



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:02 am GMT

PDB ID : 1H4P  
Title : CRYSTAL STRUCTURE OF EXO-1,3-BETA GLUCANSE FROM SACCHAROMYCES CEREVISIAE  
Authors : Ferguson, A.D.  
Deposited on : 2001-05-11  
Resolution : 1.75 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

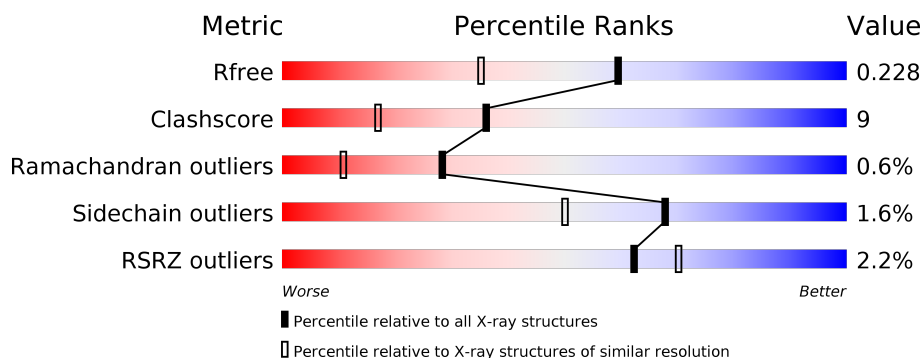
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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	408	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	408	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <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	GOL	A	1450	-	-	-	X
2	GOL	A	1451	-	-	-	X
2	GOL	A	1452	-	-	-	X
2	GOL	B	1450	-	-	-	X
2	GOL	B	1451	-	-	-	X
2	GOL	B	1452	-	-	-	X
2	GOL	B	1453	-	-	-	X
3	BMA	A	1461	-	-	X	-
4	MAN	A	1465	X	-	-	-
4	MAN	A	1466	X	-	-	-
5	NAG	B	1454	-	-	-	X
5	MAN	B	1456	X	-	-	-
5	MAN	B	1457	X	-	-	-
5	MAN	B	1458	X	-	-	-
5	MAN	B	1461	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7457 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 GLUCAN 1,3-BETA-GLUCOSIDASE I/II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3324	2120	547	645	12			
1	B	408	Total	C	N	O	S	0	0	0
			3324	2120	547	645	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ILE	THR	CONFLICT	UNP P23776
A	205	ILE	THR	CONFLICT	UNP P23776
A	223	ILE	THR	CONFLICT	UNP P23776
A	330	ILE	THR	CONFLICT	UNP P23776
A	343	ILE	THR	CONFLICT	UNP P23776
B	141	ILE	THR	CONFLICT	UNP P23776
B	205	ILE	THR	CONFLICT	UNP P23776
B	223	ILE	THR	CONFLICT	UNP P23776
B	330	ILE	THR	CONFLICT	UNP P23776
B	343	ILE	THR	CONFLICT	UNP P23776

- Molecule 2 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

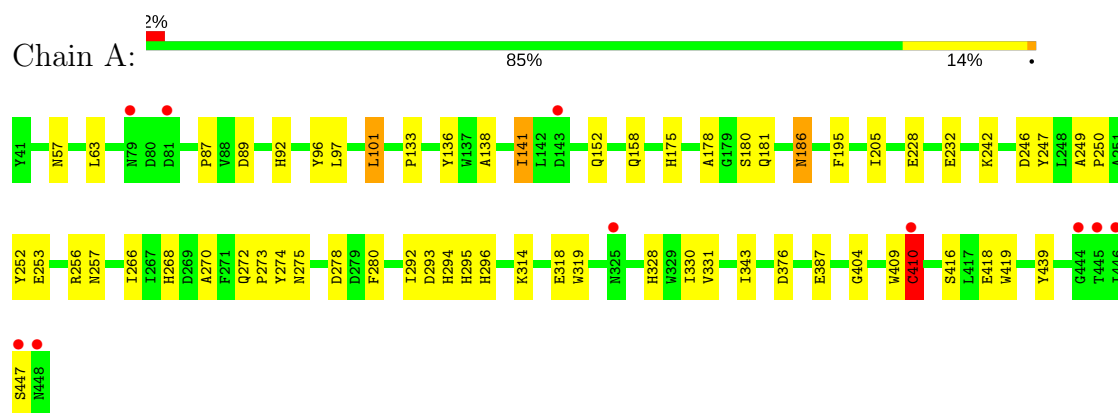
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	228	Total	O	0	0
			228	228		
7	B	228	Total	O	0	0
			228	228		

