG
2	B	201	LYS
1	A	152	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	208	LYS
1	A	36	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	223/223 (100%)	166 (74%)	57 (26%)	0	1
2	B	228/231 (99%)	162 (71%)	66 (29%)	0	1
All	All	451/454 (99%)	328 (73%)	123 (27%)	0	1

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	2	ASP
1	A	9	ASN
1	A	14	LYS
1	A	28	ARG
1	A	36	VAL
1	A	43	ARG
1	A	44	ARG
1	A	46	SER
1	A	47	GLU
1	A	51	LYS
1	A	53	ARG
1	A	66	THR
1	A	67	VAL
1	A	69	SER
1	A	73	VAL
1	A	78	LEU
1	A	82	SER
1	A	86	ASN
1	A	92	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	95	GLU
1	A	96	LEU
1	A	97	GLN
1	A	99	SER
1	A	106	THR
1	A	107	GLN
1	A	118	ASN
1	A	126	ARG
1	A	132	LEU
1	A	137	LEU
1	A	143	SER
1	A	147	ASP
1	A	152	ARG
1	A	154	LEU
1	A	157	LEU
1	A	163	GLU
1	A	179	GLN
1	A	185	THR
1	A	190	MET
1	A	195	ASN
1	A	199	SER
1	A	201	SER
1	A	210	ASN
1	A	212	SER
1	A	215	SER
1	A	219	GLN
1	A	220	LEU
1	A	221	GLN
1	A	226	THR
1	A	229	LEU
1	A	230	VAL
1	A	231	ASP
1	A	232	ASN
1	A	238	LYS
1	A	245	LEU
1	A	252	THR
1	A	254	THR
2	B	4	THR
2	B	16	VAL
2	B	24	ASP
2	B	34	THR
2	B	36	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	37	GLN
2	B	38	LEU
2	B	43	THR
2	B	44	GLN
2	B	46	ASN
2	B	48	GLN
2	B	53	ASN
2	B	55	LYS
2	B	58	ARG
2	B	60	MET
2	B	70	ASN
2	B	71	SER
2	B	75	ILE
2	B	76	MET
2	B	77	ILE
2	B	82	THR
2	B	91	GLU
2	B	95	ASP
2	B	97	SER
2	B	102	SER
2	B	103	SER
2	B	105	LEU
2	B	108	THR
2	B	115	ARG
2	B	119	LEU
2	B	120	LEU
2	B	142	THR
2	B	143	LEU
2	B	145	VAL
2	B	147	TYR
2	B	149	GLU
2	B	152	LEU
2	B	153	GLN
2	B	155	ASN
2	B	163	MET
2	B	165	ASP
2	B	170	SER
2	B	172	GLN
2	B	184	ARG
2	B	185	VAL
2	B	189	ARG
2	B	195	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	196	ASN
2	B	200	SER
2	B	202	ASP
2	B	206	ILE
2	B	208	LYS
2	B	210	GLN
2	B	216	ARG
2	B	221	SER
2	B	228	LEU
2	B	229	LYS
2	B	231	THR
2	B	236	VAL
2	B	239	SER
2	B	241	VAL
2	B	242	SER
2	B	244	GLN
2	B	260	ARG
2	B	261	THR
2	B	263	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	107	GLN
1	A	135	ASN
1	A	195	ASN
1	A	196	ASN
1	A	221	GLN
2	B	27	ASN
2	B	48	GLN
2	B	70	ASN
2	B	129	GLN
2	B	159	ASN
2	B	173	GLN
2	B	215	GLN
2	B	256	ASN
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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	B	267	3,2	14,14,15	0.45	0	17,19,21	0.65	0
3	NAG	B	268	3	14,14,15	0.60	0	17,19,21	1.16	2 (11%)
4	GAL	B	280	-	12,12,12	0.33	0	17,17,17	0.34	0
4	GAL	B	290	-	12,12,12	0.33	0	17,17,17	0.36	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	NAG	B	267	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	268	3	-	0/6/23/26	0/1/1/1
4	GAL	B	280	-	-	0/2/22/22	0/1/1/1
4	GAL	B	290	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	268	NAG	C3-C4-C5	2.08	113.97	110.24
3	B	268	NAG	C1-O5-C5	2.40	115.48	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	268	NAG	1	0
4	B	280	GAL	1	0
4	B	290	GAL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	254/254 (100%)	0.11	5 (1%) 65 56	7, 26, 48, 60	0
2	B	263/266 (98%)	0.22	4 (1%) 73 67	4, 29, 46, 63	0
All	All	517/520 (99%)	0.16	9 (1%) 70 63	4, 28, 47, 63	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	199	VAL	2.8
1	A	252	THR	2.8
2	B	154	ALA	2.5
1	A	254	THR	2.5
2	B	264	PRO	2.3
1	A	48	VAL	2.3
1	A	103	LEU	2.2
2	B	243	LEU	2.2
1	A	1	ILE	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 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
4	GAL	B	290	12/12	0.76	0.39	51,51,51,51	0
4	GAL	B	280	12/12	0.77	0.41	25,25,25,25	0
3	NAG	B	268	14/15	0.79	0.24	68,68,68,68	0
3	NAG	B	267	14/15	0.87	0.20	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.