



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 AM GMT

PDB ID : 2RI9  
Title : Penicillium citrinum alpha-1,2-mannosidase in complex with a substrate analog  
Authors : Lobsanov, Y.D.; Yoshida, T.; Desmet, T.; Nerinckx, W.; Yip, P.; Claeysens, M.; Herscovics, A.; Howell, P.L.  
Deposited on : 2007-10-10  
Resolution : 1.95 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

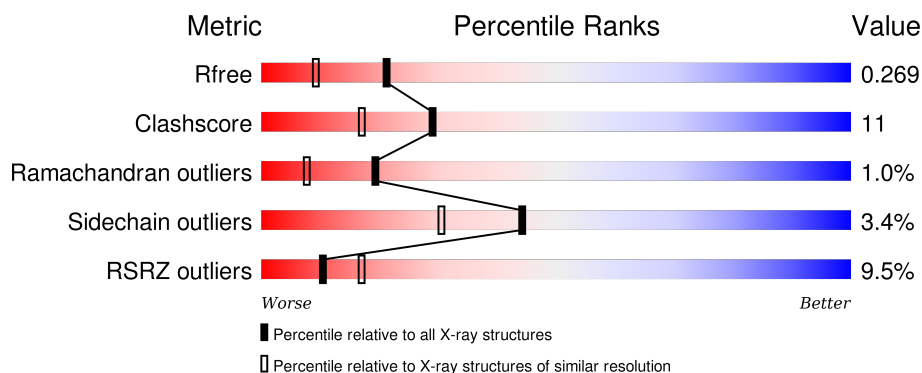
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	475	<div> <div></div> <div> <div></div> <div>88%</div> <div>11%</div> <div></div> </div> </div>
1	B	475	<div> <div>18%</div> <div>67%</div> <div>30%</div> <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
2	NAG	A	1800	-	-	-	X
2	NAG	B	2600	-	-	-	X
3	NAG	A	1700	-	-	-	X
3	NDG	A	1701	-	-	-	X
3	MAN	A	1702	X	-	-	-
3	MAN	A	1704	-	-	-	X
3	MAN	B	2702	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8503 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 Mannosyl-oligosaccharide alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	2	0
			3744	2370	624	741	9			
1	B	475	Total	C	N	O	S	0	1	0
			3736	2365	623	740	8			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	2	Total	C	O	0	2
			22	12	10		
4	B	2	Total	C	O	0	2
			22	12	10		

- Molecule 5 is a polymer of unknown type called SUGAR (O1-METHYL-MANNOSE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	1
			6	3	3		
7	A	1	Total	C	O	0	1
			6	3	3		
7	B	1	Total	C	O	0	1
			6	3	3		
7	B	1	Total	C	O	0	1
			6	3	3		

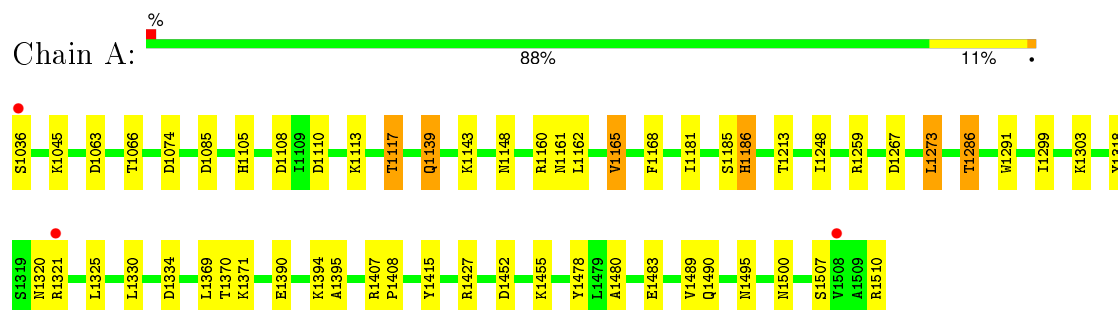
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	482	Total 483	O 483	0	1
8	B	235	Total 236	O 236	0	1

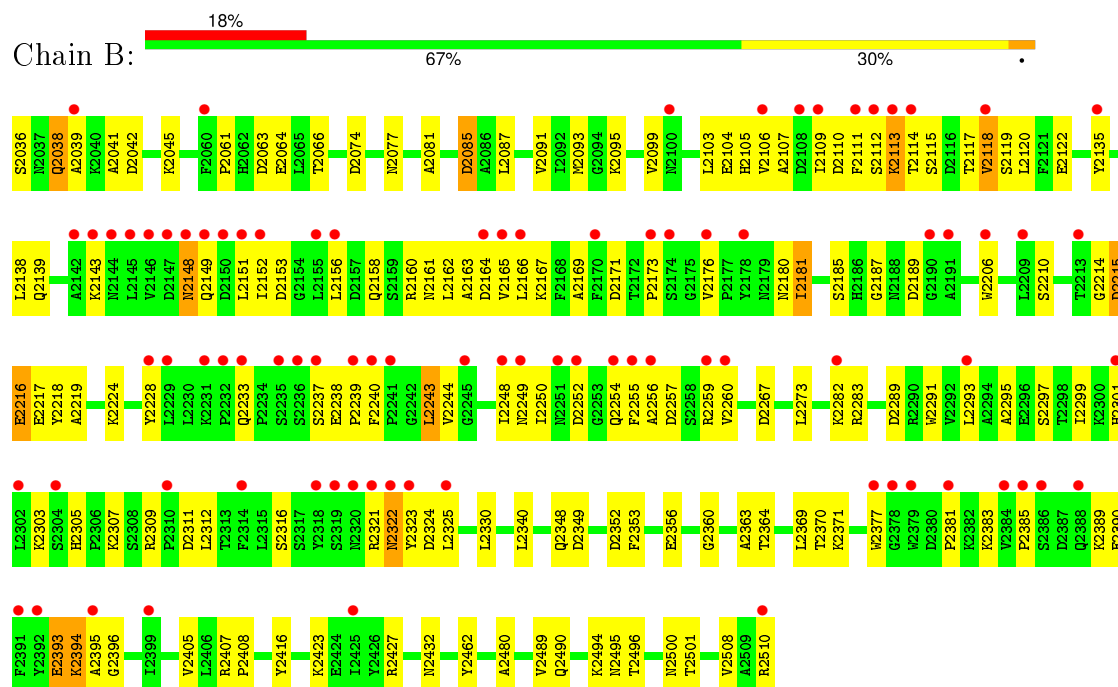
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Mannosyl-oligosaccharide alpha-1,2-mannosidase



- Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.49 Å 111.00 Å 86.23 Å 90.00° 99.17° 90.00°	Depositor
Resolution (Å)	49.83 – 1.95 49.83 – 1.97	Depositor EDS
% Data completeness (in resolution range)	93.9 (49.83-1.95) 94.0 (49.83-1.97)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 1.97 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.260 0.220 , 0.269	Depositor DCC
$R_{free}$ test set	4966 reflections (7.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 74.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 70466 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.1078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, NAG, CA, NDG, LDY, MMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.68	0/3839	0.73	2/5215 (0.0%)