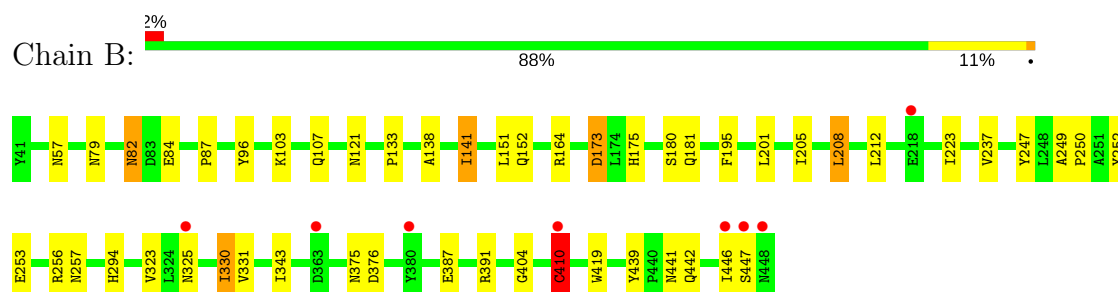
### 3 Residue-property plots [i](#)

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: GLUCAN 1,3-BETA-GLUCOSIDASE I/II



#### • Molecule 1: GLUCAN 1,3-BETA-GLUCOSIDASE I/II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.60Å 102.60Å 203.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.27 – 1.75 49.74 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.9 (36.27-1.75) 95.0 (49.74-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.75Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.206 , 0.228 0.207 , 0.228	Depositor DCC
$R_{free}$ test set	5233 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7457	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 9.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NDG, 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	0.35	1/3420 (0.0%)	0.60	0/4655
1	B	0.32	0/3420	0.61	0/4655
All	All	0.34	1/6840 (0.0%)	0.60	0/9310

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
4	A	2	0
5	B	4	0
All	All	6	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	410	CYS	CB-SG	-7.59	1.69	1.82

There are no bond angle outliers.

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1465	MAN	C1
4	A	1466	MAN	C1
5	B	1456	MAN	C1
5	B	1457	MAN	C1
5	B	1458	MAN	C1
5	B	1461	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	3324	0	3069	49	0
1	B	3324	0	3069	53	0
2	A	24	0	32	3	0
2	B	30	0	40	1	0
3	A	116	0	97	15	0
4	A	61	0	52	3	0
5	B	94	0	79	2	0
6	B	28	0	25	2	0
7	A	228	0	0	2	0
7	B	228	0	0	6	0
All	All	7457	0	6463	123	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 9.

