



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2018 – 06:31 AM EST

PDB ID : 2RI8
Title : Penicillium citrinum alpha-1,2-mannosidase complex with glycerol
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 : 2.16 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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

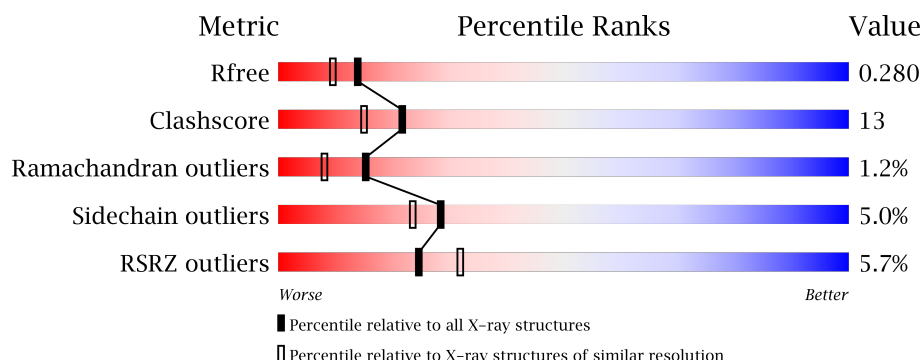
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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 ≥ 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>2%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	B	475	<div> <div>10%</div> <div>65%</div> <div>31%</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
2	NAG	B	2800	-	-	-	X
3	MAN	A	1702	X	-	-	-
3	MAN	A	1704	-	-	-	X
3	MAN	B	2702	X	-	-	-
5	GOL	A	1900	-	-	-	X
5	GOL	A	1903	-	-	-	X
5	GOL	B	2903	-	-	-	X

2 Entry composition [i](#)

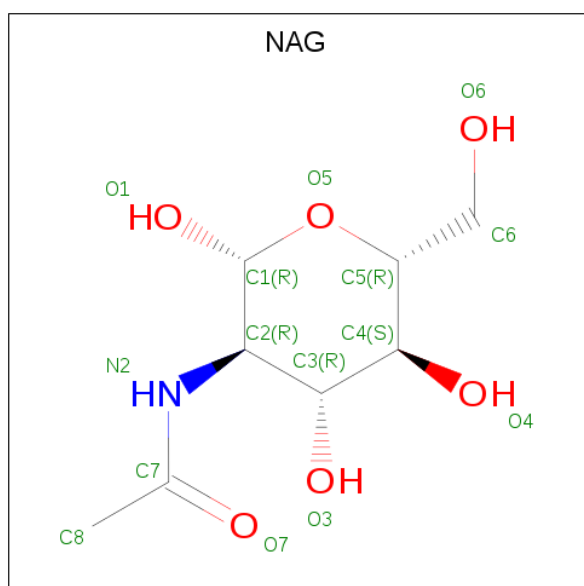
There are 6 unique types of molecules in this entry. The entry contains 8443 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			3748	2371	627	742	8			
1	B	475	Total	C	N	O	S	0	0	0
			3725	2359	619	739	8			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



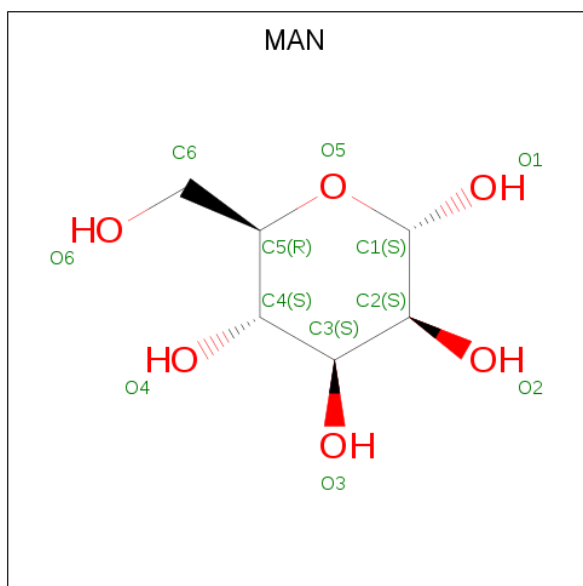
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		

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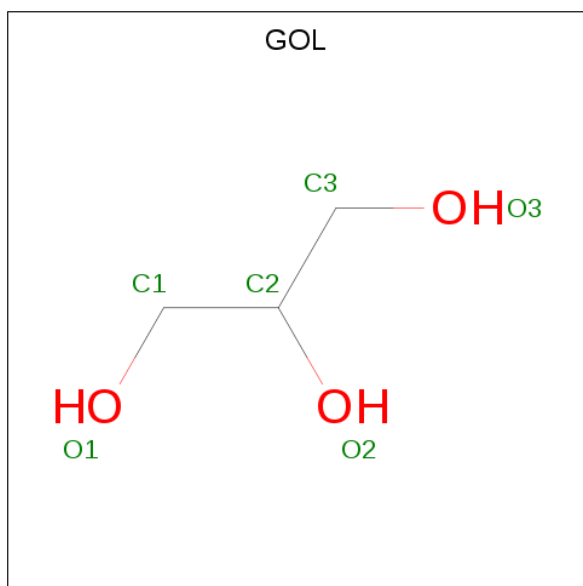
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