1	B	0.45	0/3831	0.66	2/5205 (0.0%)
All	All	0.58	0/7670	0.69	4/10420 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	1	0
3	B	1	0
All	All	2	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1066	THR	N-CA-C	-5.76	95.45	111.00
1	B	2066	THR	N-CA-C	-5.46	96.25	111.00
1	A	1334	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	2462	TYR	CB-CA-C	-5.07	100.26	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1702	MAN	C1
3	B	2702	MAN	C1

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	3744	0	3543	42	0
1	B	3736	0	3536	125	0
2	A	56	0	50	1	0
2	B	28	0	25	2	0
3	A	61	0	52	1	0
3	B	61	0	52	6	0
4	A	22	0	19	1	0
4	B	22	0	21	0	0
5	B	28	0	25	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	12	0	16	0	0
7	B	12	0	16	0	0
8	A	483	0	0	14	0
8	B	236	0	0	17	0
All	All	8503	0	7355	172	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 11.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2330:LEU:HD21	1:B:2407[B]:ARG:NH2	1.86	0.89
1:A:1330:LEU:HD21	1:A:1407[B]:ARG:NH2	1.96	0.80
1:A:1139:GLN:HA	1:A:1139:GLN:HE21	1.49	0.78
1:A:1490:GLN:H	1:A:1495:ASN:HD21	1.32	0.78
1:B:2423:LYS:HE2	1:B:2423:LYS:HA	1.67	0.77
1:B:2394:LYS:HB2	1:B:2394:LYS:NZ	2.05	0.72
1:B:2427:ARG:HD3	1:B:2480:ALA:O	1.90	0.71
1:A:1162:LEU:O	1:A:1165:VAL:HG13	1.92	0.70
1:B:2119:SER:HB3	1:B:2122:GLU:HB2	1.74	0.69
1:B:2210:SER:OG	1:B:2218:TYR:HB2	1.93	0.69
1:A:1390:GLU:HG3	8:A:673:HOH:O	1.92	0.68
1:A:1490:GLN:H	1:A:1495:ASN:ND2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2181:ILE:HD13	1:B:2181:ILE:H	1.60	0.67
1:B:2330:LEU:HD21	1:B:2407[B]:ARG:HH21	1.57	0.66
1:B:2494:LYS:HB3	8:B:646:HOH:O	1.94	0.66
1:B:2370:THR:O	1:B:2371:LYS:HB2	1.94	0.66
1:B:2244:VAL:HB	1:B:2255:PHE:CE2	2.31	0.65
1:B:2303:LYS:HE2	1:B:2305:HIS:CE1	2.31	0.64
2:A:1600:NAG:H61	8:A:207:HOH:O	1.96	0.64
1:B:2393:GLU:HG3	8:B:656:HOH:O	1.97	0.64
1:B:2161:ASN:O	1:B:2165:VAL:HG13	1.97	0.64
1:B:2135:TYR:CE2	1:B:2156:LEU:HB2	2.33	0.63
1:B:2164:ASP:HA	1:B:2167:LYS:HE2	1.81	0.63
1:B:2139:GLN:HA	8:B:605:HOH:O	2.00	0.62
1:A:1117:THR:HG22	8:A:152:HOH:O	1.98	0.62
1:A:1139:GLN:HG2	8:A:663:HOH:O	1.99	0.61
1:B:2149:GLN:HG3	1:B:2153:ASP:OD2	2.01	0.61
1:B:2113:LYS:HD2	1:B:2114:THR:N	2.16	0.60
1:A:1036:SER:N	8:A:658:HOH:O	2.34	0.60
1:B:2311:ASP:OD2	3:B:2701:NDG:H8C2	2.02	0.60
1:B:2162:LEU:O	1:B:2165:VAL:HG22	2.01	0.60
3:A:1701:NDG:H6C2	8:A:453:HOH:O	2.02	0.60
1:B:2105:HIS:O	1:B:2109:ILE:HG13	2.01	0.59