All (123) 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:A:343:ILE:HD12	1:A:419:TRP:HD1	1.22	1.00
1:B:294:HIS:HD2	1:B:330:ILE:HD11	1.25	0.97
1:B:57:ASN:HB2	1:B:410:CYS:H	1.33	0.92
1:A:292:ILE:O	1:A:330:ILE:HD12	1.72	0.90
1:B:294:HIS:HD2	1:B:330:ILE:CD1	1.90	0.85
1:A:410:CYS:HB3	1:A:419:TRP:O	1.79	0.83
1:A:343:ILE:HD12	1:A:419:TRP:CD1	2.11	0.82
1:A:278:ASP:HB2	4:A:1464:NAG:H62	1.59	0.81
3:A:1457:MAN:H62	3:A:1459:MAN:H5	1.62	0.81
1:A:141:ILE:HD13	1:A:141:ILE:H	1.46	0.81
1:B:57:ASN:O	1:B:410:CYS:HA	1.83	0.79
3:A:1460:MAN:H3	3:A:1461:BMA:H61	1.65	0.78
1:B:201:LEU:O	1:B:205:ILE:HG12	1.82	0.77
3:A:1454:NAG:H3	3:A:1461:BMA:H3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:H	1:B:141:ILE:HD13	1.51	0.76
1:B:343:ILE:HG12	7:B:2168:HOH:O	1.87	0.75
1:B:343:ILE:HG13	1:B:419:TRP:CD1	2.21	0.75
1:B:294:HIS:CD2	1:B:330:ILE:HD11	2.17	0.75
1:A:232:GLU:HA	1:A:268:HIS:CD2	2.25	0.72
1:A:158:GLN:HG2	3:A:1454:NAG:H81	1.70	0.71
1:B:343:ILE:HG13	1:B:419:TRP:HD1	1.55	0.70
1:A:343:ILE:HG13	7:A:2160:HOH:O	1.91	0.70
1:B:173:ASP:OD2	1:B:175:HIS:HD2	1.75	0.70
1:A:292:ILE:O	1:A:330:ILE:CD1	2.40	0.69
1:B:325:ASN:HB2	7:B:2159:HOH:O	1.92	0.67
1:A:232:GLU:OE2	1:A:295:HIS:HD2	1.77	0.66
1:B:387:GLU:HG3	1:B:439:TYR:OH	1.95	0.66
1:A:330:ILE:HD12	1:A:331:VAL:H	1.61	0.65
1:A:343:ILE:CD1	1:A:419:TRP:HD1	2.04	0.64
1:B:223:ILE:HG13	7:B:2100:HOH:O	1.98	0.63
3:A:1454:NAG:C3	3:A:1461:BMA:H3	2.30	0.62
1:A:87:PRO:HG3	1:A:96:TYR:CD2	2.37	0.60
1:A:387:GLU:HG3	1:A:439:TYR:OH	2.00	0.60
3:A:1456:BMA:H4	3:A:1462:BMA:C1	2.32	0.60
1:B:294:HIS:CD2	1:B:330:ILE:CD1	2.80	0.60
1:B:103:LYS:O	1:B:107:GLN:HG3	2.01	0.59
1:A:268:HIS:CD2	1:A:270:ALA:H	2.20	0.59
1:B:253:GLU:HG3	1:B:257:ASN:HD22	1.68	0.58
1:A:97:LEU:HD22	1:A:101:LEU:HD13	1.86	0.57
1:A:141:ILE:N	1:A:141:ILE:HD13	2.18	0.57
1:B:82:ASN:HD22	1:B:84:GLU:H	1.51	0.57
1:B:223:ILE:N	1:B:223:ILE:HD12	2.21	0.55