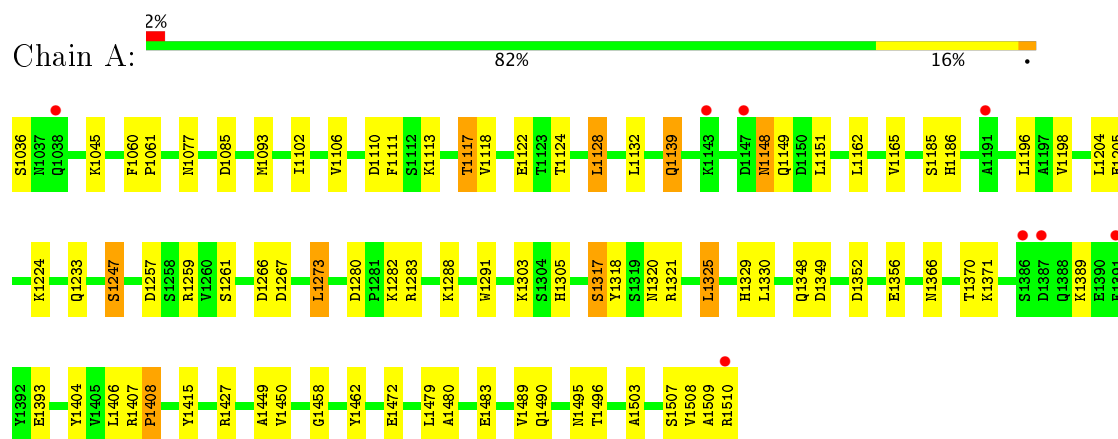
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	449	Total	O	0	0
			449	449		
6	B	243	Total	O	0	0
			243	243		

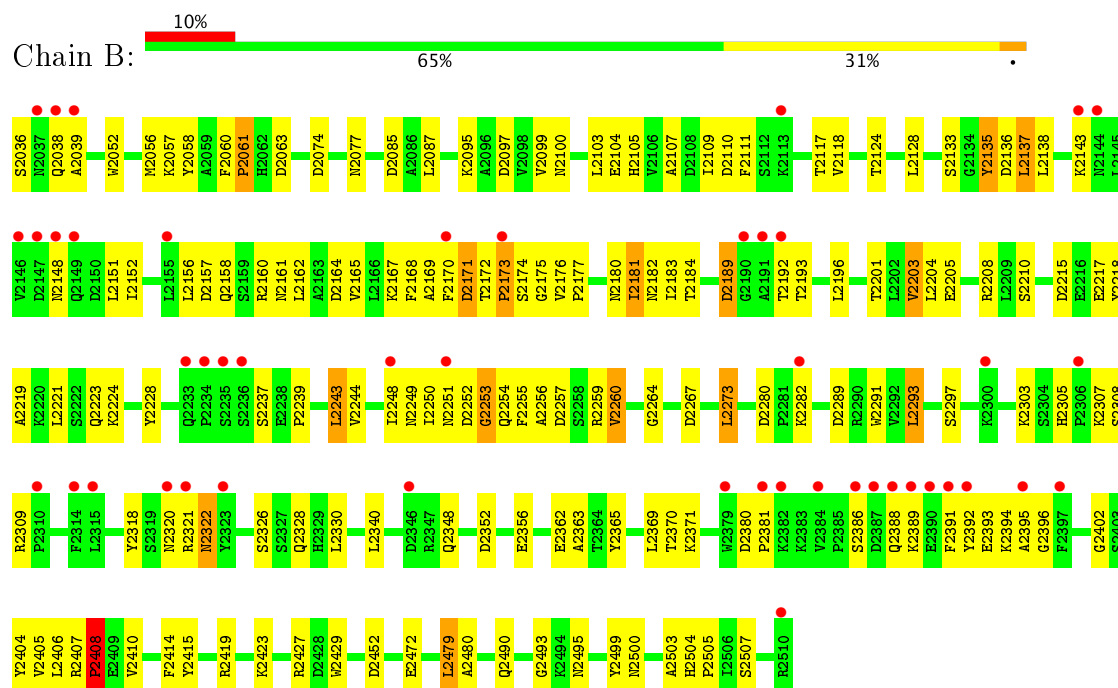
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 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, α , β , γ	56.49 Å 111.00 Å 86.23 Å 90.00° 99.17° 90.00°	Depositor
Resolution (Å)	20.32 – 2.16 20.32 – 2.18	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.32-2.16) 96.8 (20.32-2.18)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.20 (at 2.17 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.274 0.217 , 0.280	Depositor DCC
R_{free} test set	3754 reflections (7.10%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8443	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 39.54 % 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 3.1269e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GOL, CA, NAG, 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	0.52	0/3842	0.69	0/5215
1	B	0.43	0/3820	0.66	1/5190 (0.0%)
All	All	0.48	0/7662	0.68	1/10405 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2253	GLY	N-CA-C	-5.15	100.24	113.10

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	3748	0	3548	65	0
1	B	3725	0	3523	134	0
2	A	84	0	74	0	0
2	B	84	0	74	5	0
3	A	33	0	28	0	0
3	B	33	0	28	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	24	0	30	6	0
5	B	18	0	23	1	0
6	A	449	0	0	12	0
6	B	243	0	0	15	0
All	All	8443	0	7328	202	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 13.