1:B:2307:LYS:HE2	1:B:2381:PRO:HG2	1.85	0.59
1:B:2063:ASP:HB2	1:B:2074:ASP:HA	1.83	0.59
1:A:1110:ASP:OD1	1:A:1113:LYS:NZ	2.25	0.59
1:A:1139:GLN:HA	1:A:1139:GLN:NE2	2.18	0.58
1:B:2490:GLN:H	1:B:2495:ASN:HD21	1.51	0.58
1:A:1161:ASN:O	1:A:1165:VAL:HG12	2.04	0.58
1:B:2356:GLU:HG3	8:B:336:HOH:O	2.03	0.58
1:B:2321:ARG:HB2	8:B:574:HOH:O	2.02	0.58
1:B:2309:ARG:HG3	1:B:2396:GLY:CA	2.33	0.57
1:B:2103:LEU:HB3	1:B:2151:LEU:HB3	1.87	0.57
1:A:1185:SER:O	1:A:1186:HIS:HB2	2.05	0.56
1:B:2114:THR:HA	8:B:332:HOH:O	2.05	0.56
1:B:2289:ASP:O	1:B:2293:LEU:HD13	2.05	0.56
1:B:2106:VAL:HA	1:B:2109:ILE:HD12	1.87	0.56
1:B:2252:ASP:HB3	1:B:2254:GLN:HG2	1.88	0.56
1:B:2394:LYS:HZ2	1:B:2394:LYS:HB2	1.71	0.55
1:B:2496:THR:O	1:B:2508:VAL:HG22	2.07	0.55
1:B:2283:ARG:NH2	1:B:2510:ARG:HH12	2.05	0.54
4:A:1900[A]:LDY:C5	8:A:231[A]:HOH:O	2.56	0.54
1:A:1160:ARG:NH2	1:A:1213:THR:HB	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2164:ASP:O	1:B:2167:LYS:HE2	2.08	0.54
1:B:2138:LEU:O	1:B:2143:LYS:HA	2.08	0.53
1:A:1369:LEU:O	1:A:1369:LEU:HD12	2.08	0.53
1:B:2164:ASP:HA	1:B:2167:LYS:CE	2.39	0.53
1:B:2316:SER:HB3	1:B:2324:ASP:O	2.09	0.53
1:B:2045:LYS:HA	1:B:2093:MET:HE2	1.91	0.53
1:B:2045:LYS:HA	1:B:2093:MET:CE	2.39	0.53
1:B:2180:ASN:HB2	1:B:2189:ASP:HB2	1.91	0.53
1:A:1286:THR:HB	8:A:94:HOH:O	2.08	0.52
1:B:2405:VAL:HG22	1:B:2405:VAL:O	2.10	0.52
1:B:2312:LEU:HA	8:B:89:HOH:O	2.08	0.52
1:A:1299:ILE:O	1:A:1303:LYS:HE2	2.10	0.52
1:B:2214:GLY:O	1:B:2216:GLU:N	2.42	0.52
1:B:2148:ASN:HA	8:B:515:HOH:O	2.09	0.52
1:A:1286:THR:HG21	8:A:477:HOH:O	2.10	0.52
1:B:2348:GLN:HE21	1:B:2352:ASP:CG	2.12	0.52
1:B:2106:VAL:HA	1:B:2109:ILE:CD1	2.40	0.51
1:A:1394:LYS:HD3	8:A:615:HOH:O	2.10	0.51
1:B:2105:HIS:CD2	1:B:2109:ILE:HD11	2.45	0.51
1:B:2309:ARG:NH1	3:B:2701:NDG:H8C3	2.26	0.51
1:B:2041:ALA:O	1:B:2045:LYS:HG3	2.11	0.51
1:B:2348:GLN:NE2	1:B:2352:ASP:OD1	2.44	0.51
1:B:2249:ASN:HD21	1:B:2256:ALA:HB2	1.76	0.51
1:B:2249:ASN:ND2	1:B:2256:ALA:HB2	2.26	0.51
1:A:1259:ARG:HH11	1:A:1259:ARG:HG2	1.76	0.51
1:B:2273:LEU:HB3	1:B:2291:TRP:HB2	1.93	0.50
1:B:2118:VAL:O	1:B:2180:ASN:HA	2.10	0.50
1:B:2248:ILE:HD12	1:B:2248:ILE:N	2.26	0.50
1:B:2390:GLU:HB3	8:B:126:HOH:O	2.12	0.50
1:B:2038:GLN:O	1:B:2042:ASP:OD2	2.29	0.50
1:A:1427:ARG:HD3	1:A:1480:ALA:O	2.11	0.49
1:B:2405:VAL:HG13	1:B:2407[A]:ARG:HG3	1.93	0.49
1:B:2095:LYS:O	1:B:2099:VAL:HG23	2.12	0.49
1:A:1325:LEU:HD22	1:A:1325:LEU:N	2.26	0.49
1:A:1160:ARG:HD2	8:A:316:HOH:O	2.11	0.49