1:A:314:LYS:O	1:A:318:GLU:HG3	2.06	0.55
5:B:1454:NAG:H61	5:B:1455:NAG:N2	2.22	0.55
1:B:87:PRO:HG3	1:B:96:TYR:CD2	2.42	0.55
1:B:79:ASN:HD21	1:B:82:ASN:ND2	2.05	0.55
3:A:1460:MAN:C3	3:A:1461:BMA:H61	2.36	0.54
1:B:205:ILE:CD1	1:B:247:TYR:HD1	2.21	0.54
1:B:82:ASN:C	1:B:82:ASN:HD22	2.11	0.54
1:B:205:ILE:HD11	1:B:247:TYR:HD1	1.72	0.53
1:A:181:GLN:HA	1:A:195:PHE:HB2	1.90	0.53
1:B:330:ILE:HG12	1:B:331:VAL:N	2.22	0.53
1:B:103:LYS:HE2	1:B:151:LEU:HD11	1.91	0.53
1:B:141:ILE:N	1:B:141:ILE:HD13	2.23	0.53
1:B:391:ARG:HH11	1:B:442:GLN:NE2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:CD1	7:B:2165:HOH:O	2.58	0.52
3:A:1461:BMA:O6	3:A:1462:BMA:H4	2.11	0.51
5:B:1456:MAN:H4	5:B:1458:MAN:O2	2.10	0.51
3:A:1454:NAG:HN2	3:A:1461:BMA:H3	1.76	0.51
1:A:343:ILE:CD1	1:A:416:SER:OG	2.58	0.50
6:B:1462:NAG:H83	6:B:1462:NAG:O3	2.12	0.50
1:B:330:ILE:O	1:B:404:GLY:HA3	2.12	0.50
1:B:237:VAL:HG12	1:B:237:VAL:O	2.10	0.50
3:A:1455:BMA:H2	3:A:1456:BMA:H2	1.93	0.50
1:A:92:HIS:HE1	7:A:2032:HOH:O	1.95	0.49
3:A:1457:MAN:C6	3:A:1459:MAN:H5	2.38	0.49
1:B:391:ARG:HH11	1:B:442:GLN:HE21	1.60	0.49
1:A:330:ILE:HD12	1:A:331:VAL:N	2.26	0.49
1:B:205:ILE:HD13	1:B:247:TYR:CD1	2.48	0.49
1:B:208:LEU:HD22	1:B:212:LEU:HG	1.95	0.49
3:A:1455:BMA:O3	3:A:1462:BMA:H61	2.13	0.48
1:A:253:GLU:CD	1:A:257:ASN:HD22	2.16	0.48
1:B:173:ASP:OD2	1:B:175:HIS:CD2	2.62	0.48
1:A:249:ALA:HB3	1:A:250:PRO:HD3	1.96	0.48
1:A:293:ASP:OD2	1:A:295:HIS:HE1	1.97	0.48
1:B:323:VAL:HG11	1:B:330:ILE:CD1	2.44	0.48
1:A:409:TRP:O	1:A:410:CYS:HB2	2.14	0.47
1:A:252:TYR:CE1	1:A:256:ARG:HG3	2.49	0.47
1:A:228:GLU:HA	1:A:266:ILE:HB	1.95	0.47
1:B:330:ILE:HD11	7:B:2165:HOH:O	2.15	0.47
1:A:205:ILE:HD11	1:A:247:TYR:CD1	2.49	0.47
1:B:164:ARG:HB2	1:B:223:ILE:HG12	1.97	0.46
3:A:1457:MAN:H2	3:A:1461:BMA:C1	2.46	0.46
1:B:82:ASN:ND2	1:B:84:GLU:H	2.11	0.46
4:A:1463:NAG:H83	4:A:1463:NAG:O3	2.15	0.46
1:B:253:GLU:HG3	1:B:257:ASN:ND2	2.31	0.46