All (202) 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:2264:GLY:H	1:B:2328:GLN:HE22	1.10	0.97
1:B:2158:GLN:HA	1:B:2161:ASN:HD22	1.32	0.94
1:B:2423:LYS:HE2	1:B:2423:LYS:HA	1.49	0.93
1:A:1349:ASP:HB3	5:A:1904:GOL:H11	1.50	0.90
1:B:2307:LYS:HE2	1:B:2381:PRO:HG2	1.58	0.85
1:B:2289:ASP:O	1:B:2293:LEU:HD13	1.77	0.84
1:A:1490:GLN:H	1:A:1495:ASN:HD21	1.29	0.81
1:B:2499:TYR:CE2	1:B:2505:PRO:HG3	2.16	0.80
1:A:1117:THR:HG22	6:A:156:HOH:O	1.84	0.76
1:A:1320:ASN:HB3	1:A:1321:ARG:HH12	1.51	0.75
1:A:1389:LYS:O	1:A:1393:GLU:HG2	1.87	0.75
1:B:2158:GLN:HA	1:B:2161:ASN:ND2	2.01	0.75
1:B:2162:LEU:O	1:B:2165:VAL:HG22	1.86	0.74
1:A:1122:GLU:OE2	5:A:1903:GOL:H11	1.87	0.74
1:B:2330:LEU:HD21	1:B:2407:ARG:NH2	2.02	0.74
1:B:2264:GLY:H	1:B:2328:GLN:NE2	1.86	0.74
1:B:2174:SER:HB3	1:B:2252:ASP:O	1.89	0.72
1:A:1259:ARG:HD3	1:B:2386:SER:OG	1.90	0.72
1:B:2252:ASP:HB3	1:B:2254:GLN:HG2	1.72	0.71
1:B:2260:VAL:HG13	1:B:2318:TYR:HB3	1.72	0.71
1:B:2303:LYS:HE2	1:B:2305:HIS:CE1	2.26	0.71
1:B:2063:ASP:HB2	1:B:2074:ASP:HA	1.72	0.70
1:A:1282:LYS:HD2	1:A:1510[B]:ARG:NH1	2.06	0.70
1:B:2427:ARG:HD3	1:B:2480:ALA:O	1.92	0.69
1:B:2173:PRO:HG2	1:B:2251:ASN:OD1	1.92	0.69
1:B:2249:ASN:HD21	1:B:2256:ALA:HB2	1.58	0.69
1:B:2252:ASP:CB	1:B:2254:GLN:HG2	2.21	0.69
5:A:1904:GOL:H2	6:A:677:HOH:O	1.91	0.69
1:B:2307:LYS:HE2	1:B:2381:PRO:CG	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2135:TYR:CE2	1:B:2156:LEU:HB2	2.27	0.69
1:B:2109:ILE:HG22	1:B:2110:ASP:N	2.09	0.68
1:B:2405:VAL:HG23	1:B:2407:ARG:HG3	1.76	0.68
1:A:1450:VAL:HG22	1:A:1458:GLY:O	1.94	0.67
1:B:2490:GLN:H	1:B:2495:ASN:HD21	1.44	0.66
1:B:2161:ASN:O	1:B:2165:VAL:HG13	1.95	0.66
1:A:1490:GLN:H	1:A:1495:ASN:ND2	1.93	0.65
1:A:1273:LEU:HB3	1:A:1291:TRP:HB2	1.79	0.65
1:A:1280:ASP:OD1	1:A:1282:LYS:HB3	1.98	0.64
1:A:1510[A]:ARG:NH1	1:A:1510[A]:ARG:HB3	2.12	0.64
1:B:2273:LEU:HD23	1:B:2291:TRP:HA	1.80	0.62
1:A:1303:LYS:HE3	1:A:1305:HIS:CE1	2.35	0.62
1:B:2182:ASN:OD1	1:B:2184:THR:HB	1.99	0.62
1:B:2249:ASN:ND2	1:B:2256:ALA:HB2	2.13	0.62
1:B:2077:ASN:ND2	1:B:2118:VAL:HG12	2.14	0.62
5:A:1903:GOL:H31	6:A:383:HOH:O	2.00	0.61
1:B:2192:THR:O	1:B:2193:THR:HG23	2.01	0.61
1:A:1111:PHE:CD2	1:A:1162:LEU:HD13	2.36	0.60
2:B:2700:NAG:H61	2:B:2701:NAG:H82	1.84	0.60
1:B:2219:ALA:O	1:B:2223:GLN:HG3	2.02	0.60
1:B:2370:THR:O	1:B:2371:LYS:HB2	2.01	0.59
1:A:1510[A]:ARG:CZ	1:A:1510[A]:ARG:HB3	2.31	0.59