1:B:2036:SER:O	1:B:2039:ALA:N	2.45	0.49
1:A:1452:ASP:OD2	1:A:1455:LYS:HD2	2.13	0.49
1:B:2077:ASN:ND2	1:B:2118:VAL:HG12	2.28	0.48
1:B:2233:GLN:HB2	1:B:2254:GLN:HE22	1.78	0.48
1:B:2160:ARG:NH2	8:B:713:HOH:O	2.47	0.48
1:B:2312:LEU:CD2	3:B:2701:NDG:H8C1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2237:SER:C	1:B:2239:PRO:HD3	2.34	0.48
3:B:2704:MAN:H3	8:B:375:HOH:O	2.14	0.48
1:B:2364:THR:HG21	1:B:2377:TRP:CE2	2.49	0.48
1:A:1370:THR:O	1:A:1371:LYS:HB2	2.13	0.48
1:B:2210:SER:OG	1:B:2219:ALA:N	2.43	0.48
1:B:2160:ARG:HG3	1:B:2218:TYR:OH	2.14	0.48
1:B:2349:ASP:OD1	1:B:2349:ASP:N	2.47	0.48
1:B:2407[B]:ARG:HD2	8:B:383[B]:HOH:O	2.13	0.47
1:A:1273:LEU:HB3	1:A:1291:TRP:HB2	1.95	0.47
1:B:2282:LYS:HG2	1:B:2283:ARG:N	2.28	0.47
1:B:2360:GLY:O	1:B:2363:ALA:HB3	2.14	0.47
1:A:1105:HIS:HD2	8:A:55:HOH:O	1.97	0.47
1:B:2110:ASP:OD2	1:B:2112:SER:OG	2.31	0.47
1:B:2325:LEU:HD12	1:B:2325:LEU:N	2.29	0.47
1:B:2087:LEU:O	1:B:2091:VAL:HG23	2.14	0.47
1:A:1510:ARG:NH1	1:A:1510:ARG:HB3	2.29	0.47
1:B:2301:HIS:O	1:B:2323:TYR:HE2	1.97	0.46
1:B:2185:SER:C	1:B:2187:GLY:N	2.67	0.46
1:B:2045:LYS:HG2	1:B:2093:MET:HE2	1.96	0.46
1:A:1318:TYR:CE1	1:A:1321:ARG:HA	2.50	0.46
1:A:1415:TYR:HE1	1:A:1489:VAL:HG23	1.79	0.46
1:B:2148:ASN:CG	1:B:2151:LEU:HG	2.36	0.46
1:B:2312:LEU:HD23	3:B:2701:NDG:H8C1	1.97	0.46
5:B:2801:NDG:O7	5:B:2801:NDG:H3	2.15	0.46
1:B:2369:LEU:HD23	1:B:2369:LEU:C	2.36	0.46
1:B:2181:ILE:HD13	1:B:2181:ILE:N	2.30	0.46
1:B:2243:LEU:HB3	1:B:2260:VAL:HG21	1.97	0.46
1:B:2330:LEU:CD2	1:B:2407[B]:ARG:HH21	2.26	0.45
1:B:2238:GLU:HG3	1:B:2240:PHE:O	2.16	0.45
1:A:1168:PHE:CZ	1:A:1181:ILE:HD12	2.51	0.45
1:A:1407[A]:ARG:NH2	8:A:449:HOH:O	2.48	0.45
1:B:2490:GLN:H	1:B:2495:ASN:ND2	2.14	0.45
1:B:2176:VAL:O	1:B:2250:ILE:HG23	2.17	0.45
1:B:2164:ASP:CA	1:B:2167:LYS:HE2	2.45	0.45
1:B:2036:SER:O	1:B:2039:ALA:HB3	2.16	0.45
1:B:2045:LYS:HB3	1:B:2045:LYS:NZ	2.32	0.45
1:B:2257:ASP:OD2	1:B:2259:ARG:HB3	2.17	0.44
1:A:1394:LYS:HG3	1:A:1395:ALA:N	2.33	0.44
1:B:2064:GLU:HB2	8:B:183:HOH:O	2.17	0.44
1:B:2432:ASN:OD1	8:B:704:HOH:O	2.21	0.44
1:B:2110:ASP:C	1:B:2112:SER:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2416:TYR:CE2	1:B:2489:VAL:HG11	2.52	0.44
1:B:2394:LYS:HG3	1:B:2395:ALA:N	2.33	0.43
1:A:1325:LEU:H	1:A:1325:LEU:HD22	1.84	0.43
1:B:2250:ILE:O	1:B:2250:ILE:HG22	2.17	0.43
1:B:2322:ASN:HB2	8:B:280:HOH:O	2.18	0.43
1:B:2299:ILE:HG12	1:B:2353:PHE:CD2	2.53	0.43
1:A:1139:GLN:O	1:A:1143:LYS:HD3	2.18	0.43
1:B:2106:VAL:O	1:B:2158:GLN:NE2	2.52	0.43