1:B:205:ILE:CD1	1:B:247:TYR:CD1	2.98	0.46
1:A:294:HIS:CD2	1:A:330:ILE:CD1	2.99	0.46
1:A:280:PHE:O	1:A:328:HIS:CE1	2.69	0.46
1:A:242:LYS:O	1:A:246:ASP:HB2	2.17	0.45
1:A:409:TRP:O	1:A:410:CYS:CB	2.65	0.45
1:A:138:ALA:HB1	1:A:152:GLN:HB2	1.99	0.45
1:B:79:ASN:HD21	1:B:82:ASN:HD21	1.63	0.45
2:B:1449:GOL:H31	7:B:2166:HOH:O	2.17	0.44
1:A:136:TYR:CE2	1:A:178:ALA:HA	2.52	0.44
1:A:343:ILE:HD11	1:A:418:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HB3	1:A:101:LEU:HB3	1.99	0.44
1:B:343:ILE:HD13	1:B:375:ASN:HD22	1.83	0.44
1:A:272:GLN:HE21	1:A:273:PRO:HD2	1.83	0.44
1:B:252:TYR:CZ	1:B:256:ARG:HG3	2.52	0.44
1:A:343:ILE:CD1	1:A:376:ASP:OD1	2.65	0.43
3:A:1456:BMA:C4	3:A:1462:BMA:C1	2.95	0.43
1:A:133:PRO:HB3	1:A:175:HIS:CG	2.53	0.43
1:A:296:HIS:HB3	1:A:319:TRP:CZ3	2.54	0.43
1:B:138:ALA:HB1	1:B:152:GLN:HB2	1.99	0.43
1:A:57:ASN:HB2	1:A:410:CYS:H	1.82	0.43
6:B:1462:NAG:H62	6:B:1463:NDG:N2	2.34	0.42
1:A:63:LEU:HD13	1:A:175:HIS:HB3	2.02	0.42
1:B:133:PRO:HB3	1:B:175:HIS:CG	2.55	0.42
4:A:1465:MAN:O4	4:A:1466:MAN:H2	2.20	0.42
1:A:330:ILE:O	1:A:404:GLY:HA3	2.20	0.42
1:B:446:ILE:HG22	1:B:447:SER:N	2.34	0.42
2:A:1452:GOL:C1	1:B:121:ASN:HD21	2.32	0.42
1:B:249:ALA:N	1:B:250:PRO:HD2	2.35	0.42
1:B:343:ILE:CD1	1:B:376:ASP:OD1	2.68	0.41
1:B:223:ILE:N	1:B:223:ILE:CD1	2.84	0.41
1:A:296:HIS:HB3	1:A:319:TRP:CH2	2.55	0.41
1:B:181:GLN:HA	1:B:195:PHE:HB2	2.02	0.41
2:A:1452:GOL:O1	1:B:121:ASN:ND2	2.52	0.41
1:A:89:ASP:OD1	1:A:92:HIS:HD2	2.04	0.41
1:A:186:ASN:OD1	2:A:1450:GOL:H12	2.21	0.40
3:A:1460:MAN:O3	3:A:1460:MAN:H61	2.22	0.40
1:A:274:TYR:O	1:A:275:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/408 (100%)	387 (95%)	16 (4%)	3 (1%)	25	9
1	B	406/408 (100%)	387 (95%)	17 (4%)	2 (0%)	32	13
All	All	812/816 (100%)	774 (95%)	33 (4%)	5 (1%)	28	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	410	CYS
1	A	410	CYS
1	A	447	SER
1	A	180	SER
1	B	180	SER