1:A:1320:ASN:HB3	1:A:1321:ARG:NH1	2.17	0.59
1:A:1036:SER:N	6:A:412:HOH:O	2.36	0.59
1:B:2124:THR:CG2	1:B:2205:GLU:HG3	2.32	0.59
1:A:1162:LEU:O	1:A:1165:VAL:HG12	2.03	0.59
1:B:2100:ASN:O	1:B:2104:GLU:HG2	2.02	0.59
1:B:2405:VAL:HG23	1:B:2407:ARG:CG	2.32	0.59
1:A:1139:GLN:HE22	1:A:1149:GLN:HE22	1.49	0.58
1:B:2176:VAL:O	1:B:2250:ILE:HG23	2.03	0.58
1:B:2309:ARG:NH1	2:B:2701:NAG:H81	2.18	0.58
1:B:2036:SER:O	1:B:2039:ALA:N	2.36	0.58
1:A:1045:LYS:HE2	1:A:1093:MET:O	2.04	0.57
1:A:1124:THR:CG2	1:A:1205:GLU:HG3	2.34	0.57
1:B:2180:ASN:HB2	1:B:2189:ASP:HB2	1.86	0.57
1:B:2164:ASP:HA	1:B:2167:LYS:HD3	1.86	0.57
1:B:2109:ILE:CG2	1:B:2110:ASP:N	2.69	0.56
1:B:2429:TRP:HE1	2:B:2700:NAG:C8	2.17	0.56
1:B:2111:PHE:CD2	1:B:2162:LEU:HD13	2.40	0.56
1:B:2352:ASP:O	1:B:2356:GLU:HG3	2.06	0.56
1:B:2104:GLU:O	1:B:2107:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2326:SER:HB2	6:B:691:HOH:O	2.06	0.56
1:A:1198:VAL:HG22	6:A:28:HOH:O	2.05	0.56
1:A:1282:LYS:HD2	1:A:1510[B]:ARG:HH12	1.70	0.56
1:A:1404:TYR:CE2	1:A:1406:LEU:HA	2.40	0.55
1:B:2210:SER:OG	1:B:2218:TYR:HB2	2.07	0.55
1:B:2135:TYR:HE2	1:B:2156:LEU:HB2	1.68	0.55
1:B:2203:VAL:HG22	6:B:85:HOH:O	2.07	0.55
1:B:2490:GLN:H	1:B:2495:ASN:ND2	2.04	0.54
1:B:2237:SER:C	1:B:2239:PRO:HD3	2.28	0.54
1:B:2308:SER:HB3	1:B:2392:TYR:CE2	2.43	0.54
1:A:1124:THR:HG22	1:A:1205:GLU:HG3	1.89	0.53
1:A:1349:ASP:HB3	5:A:1904:GOL:C1	2.32	0.53
1:B:2170:PHE:O	1:B:2172:THR:HG23	2.09	0.53
1:B:2264:GLY:N	1:B:2328:GLN:HE22	1.93	0.53
1:B:2237:SER:OG	1:B:2255:PHE:HB2	2.09	0.52
1:B:2182:ASN:C	1:B:2184:THR:H	2.11	0.52
1:B:2170:PHE:CD2	1:B:2177:PRO:HB3	2.45	0.52
1:A:1330:LEU:HD21	1:A:1407:ARG:NH1	2.24	0.52
1:B:2243:LEU:HD22	1:B:2297:SER:HB3	1.92	0.52
1:B:2160:ARG:HD2	6:B:700:HOH:O	2.10	0.52
1:B:2404:TYR:CE2	1:B:2406:LEU:HA	2.46	0.51
1:B:2254:GLN:NE2	6:B:684:HOH:O	2.43	0.51
1:B:2228:TYR:CD1	1:B:2253:GLY:HA3	2.45	0.51
1:B:2208:ARG:NH2	1:B:2507:SER:HB2	2.25	0.51
1:B:2389:LYS:NZ	1:B:2389:LYS:HB2	2.26	0.51
1:B:2168:PHE:O	6:B:284:HOH:O	2.18	0.51
1:B:2224:LYS:NZ	1:B:2228:TYR:OH	2.40	0.51
1:B:2077:ASN:HD21	1:B:2118:VAL:HG12	1.76	0.50
1:B:2105:HIS:O	1:B:2109:ILE:HG13	2.12	0.50
1:B:2250:ILE:O	1:B:2250:ILE:HG22	2.10	0.50
1:B:2499:TYR:CZ	1:B:2505:PRO:HG3	2.46	0.50
1:A:1162:LEU:O	1:A:1165:VAL:CG1	2.59	0.49
1:B:2280:ASP:OD2	1:B:2282:LYS:HB3	2.12	0.49
1:A:1348:GLN:NE2	1:A:1352:ASP:OD1	2.38	0.49