1:B:2138:LEU:HD13	1:B:2152:ILE:HG12	2.01	0.43
1:A:1045:LYS:HE3	1:A:1478:TYR:CE1	2.54	0.43
1:B:2224:LYS:NZ	1:B:2228:TYR:CE2	2.86	0.43
1:A:1108:ASP:HB2	8:A:334:HOH:O	2.19	0.43
1:B:2321:ARG:N	1:B:2321:ARG:HD2	2.34	0.42
1:B:2077:ASN:HB3	1:B:2114:THR:OG1	2.19	0.42
1:B:2243:LEU:HD22	1:B:2297:SER:CB	2.49	0.42
1:B:2185:SER:HB3	2:B:2600:NAG:H61	2.01	0.42
1:B:2109:ILE:HG22	1:B:2110:ASP:N	2.33	0.42
1:B:2167:LYS:C	1:B:2169:ALA:N	2.73	0.42
1:B:2295:ALA:O	1:B:2299:ILE:HG13	2.20	0.42
1:B:2423:LYS:HE2	8:B:379:HOH:O	2.19	0.42
1:B:2427:ARG:CD	1:B:2480:ALA:O	2.62	0.42
1:B:2237:SER:OG	1:B:2255:PHE:HB2	2.20	0.42
1:A:1248:ILE:HD12	1:A:1248:ILE:N	2.36	0.41
1:A:1063:ASP:HB2	1:A:1074:ASP:HA	2.02	0.41
1:B:2163:ALA:HB1	1:B:2206:TRP:CZ3	2.55	0.41
1:B:2259:ARG:HG3	1:B:2259:ARG:HH11	1.86	0.41
1:B:2104:GLU:O	1:B:2107:ALA:HB3	2.20	0.41
1:A:1320:ASN:HB3	1:A:1321:ARG:HH12	1.85	0.41
1:B:2081:ALA:O	1:B:2085:ASP:HB2	2.20	0.41
1:B:2215:ASP:O	1:B:2217:GLU:N	2.54	0.41
1:B:2216:GLU:HB3	8:B:689:HOH:O	2.19	0.41
1:A:1415:TYR:CE1	1:A:1489:VAL:HG23	2.56	0.40
1:B:2383:LYS:O	1:B:2385:PRO:HD3	2.21	0.40
1:B:2311:ASP:OD2	3:B:2701:NDG:C8	2.68	0.40
1:A:1259:ARG:NH1	1:A:1259:ARG:HG2	2.35	0.40
1:B:2115:SER:O	2:B:2600:NAG:H81	2.22	0.40
1:B:2120:LEU:HD12	1:B:2166:LEU:HD13	2.02	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	475/475 (100%)	457 (96%)	15 (3%)	3 (1%)	30	16
1	B	474/475 (100%)	429 (90%)	39 (8%)	6 (1%)	15	4
All	All	949/950 (100%)	886 (93%)	54 (6%)	9 (1%)	19	9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2215	ASP
1	A	1267	ASP
1	B	2148	ASN
1	B	2267	ASP
1	B	2216	GLU
1	B	2111	PHE
1	B	2173	PRO
1	A	1186	HIS
1	A	1148	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/400 (100%)	392 (98%)	10 (2%)	55	45
1	B	401/400 (100%)	384 (96%)	17 (4%)	36	21
All	All	803/800 (100%)	776 (97%)	27 (3%)	44	30

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1085	ASP
1	A	1117	THR
1	A	1139	GLN
1	A	1165	VAL
1	A	1273	LEU
1	A	1286	THR
1	A	1408	PRO
1	A	1483	GLU
1	A	1500	ASN
1	A	1507	SER
1	B	2038	GLN
1	B	2061	PRO
1	B	2085	ASP
1	B	2113	LYS
1	B	2117	THR
1	B	2118	VAL
1	B	2171	ASP
1	B	2181	ILE
1	B	2243	LEU
1	B	2322	ASN
1	B	2340	LEU
1	B	2389	LYS
1	B	2393	GLU
1	B	2394	LYS
1	B	2408	PRO
1	B	2500	ASN
1	B	2501	THR

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	1037	ASN
1	A	1105	HIS
1	A	1139	GLN
1	A	1144	ASN
1	A	1223	GLN
1	A	1322	ASN
1	A	1432	ASN
1	A	1490	GLN
1	A	1495	ASN
1	B	2223	GLN

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Mol	Chain	Res	Type