### 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	352/352 (100%)	348 (99%)	4 (1%)	78	64
1	B	352/352 (100%)	345 (98%)	7 (2%)	60	38
All	All	704/704 (100%)	693 (98%)	11 (2%)	68	50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	141	ILE
1	A	186	ASN
1	A	410	CYS
1	B	82	ASN
1	B	141	ILE
1	B	173	ASP
1	B	208	LEU
1	B	330	ILE
1	B	410	CYS
1	B	441	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	107	GLN
1	A	125	GLN
1	A	186	ASN
1	A	257	ASN
1	A	268	HIS
1	A	272	GLN
1	A	284	ASN
1	A	295	HIS
1	A	364	GLN
1	A	422	GLN
1	B	82	ASN
1	B	107	GLN
1	B	121	ASN
1	B	166	ASN
1	B	175	HIS
1	B	200	ASN
1	B	257	ASN
1	B	364	GLN
1	B	422	GLN
1	B	441	ASN
1	B	442	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 ⓘ

25 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	$\# Z  > 2$
3	NAG	A	1453	1,3	14,14,15	0.60	0	15,19,21	0.78	1 (6%)
3	NAG	A	1454	3	14,14,15	0.53	0	15,19,21	0.85	0
3	BMA	A	1455	3	11,11,12	0.56	0	13,15,17	0.64	0
3	BMA	A	1456	3	11,11,12	0.78	0	13,15,17	0.70	0
3	MAN	A	1457	3	11,11,12	0.64	0	13,15,17	0.73	1 (7%)
3	BMA	A	1458	3	11,11,12	0.60	0	13,15,17	0.46	0
3	MAN	A	1459	3	11,11,12	0.48	0	13,15,17	0.66	0
3	MAN	A	1460	3	11,11,12	0.59	0	13,15,17	0.69	1 (7%)
3	BMA	A	1461	3	11,11,12	0.56	0	13,15,17	0.91	1 (7%)
3	BMA	A	1462	3	11,11,12	0.61	0	13,15,17	0.91	1 (7%)
4	NAG	A	1463	1,4	14,14,15	0.52	0	15,19,21	0.71	0
4	NAG	A	1464	4	14,14,15	0.61	0	15,19,21	0.77	0
4	MAN	A	1465	4	11,11,12	0.64	0	13,15,17	0.34	0
4	MAN	A	1466	4	11,11,12	0.54	0	13,15,17	0.50	0
4	BMA	A	1467	4	11,11,12	0.61	0	13,15,17	0.55	0
5	NAG	B	1454	1,5	14,14,15	0.59	0	15,19,21	0.71	0
5	NAG	B	1455	5	14,14,15	0.50	0	15,19,21	0.67	0
5	MAN	B	1456	5	11,11,12	0.54	0	13,15,17	0.31	0
5	MAN	B	1457	5	11,11,12	0.58	0	13,15,17	0.53	0
5	MAN	B	1458	5	11,11,12	0.71	0	13,15,17	0.77	0
5	BMA	B	1459	5	11,11,12	0.56	0	13,15,17	0.47	0
5	BMA	B	1460	5	11,11,12	0.54	0	13,15,17	0.49	0
5	MAN	B	1461	5	11,11,12	0.49	0	13,15,17	0.48	0
6	NAG	B	1462	1,6	14,14,15	0.56	0	15,19,21	0.82	1 (6%)
6	NDG	B	1463	6	14,14,15	0.59	0	15,19,21	0.72	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	A	1453	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1454	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1455	3	-	0/2/19/22	0/1/1/1
3	BMA	A	1456	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1457	3	-	0/2/19/22	0/1/1/1
3	BMA	A	1458	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	1459	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1460	3	-	0/2/19/22	0/1/1/1
3	BMA	A	1461	3	-	0/2/19/22	1/1/1/1
3	BMA	A	1462	3	-	0/2/19/22	1/1/1/1
4	NAG	A	1463	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1464	4	-	0/6/23/26	0/1/1/1
4	MAN	A	1465	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	1466	4	1/1/4/5	0/2/19/22	0/1/1/1
4	BMA	A	1467	4	-	0/2/19/22	0/1/1/1
5	NAG	B	1454	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1455	5	-	1/6/23/26	0/1/1/1
5	MAN	B	1456	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	1457	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	1458	5	1/1/4/5	0/2/19/22	0/1/1/1
5	BMA	B	1459	5	-	0/2/19/22	0/1/1/1
5	BMA	B	1460	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1461	5	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	B	1462	1,6	-	0/6/23/26	0/1/1/1
6	NDG	B	1463	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1462	NAG	C2-N2-C7	-2.19	119.75	122.94
3	A	1453	NAG	C2-N2-C7	-2.04	119.96	122.94
3	A	1457	MAN	C1-O5-C5	2.00	114.92	112.17
3	A	1460	MAN	C1-O5-C5	2.12	115.09	112.17
3	A	1461	BMA	C1-O5-C5	2.71	115.90	112.17
3	A	1462	BMA	C1-O5-C5	2.75	115.96	112.17