1:B:2217:GLU:O	1:B:2221:LEU:HG	2.12	0.49
1:B:2052:TRP:NE1	1:B:2056:MET:HE2	2.28	0.49
1:B:2060:PHE:CD1	1:B:2061:PRO:HA	2.47	0.49
1:B:2309:ARG:HG3	1:B:2396:GLY:HA3	1.95	0.49
1:A:1389:LYS:NZ	6:A:693:HOH:O	2.46	0.48
1:B:2394:LYS:HE2	6:B:582:HOH:O	2.12	0.48
1:B:2157:ASP:O	1:B:2161:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:SER:HB2	1:A:1257:ASP:OD1	2.13	0.48
1:A:1450:VAL:HG21	1:A:1458:GLY:HA3	1.95	0.48
1:A:1128:LEU:HD13	1:A:1205:GLU:HB2	1.96	0.48
1:B:2143:LYS:HD3	6:B:429:HOH:O	2.13	0.48
1:A:1449:ALA:HB3	1:A:1462:TYR:HB2	1.96	0.48
1:B:2095:LYS:O	1:B:2099:VAL:HG23	2.13	0.47
1:B:2124:THR:HG23	1:B:2205:GLU:HG3	1.96	0.47
1:A:1370:THR:O	1:A:1371:LYS:HB2	2.13	0.47
1:B:2388:GLN:HG2	1:B:2391:PHE:HB3	1.95	0.47
1:A:1128:LEU:HD22	1:A:1132:LEU:CD1	2.45	0.47
1:B:2201:THR:O	1:B:2201:THR:HG22	2.14	0.47
1:B:2429:TRP:HE1	2:B:2700:NAG:H81	1.80	0.47
1:B:2248:ILE:N	1:B:2248:ILE:HD12	2.30	0.47
1:B:2363:ALA:HB2	2:B:2700:NAG:H62	1.96	0.47
5:B:2903:GOL:H32	6:B:478:HOH:O	2.15	0.47
1:B:2133:SER:HB2	1:B:2504:HIS:HB3	1.97	0.46
1:B:2117:THR:HG22	1:B:2118:VAL:N	2.29	0.46
1:B:2493:GLY:HA2	6:B:83:HOH:O	2.15	0.46
1:B:2405:VAL:HG22	6:B:45:HOH:O	2.16	0.46
1:A:1077:ASN:ND2	1:A:1118:VAL:HG22	2.30	0.46
1:A:1510[A]:ARG:NH1	1:A:1510[A]:ARG:CB	2.78	0.46
1:B:2138:LEU:O	1:B:2143:LYS:HA	2.16	0.46
1:B:2257:ASP:OD2	1:B:2259:ARG:N	2.37	0.46
1:A:1404:TYR:CZ	1:A:1406:LEU:HA	2.50	0.46
1:B:2182:ASN:ND2	6:B:247:HOH:O	2.31	0.45
1:A:1320:ASN:O	1:A:1321:ARG:HB2	2.17	0.45
1:B:2103:LEU:HB3	1:B:2151:LEU:HB3	1.98	0.45
1:B:2252:ASP:HB2	1:B:2254:GLN:HG2	1.96	0.45
1:B:2251:ASN:HB2	6:B:398:HOH:O	2.16	0.45
1:B:2309:ARG:HG3	1:B:2396:GLY:CA	2.47	0.45
1:A:1283:ARG:NH1	6:A:252:HOH:O	2.46	0.45
1:B:2109:ILE:CG2	1:B:2110:ASP:H	2.29	0.45
1:A:1407:ARG:NH2	5:A:1903:GOL:O3	2.49	0.45
1:A:1185:SER:O	1:A:1186:HIS:HB2	2.17	0.45
1:A:1325:LEU:HD22	1:A:1325:LEU:H	1.80	0.45
1:B:2472:GLU:HG2	1:B:2503:ALA:HB3	1.99	0.45
1:B:2167:LYS:C	1:B:2169:ALA:N	2.68	0.45
1:B:2321:ARG:HD2	1:B:2321:ARG:N	2.32	0.45
1:A:1496:THR:O	1:A:1508:VAL:HG22	2.18	0.44
1:B:2322:ASN:HB2	6:B:302:HOH:O	2.17	0.44
1:B:2408:PRO:HG3	1:B:2472:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:ALA:O	1:A:1510[A]:ARG:C	2.54	0.44
1:A:1317:SER:HB2	6:A:46:HOH:O	2.17	0.44
1:B:2205:GLU:CD	1:B:2205:GLU:H	2.21	0.44
1:B:2273:LEU:HB3	1:B:2291:TRP:HB2	2.00	0.44
1:A:1102:ILE:O	1:A:1106:VAL:HG23	2.18	0.44