1	B	2249	ASN
1	B	2348	GLN
1	B	2432	ASN
1	B	2490	GLN
1	B	2495	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

22 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	$\# Z  > 2$
2	NAG	A	1600	1,2	14,14,15	0.58	0	15,19,21	0.85	0
2	NAG	A	1601	2	14,14,15	0.58	0	15,19,21	0.80	1 (6%)
3	NAG	A	1700	1,3	14,14,15	1.15	1 (7%)	15,19,21	0.90	1 (6%)
3	NDG	A	1701	3	14,14,15	1.05	1 (7%)	15,19,21	1.01	1 (6%)
3	MAN	A	1702	3	11,11,12	0.46	0	14,15,17	0.56	0
3	MAN	A	1703	3	11,11,12	0.44	0	14,15,17	0.71	0
3	MAN	A	1704	3	11,11,12	0.57	0	14,15,17	0.65	0
2	NAG	A	1800	1,2	14,14,15	0.83	1 (7%)	15,19,21	0.81	0
2	NAG	A	1801	2	14,14,15	0.71	1 (7%)	15,19,21	0.77	0
4	LDY	A	1900[A]	4,6	9,9,10	0.99	0	12,12,14	1.34	1 (8%)
4	MMA	A	1901[A]	4	13,13,13	0.66	0	18,18,18	0.86	1 (5%)
2	NAG	B	2600	1,2	14,14,15	0.65	0	15,19,21	0.70	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	2601	2	14,14,15	0.65	0	15,19,21	0.78	1 (6%)
3	NAG	B	2700	1,3	14,14,15	0.78	0	15,19,21	0.73	0
3	NDG	B	2701	3	14,14,15	0.78	0	15,19,21	1.13	2 (13%)
3	MAN	B	2702	3	11,11,12	0.49	0	14,15,17	0.52	0
3	MAN	B	2703	3	11,11,12	0.47	0	14,15,17	0.64	1 (7%)
3	MAN	B	2704	3	11,11,12	0.42	0	14,15,17	0.71	1 (7%)
5	NAG	B	2800	1,5	14,14,15	0.96	1 (7%)	15,19,21	0.74	0
5	NDG	B	2801	5	14,14,15	0.76	0	15,19,21	0.92	1 (6%)
4	LDY	B	2900[A]	4,6	9,9,10	0.95	0	12,12,14	0.89	1 (8%)
4	MMA	B	2901[A]	4	13,13,13	0.63	0	18,18,18	0.74	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
2	NAG	A	1600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1601	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1700	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	1701	3	-	0/6/23/26	0/1/1/1
3	MAN	A	1702	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	1703	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1704	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1801	2	-	0/6/23/26	0/1/1/1
4	LDY	A	1900[A]	4,6	-	0/0/14/17	0/1/1/1
4	MMA	A	1901[A]	4	-	0/4/24/24	0/1/1/1
2	NAG	B	2600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2601	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2700	1,3	-	0/6/23/26	0/1/1/1
3	NDG	B	2701	3	-	0/6/23/26	0/1/1/1
3	MAN	B	2702	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	B	2703	3	-	0/2/19/22	0/1/1/1
3	MAN	B	2704	3	-	0/2/19/22	0/1/1/1
5	NAG	B	2800	1,5	-	0/6/23/26	0/1/1/1
5	NDG	B	2801	5	-	0/6/23/26	0/1/1/1
4	LDY	B	2900[A]	4,6	-	0/0/14/17	0/1/1/1
4	MMA	B	2901[A]	4	-	0/4/24/24	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1801	NAG	C1-C2	2.04	1.55	1.52