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1457	MAN	C1
5	B	1456	MAN	C1
4	A	1466	MAN	C1
5	B	1458	MAN	C1
4	A	1465	MAN	C1
5	B	1461	MAN	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1455	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1461	BMA	C1-C2-C3-C4-C5-O5
3	A	1462	BMA	C1-C2-C3-C4-C5-O5

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1454	NAG	4	0
3	A	1455	BMA	2	0
3	A	1456	BMA	3	0
3	A	1457	MAN	3	0
3	A	1459	MAN	2	0
3	A	1460	MAN	3	0
3	A	1461	BMA	7	0
3	A	1462	BMA	4	0
4	A	1463	NAG	1	0
4	A	1464	NAG	1	0
4	A	1465	MAN	1	0
4	A	1466	MAN	1	0
5	B	1454	NAG	1	0
5	B	1455	NAG	1	0
5	B	1456	MAN	1	0
5	B	1458	MAN	1	0
6	B	1462	NAG	2	0
6	B	1463	NDG	1	0

## 5.6 Ligand geometry

9 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
2	GOL	A	1449	-	5,5,5	0.94	0	5,5,5	0.32	0
2	GOL	A	1450	-	5,5,5	0.87	0	5,5,5	0.37	0
2	GOL	A	1451	-	5,5,5	0.90	0	5,5,5	0.32	0
2	GOL	A	1452	-	5,5,5	0.90	0	5,5,5	0.38	0
2	GOL	B	1449	-	5,5,5	0.98	0	5,5,5	0.27	0
2	GOL	B	1450	-	5,5,5	0.87	0	5,5,5	0.40	0
2	GOL	B	1451	-	5,5,5	0.92	0	5,5,5	0.31	0
2	GOL	B	1452	-	5,5,5	0.92	0	5,5,5	0.38	0
2	GOL	B	1453	-	5,5,5	0.87	0	5,5,5	0.34	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	GOL	A	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1450	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1451	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1452	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1449	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1450	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1451	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1452	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1453	-	-	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1450	GOL	1	0
2	A	1452	GOL	2	0
2	B	1449	GOL	1	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	408/408 (100%)	0.10	10 (2%) 58 64	15, 24, 37, 80	0
1	B	408/408 (100%)	0.09	8 (1%) 65 73	15, 24, 37, 78	0
All	All	816/816 (100%)	0.10	18 (2%) 62 70	15, 24, 37, 80	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	SER	12.1
1	A	447	SER	12.1
1	B	448	ASN	12.0
1	A	448	ASN	10.4
1	B	446	ILE	9.6
1	A	446	ILE	9.1
1	B	410	CYS	4.0
1	A	445	THR	3.8
1	B	363	ASP	3.4
1	B	218	GLU	2.9
1	A	410	CYS	2.9
1	A	79	ASN	2.8
1	A	143	ASP	2.5
1	A	81	ASP	2.5
1	B	380	TYR	2.4
1	A	325	ASN	2.3
1	B	325	ASN	2.2
1	A	444	GLY	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

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(Å <sup>2</sup> )	Q<0.9
5	NAG	B	1454	14/15	0.72	0.23	6.48	49,52,54,58	0
6	NDG	B	1463	14/15	0.53	0.68	-	73,75,76,76	0
5	MAN	B	1457	11/12	0.58	0.41	-	84,85,86,87	0
3	MAN	A	1457	11/12	0.36	0.60	-	88,91,92,93	0
5	BMA	B	1459	11/12	0.17	0.77	-	91,91,91,91	0
3	BMA	A	1461	11/12	0.53	0.93	-	95,95,96,96	0
5	MAN	B	1456	11/12	0.59	0.32	-	76,79,82,84	0
3	BMA	A	1462	11/12	0.37	0.99	-	91,92,93,93	0
5	NAG	B	1455	14/15	0.55	0.32	-	62,65,67,72	0
4	MAN	A	1466	11/12	0.33	0.80	-	95,96,96,96	0
4	NAG	A	1463	14/15	0.55	0.48	-	69,72,75,80	0
4	NAG	A	1464	14/15	0.21	0.76	-	84,86,88,91	0
5	MAN	B	1458	11/12	0.36	0.61	-	86,88,89,90	0
3	BMA	A	1456	11/12	0.35	0.62	-	85,87,88,90	0
3	MAN	A	1460	11/12	0.26	0.67	-	94,94,95,95	0
3	BMA	A	1458	11/12	0.30	0.56	-	93,94,94,95	0
5	BMA	B	1460	11/12	0.13	0.61	-	90,90,90,91	0
3	BMA	A	1455	11/12	0.58	0.26	-	74,79,82,86	0
4	BMA	A	1467	11/12	-0.25	1.17	-	98,99,99,99	0
3	NAG	A	1454	14/15	0.73	0.38	-	57,60,64,69	0
3	NAG	A	1453	14/15	0.77	0.28	-	42,46,48,51	0
4	MAN	A	1465	11/12	0.22	0.94	-	93,95,96,98	0
5	MAN	B	1461	11/12	0.14	0.84	-	88,89,89,90	0
6	NAG	B	1462	14/15	0.67	0.35	-	61,65,67,70	0
3	MAN	A	1459	11/12	0.20	0.64	-	95,96,96,96	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
2	GOL	B	1452	6/6	0.76	0.31	19.79	49,54,55,56	0
2	GOL	A	1452	6/6	0.55	0.27	17.09	50,52,55,56	0
2	GOL	B	1451	6/6	0.64	0.23	15.62	56,57,57,57	0
2	GOL	B	1453	6/6	0.65	0.22	9.19	61,62,63,64	0
2	GOL	A	1450	6/6	0.74	0.26	8.88	40,41,43,43	0
2	GOL	B	1450	6/6	0.90	0.14	5.11	24,29,31,35	0
2	GOL	A	1451	6/6	0.57	0.22	4.36	57,58,58,58	0
2	GOL	B	1449	6/6	0.82	0.13	1.69	36,40,42,42	0
2	GOL	A	1449	6/6	0.95	0.12	1.58	28,30,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.