1:A:1329:HIS:HB3	6:A:182:HOH:O	2.18	0.44
1:A:1233:GLN:HG2	6:A:259:HOH:O	2.18	0.43
1:B:2138:LEU:HD13	1:B:2152:ILE:HG12	1.99	0.43
1:A:1366:ASN:HB2	6:A:596:HOH:O	2.18	0.43
1:B:2136:ASP:HB3	1:B:2507:SER:OG	2.19	0.43
1:A:1060:PHE:CD1	1:A:1061:PRO:HA	2.54	0.43
1:B:2192:THR:O	1:B:2193:THR:CG2	2.65	0.43
1:A:1205:GLU:CD	1:A:1205:GLU:H	2.21	0.43
1:A:1110:ASP:OD1	1:A:1113:LYS:HE3	2.19	0.43
1:B:2252:ASP:HB2	1:B:2254:GLN:H	1.83	0.43
1:B:2415:TYR:O	1:B:2419:ARG:HG2	2.17	0.43
1:B:2479:LEU:HD12	1:B:2479:LEU:HA	1.81	0.43
1:B:2057:LYS:HD3	1:B:2058:TYR:CE1	2.54	0.43
1:B:2423:LYS:HA	1:B:2423:LYS:CE	2.33	0.43
1:B:2224:LYS:NZ	1:B:2228:TYR:CE2	2.87	0.43
1:B:2133:SER:O	1:B:2137:LEU:HB2	2.18	0.42
1:B:2160:ARG:NH2	1:B:2215:ASP:HB2	2.34	0.42
1:B:2479:LEU:HD21	1:B:2499:TYR:OH	2.19	0.42
1:A:1124:THR:CG2	1:A:1205:GLU:CG	2.98	0.42
1:B:2380:ASP:HA	1:B:2381:PRO:HD3	1.90	0.42
1:B:2348:GLN:NE2	1:B:2352:ASP:OD1	2.52	0.42
1:A:1303:LYS:HE3	1:A:1305:HIS:HE1	1.83	0.42
1:B:2167:LYS:C	1:B:2169:ALA:H	2.22	0.42
1:B:2138:LEU:HB3	1:B:2152:ILE:HD13	2.02	0.42
1:A:1148:ASN:HB3	1:A:1151:LEU:HB2	2.02	0.42
1:A:1472:GLU:HG2	1:A:1503:ALA:HB3	2.01	0.42
1:B:2124:THR:HG22	1:B:2205:GLU:HG3	2.01	0.41
1:B:2168:PHE:CZ	1:B:2181:ILE:HG13	2.55	0.41
1:A:1415:TYR:HE1	1:A:1489:VAL:HG23	1.85	0.41
1:B:2109:ILE:HG22	1:B:2110:ASP:H	1.85	0.41
1:B:2362:GLU:HB2	1:B:2414:PHE:CZ	2.55	0.41
1:B:2369:LEU:O	1:B:2369:LEU:HD23	2.21	0.41
1:B:2394:LYS:HG3	1:B:2395:ALA:H	1.85	0.41
1:A:1427:ARG:HD3	1:A:1480:ALA:O	2.21	0.41
1:B:2388:GLN:NE2	6:B:147:HOH:O	2.53	0.41
1:A:1261:SER:HB2	1:A:1317:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2244:VAL:HB	1:B:2255:PHE:CE2	2.56	0.41
1:A:1128:LEU:HD22	1:A:1132:LEU:HD11	2.01	0.41
1:A:1224:LYS:HA	6:A:281:HOH:O	2.21	0.41
1:B:2175:GLY:CA	6:B:129:HOH:O	2.69	0.40
1:B:2365:TYR:CE1	1:B:2410:VAL:HG21	2.56	0.40
1:B:2402:GLY:O	1:B:2452:ASP:HA	2.21	0.40
1:A:1318:TYR:CE1	1:A:1321:ARG:HA	2.56	0.40
1:B:2168:PHE:C	1:B:2168:PHE:CD1	2.94	0.40
1:B:2105:HIS:CE1	1:B:2109:ILE:HD11	2.56	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	474/475 (100%)	449 (95%)	22 (5%)	3 (1%)	28	20
1	B	473/475 (100%)	428 (90%)	37 (8%)	8 (2%)	11	4
All	All	947/950 (100%)	877 (93%)	59 (6%)	11 (1%)	15	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1267	ASP
1	B	2171	ASP
1	B	2189	ASP
1	B	2267	ASP
1	B	2173	PRO
1	B	2183	ILE
1	A	1148	ASN
1	B	2320	ASN
1	B	2408	PRO