2	A	1800	NAG	C1-C2	2.27	1.55	1.52
5	B	2800	NAG	C1-C2	2.33	1.55	1.52
3	A	1701	NDG	C1-C2	2.73	1.56	1.52
3	A	1700	NAG	C1-C2	2.78	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2701	NDG	C2-N2-C7	-2.89	119.33	123.04
3	A	1701	NDG	C2-N2-C7	-2.72	119.54	123.04
5	B	2801	NDG	C2-N2-C7	-2.60	119.70	123.04
3	B	2701	NDG	C4-C3-C2	-2.50	107.34	111.23
2	B	2600	NAG	C2-N2-C7	-2.31	120.07	123.04
2	B	2601	NAG	C2-N2-C7	-2.23	120.17	123.04
2	A	1601	NAG	C2-N2-C7	-2.10	120.34	123.04
3	A	1700	NAG	C2-N2-C7	-2.01	120.45	123.04
3	B	2703	MAN	C1-O5-C5	2.05	114.85	112.25
4	A	1901[A]	MMA	C7-O1-C1	2.18	116.86	113.29
3	B	2704	MAN	C1-O5-C5	2.34	115.22	112.25
4	B	2900[A]	LDY	C1-C2-C3	2.57	112.58	109.54
4	A	1900[A]	LDY	C1-C2-C3	4.03	114.31	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	2702	MAN	C1
3	A	1702	MAN	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1600	NAG	1	0
3	A	1701	NDG	1	0
4	A	1900[A]	LDY	1	0
2	B	2600	NAG	2	0
3	B	2701	NDG	5	0
3	B	2704	MAN	1	0
5	B	2801	NDG	1	0

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
7	GOL	A	1902[B]	-	5,5,5	0.27	0	5,5,5	0.37	0
7	GOL	A	1903[B]	6	5,5,5	0.27	0	5,5,5	0.36	0
7	GOL	B	2902[B]	-	5,5,5	0.25	0	5,5,5	0.34	0
7	GOL	B	2903[B]	6	5,5,5	0.31	0	5,5,5	0.33	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
7	GOL	A	1902[B]	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1903[B]	6	-	0/4/4/4	0/0/0/0
7	GOL	B	2902[B]	-	-	0/4/4/4	0/0/0/0
7	GOL	B	2903[B]	6	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	475/475 (100%)	-0.01	3 (0%) 90 94	5, 15, 32, 46	0
1	B	475/475 (100%)	0.95	87 (18%) 2 2	10, 37, 62, 74	0
All	All	950/950 (100%)	0.47	90 (9%) 10 17	5, 23, 58, 74	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2323	TYR	6.6
1	B	2255	PHE	5.2
1	B	2149	GLN	5.1
1	B	2113	LYS	4.7
1	B	2381	PRO	4.7
1	B	2147	ASP	4.3
1	B	2321	ARG	4.1
1	B	2302	LEU	4.1
1	B	2510	ARG	4.0
1	B	2146	VAL	3.9
1	B	2256	ALA	3.9
1	B	2235	SER	3.9
1	B	2379	TRP	3.8
1	B	2151	LEU	3.7
1	B	2148	ASN	3.6
1	B	2233	GLN	3.6
1	B	2239	PRO	3.6
1	B	2252	ASP	3.5
1	B	2301	HIS	3.4
1	B	2178	TYR	3.4
1	B	2310	PRO	3.4
1	B	2206	TRP	3.4
1	B	2190	GLY	3.4
1	B	2156	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	2114	THR	3.3
1	B	2106	VAL	3.3
1	B	2118	VAL	3.3
1	B	2109	ILE	3.3
1	B	2236	SER	3.2
1	B	2384	VAL	3.2
1	B	2039	ALA	3.2
1	B	2319	SER	3.2
1	B	2391	PHE	3.2
1	B	2237	SER	3.2
1	B	2254	GLN	3.1
1	B	2143	LYS	3.1
1	B	2249	ASN	2.9
1	B	2232	PRO	2.9
1	B	2060	PHE	2.8
1	B	2155	LEU	2.8