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Mol	Chain	Res	Type
1	A	1408	PRO
1	B	2148	ASN

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	402/400 (100%)	385 (96%)	17 (4%)	34	32
1	B	400/400 (100%)	377 (94%)	23 (6%)	23	18
All	All	802/800 (100%)	762 (95%)	40 (5%)	28	23

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1085	ASP
1	A	1117	THR
1	A	1128	LEU
1	A	1139	GLN
1	A	1196	LEU
1	A	1204	LEU
1	A	1247	SER
1	A	1266	ASP
1	A	1273	LEU
1	A	1288	LYS
1	A	1317	SER
1	A	1325	LEU
1	A	1356	GLU
1	A	1408	PRO
1	A	1479	LEU
1	A	1483	GLU
1	A	1507	SER
1	B	2038	GLN
1	B	2061	PRO
1	B	2085	ASP
1	B	2087	LEU

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Mol	Chain	Res	Type
1	B	2097	ASP
1	B	2128	LEU
1	B	2135	TYR
1	B	2137	LEU
1	B	2171	ASP
1	B	2181	ILE
1	B	2196	LEU
1	B	2203	VAL
1	B	2204	LEU
1	B	2243	LEU
1	B	2260	VAL
1	B	2273	LEU
1	B	2293	LEU
1	B	2322	ASN
1	B	2340	LEU
1	B	2393	GLU
1	B	2408	PRO
1	B	2479	LEU
1	B	2500	ASN

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	1037	ASN
1	A	1105	HIS
1	A	1139	GLN
1	A	1144	ASN
1	A	1223	GLN
1	A	1249	ASN
1	A	1301	HIS
1	A	1305	HIS
1	A	1322	ASN
1	A	1418	HIS
1	A	1432	ASN
1	A	1490	GLN
1	A	1495	ASN
1	B	2037	ASN
1	B	2105	HIS
1	B	2139	GLN
1	B	2161	ASN
1	B	2223	GLN
1	B	2249	ASN

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Mol	Chain	Res	Type
1	B	2301	HIS
1	B	2328	GLN
1	B	2388	GLN
1	B	2418	HIS
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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	$\# Z > 2$
2	NAG	A	1600	1,2	14,14,15	0.56	0	15,19,21	1.05	0
2	NAG	A	1601	2	14,14,15	0.62	0	15,19,21	0.80	0
2	NAG	A	1700	1,2	14,14,15	0.89	1 (7%)	15,19,21	0.83	0
2	NAG	A	1701	3,2	14,14,15	0.84	1 (7%)	15,19,21	0.62	0
3	MAN	A	1702	3,2	11,11,12	0.51	0	13,15,17	0.52	0
3	MAN	A	1703	3	11,11,12	0.50	0	13,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	A	1704	3	11,11,12	0.54	0	13,15,17	0.69	0
2	NAG	A	1800	1,2	14,14,15	0.63	0	15,19,21	0.73	0
2	NAG	A	1801	2	14,14,15	0.61	0	15,19,21	0.60	0
5	GOL	A	1900	-	5,5,5	0.34	0	5,5,5	0.36	0
5	GOL	A	1901	4	5,5,5	0.36	0	5,5,5	0.32	0
5	GOL	A	1903	-	5,5,5	0.21	0	5,5,5	0.33	0
5	GOL	A	1904	-	5,5,5	0.30	0	5,5,5	0.43	0
2	NAG	B	2600	1,2	14,14,15	0.62	0	15,19,21	0.84	0
2	NAG	B	2601	2	14,14,15	0.59	0	15,19,21	0.68	0
2	NAG	B	2700	1,2	14,14,15	0.73	0	15,19,21	0.98	0
2	NAG	B	2701	3,2	14,14,15	0.64	0	15,19,21	0.74	0
3	MAN	B	2702	3,2	11,11,12	0.56	0	13,15,17	0.50	0
3	MAN	B	2703	3	11,11,12	0.45	0	13,15,17	0.69	1 (7%)
3	MAN	B	2704	3	11,11,12	0.49	0	13,15,17	0.71	1 (7%)
2	NAG	B	2800	1,2	14,14,15	0.61	0	15,19,21	0.80	0
2	NAG	B	2801	2	14,14,15	0.52	0	15,19,21	0.73	0
5	GOL	B	2900	-	5,5,5	0.21	0	5,5,5	0.37	0
5	GOL	B	2901	4	5,5,5	0.36	0	5,5,5	0.33	0
5	GOL	B	2903	-	5,5,5	0.30	0	5,5,5	0.43	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
2	NAG	A	1700	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1701	3,2	-	0/6/23/26	0/1/1/1
3	MAN	A	1702	3,2	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
5	GOL	A	1900	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1901	4	-	0/4/4/4	0/0/0/0
5	GOL	A	1903	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1904	-	-	0/4/4/4	0/0/0/0
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
2	NAG	B	2700	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2701	3,2	-	0/6/23/26	0/1/1/1
3	MAN	B	2702	3,2	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
2	NAG	B	2800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2801	2	-	0/6/23/26	0/1/1/1
5	GOL	B	2900	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2901	4	-	0/4/4/4	0/0/0/0
5	GOL	B	2903	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1700	NAG	C1-C2	2.30	1.55	1.52
2	A	1701	NAG	C1-C2	2.65	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2703	MAN	C1-O5-C5	2.06	115.00	112.17
3	B	2704	MAN	C1-O5-C5	2.12	115.09	112.17

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 torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1903	GOL	3	0
5	A	1904	GOL	3	0
2	B	2700	NAG	4	0
2	B	2701	NAG	2	0
5	B	2903	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	475/475 (100%)	-0.15	8 (1%) 70 76	7, 18, 38, 57	0
1	B	475/475 (100%)	0.49	46 (9%) 8 12	13, 30, 63, 79	0
All	All	950/950 (100%)	0.17	54 (5%) 24 32	7, 23, 52, 79	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2147	ASP	4.0
1	B	2391	PHE	3.8
1	B	2384	VAL	3.7
1	B	2320	ASN	3.6
1	A	1387	ASP	3.4
1	B	2038	GLN	3.3
1	B	2382	LYS	3.3
1	B	2386	SER	3.2
1	B	2392	TYR	3.2
1	B	2381	PRO	3.2
1	B	2236	SER	3.1
1	B	2300	LYS	3.1
1	B	2395	ALA	3.1
1	B	2321	ARG	3.0
1	B	2235	SER	2.9
1	B	2233	GLN	2.9
1	A	1510[A]	ARG	2.9
1	B	2310	PRO	2.9
1	B	2387	ASP	2.8
1	B	2173	PRO	2.8
1	B	2113	LYS	2.7
1	B	2314	PHE	2.7
1	B	2039	ALA	2.7
1	B	2397	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1038	GLN	2.7
1	B	2191	ALA	2.6
1	B	2146	VAL	2.6
1	B	2251	ASN	2.5
1	B	2192	THR	2.5
1	B	2510	ARG	2.5
1	B	2148	ASN	2.4
1	B	2282	LYS	2.4
1	B	2144	ASN	2.4
1	B	2379	TRP	2.4
1	B	2234	PRO	2.3
1	A	1386	SER	2.3
1	B	2155	LEU	2.3
1	B	2143	LYS	2.3
1	B	2323	TYR	2.3
1	B	2389	LYS	2.3
1	B	2170	PHE	2.3
1	B	2390	GLU	2.2
1	B	2346	ASP	2.2
1	A	1391	PHE	2.2
1	B	2190	GLY	2.2
1	B	2149	GLN	2.2
1	B	2388	GLN	2.2
1	B	2037	ASN	2.2
1	A	1147	ASP	2.2
1	A	1143	LYS	2.1
1	A	1191	ALA	2.1
1	B	2306	PRO	2.1
1	B	2248	ILE	2.0
1	B	2315	LEU	2.0

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 ⓘ

There are no carbohydrates in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	B	2903	6/6	0.83	0.17	10.47	34,44,45,46	0
2	NAG	B	2600	14/15	0.69	0.33	8.68	56,58,62,65	0
5	GOL	A	1903	6/6	0.88	0.23	8.10	42,44,44,45	0
3	MAN	A	1704	11/12	0.85	0.17	7.30	29,30,31,31	10
2	NAG	B	2800	14/15	0.90	0.17	4.09	26,34,40,45	0
5	GOL	A	1900	6/6	0.93	0.15	3.60	21,29,30,32	0
2	NAG	A	1800	14/15	0.91	0.14	3.40	20,25,31,38	0
3	MAN	B	2704	11/12	0.87	0.22	1.56	41,43,45,45	10
5	GOL	B	2900	6/6	0.87	0.14	1.40	33,34,35,36	0
2	NAG	A	1600	14/15	0.86	0.17	1.33	28,31,36,42	0
2	NAG	A	1700	14/15	0.95	0.13	1.13	20,24,29,29	0
2	NAG	B	2701	14/15	0.85	0.18	0.74	39,42,43,44	0
2	NAG	A	1701	14/15	0.91	0.12	0.02	26,28,32,32	0
2	NAG	B	2700	14/15	0.93	0.14	-0.65	36,38,39,39	0
5	GOL	A	1901	6/6	0.98	0.06	-1.71	6,11,11,12	0
5	GOL	B	2901	6/6	0.97	0.07	-1.90	13,14,15,17	0
4	CA	B	1551	1/1	0.99	0.06	-2.44	14,14,14,14	0
4	CA	A	1550	1/1	1.00	0.04	-7.57	12,12,12,12	0
2	NAG	B	2601	14/15	0.72	0.34	-	68,69,70,70	0
2	NAG	A	1801	14/15	0.81	0.30	-	45,50,53,54	0
3	MAN	B	2703	11/12	0.83	0.27	-	47,49,50,52	11
5	GOL	A	1904	6/6	0.56	0.36	-	62,63,64,64	0
3	MAN	A	1702	11/12	0.90	0.13	-	30,32,37,41	11
2	NAG	B	2801	14/15	0.77	0.35	-	48,52,56,56	0
3	MAN	B	2702	11/12	0.88	0.19	-	40,43,45,45	11
3	MAN	A	1703	11/12	0.80	0.23	-	45,48,50,51	11
2	NAG	A	1601	14/15	0.82	0.29	-	48,51,55,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.