1	B	2108	ASP	2.8
1	B	2170	PHE	2.8
1	B	2144	ASN	2.7
1	B	2135	TYR	2.7
1	B	2248	ILE	2.7
1	B	2145	LEU	2.7
1	B	2392	TYR	2.7
1	B	2152	ILE	2.6
1	B	2293	LEU	2.6
1	B	2251	ASN	2.6
1	B	2174	SER	2.6
1	B	2314	PHE	2.6
1	B	2385	PRO	2.6
1	A	1321	ARG	2.6
1	B	2150	ASP	2.6
1	B	2241	PRO	2.5
1	B	2228	TYR	2.5
1	B	2318	TYR	2.5
1	B	2142	ALA	2.5
1	B	2111	PHE	2.5
1	B	2176	VAL	2.5
1	B	2425	ILE	2.5
1	B	2386	SER	2.4
1	B	2259	ARG	2.4
1	B	2240	PHE	2.4
1	B	2245	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2112	SER	2.4
1	B	2229	LEU	2.3
1	B	2100	ASN	2.3
1	B	2322	ASN	2.3
1	B	2165	VAL	2.3
1	B	2260	VAL	2.3
1	B	2213	THR	2.3
1	B	2231	LYS	2.3
1	A	1036	SER	2.2
1	B	2166	LEU	2.2
1	B	2325	LEU	2.2
1	B	2173	PRO	2.1
1	B	2395	ALA	2.1
1	B	2320	ASN	2.1
1	B	2191	ALA	2.1
1	B	2164	ASP	2.1
1	B	2388	GLN	2.1
1	B	2378	GLY	2.1
1	B	2304	SER	2.1
1	B	2399	ILE	2.0
1	B	2209	LEU	2.0
1	B	2282	LYS	2.0
1	B	2377	TRP	2.0
1	A	1508	VAL	2.0

## 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1700	14/15	0.91	0.12	5.98	18,20,28,29	0
3	MAN	A	1704	11/12	0.84	0.14	4.13	25,29,31,33	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	2600	14/15	0.45	0.33	3.40	60,62,65,68	0
2	NAG	A	1800	14/15	0.95	0.11	3.10	15,18,21,25	0
3	NDG	A	1701	14/15	0.91	0.13	2.19	21,25,30,30	0
3	NAG	B	2700	14/15	0.73	0.22	1.37	47,49,53,54	0
3	NDG	B	2701	14/15	0.70	0.21	1.02	53,54,56,56	0
4	MMA	B	2901[A]	13/13	0.87	0.14	0.79	24,26,29,29	13
4	LDY	B	2900[A]	9/10	0.94	0.12	0.67	15,18,20,22	9
2	NAG	A	1600	14/15	0.90	0.14	0.56	26,29,32,35	0
3	MAN	B	2704	11/12	0.76	0.17	0.30	52,54,54,56	10
5	NAG	B	2800	14/15	0.86	0.12	0.09	30,35,40,44	0
4	MMA	A	1901[A]	13/13	0.92	0.14	0.07	13,15,19,20	13
4	LDY	A	1900[A]	9/10	0.98	0.14	-0.39	4,10,13,16	9
2	NAG	A	1801	14/15	0.91	0.18	-	31,35,39,40	0
3	MAN	B	2703	11/12	0.72	0.23	-	58,59,60,60	11
2	NAG	A	1601	14/15	0.86	0.24	-	41,45,47,48	0
3	MAN	B	2702	11/12	0.69	0.25	-	54,55,58,59	11
3	MAN	A	1702	11/12	0.93	0.10	-	25,29,33,38	11
3	MAN	A	1703	11/12	0.77	0.19	-	42,46,48,48	11
2	NAG	B	2601	14/15	0.65	0.27	-	70,71,72,73	0
5	NDG	B	2801	14/15	0.80	0.22	-	48,50,54,55	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CA	B	2551	1/1	0.99	0.10	0.22	15,15,15,15	0
7	GOL	B	2903[B]	6/6	0.96	0.10	-0.26	11,11,12,12	6
7	GOL	A	1903[B]	6/6	0.98	0.14	-0.26	6,7,7,7	6
7	GOL	A	1902[B]	6/6	0.95	0.12	-0.55	25,26,27,27	6
7	GOL	B	2902[B]	6/6	0.93	0.10	-1.27	34,35,35,35	6
6	CA	A	1550	1/1	1.00	0.11	-2.01	8,8,8,8	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.