



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:48 am GMT

PDB ID : 3OVW  
Title : ENDOGLUCANASE I NATIVE STRUCTURE  
Authors : Davies, G.J.; Schulein, M.  
Deposited on : 1997-10-06  
Resolution : 2.30 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

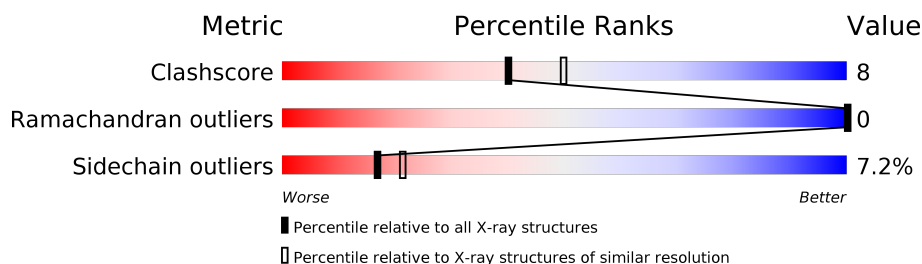
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	411	 75% 18% . .
1	B	411	 75% 18% . . .

## 2 Entry composition [i](#)

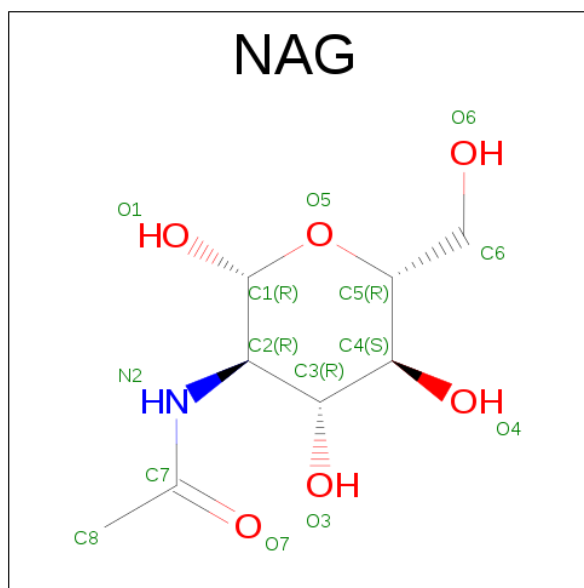
There are 3 unique types of molecules in this entry. The entry contains 6548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOGLUCANASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3035	1878	536	592	29			
1	B	400	Total	C	N	O	S	0	0	0
			3035	1878	536	592	29			

- Molecule 2 is SUGAR (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	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 water.

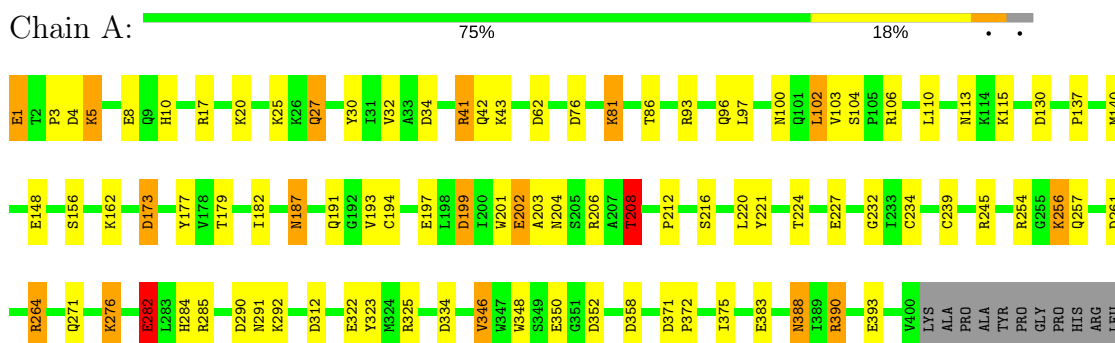
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	227	Total 227	O 227	0	0
3	B	195	Total 195	O 195	0	0

### 3 Residue-property plots

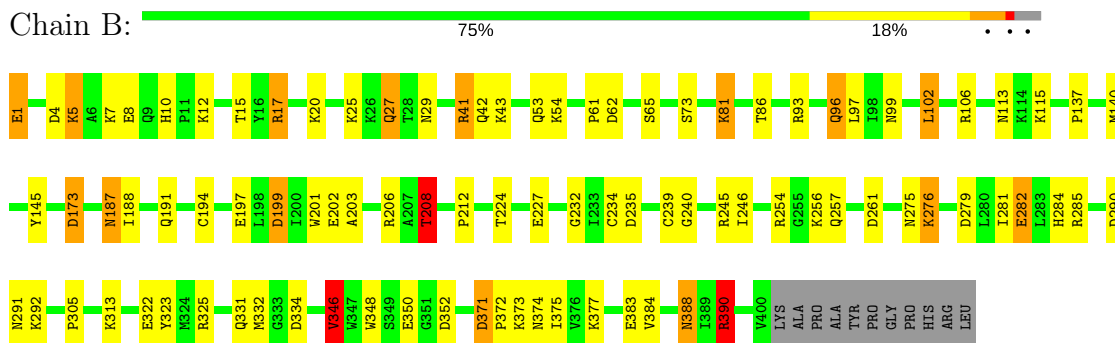
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: ENDOGLUCANASE I



#### • Molecule 1: ENDOGLUCANASE I



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.42Å 81.94Å 90.99Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	18.00 – 2.30	Depositor
% Data completeness (in resolution range)	91.0 (18.00-2.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.158 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.65	0/3089	1.55	50/4173 (1.2%)
1	B	0.65	0/3089	1.57	43/4173 (1.0%)
All	All	0.65	0/6178	1.56	93/8346 (1.1%)

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
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	B	17	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	A	285	ARG	NE-CZ-NH2	10.49	125.55	120.30
1	B	323	TYR	CB-CG-CD2	10.19	127.12	121.00
1	A	371	ASP	CB-CG-OD1	10.10	127.39	118.30
1	B	323	TYR	CB-CG-CD1	-9.96	115.02	121.00
1	A	173	ASP	CB-CG-OD1	9.64	126.97	118.30
1	B	282	GLU	OE1-CD-OE2	-9.54	111.85	123.30
1	B	371	ASP	CB-CG-OD1	9.46	126.82	118.30
1	A	346	VAL	CB-CA-C	-9.44	93.46	111.40
1	A	17	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	B	1	PCA	O-C-N	-9.19	108.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLU	OE1-CD-OE2	9.09	134.21	123.30
1	B	106	ARG	NE-CZ-NH1	-8.99	115.80	120.30
1	B	390	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	245	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	B	202	GLU	OE1-CD-OE2	8.58	133.60	123.30
1	B	245	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	B	206	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	B	199	ASP	CB-CG-OD1	8.21	125.69	118.30
1	B	383	GLU	OE1-CD-OE2	-7.71	114.04	123.30
1	A	34	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	B	206	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	B	346	VAL	CB-CA-C	-7.61	96.94	111.40
1	A	221	TYR	CB-CG-CD1	7.60	125.56	121.00
1	A	41	ARG	CD-NE-CZ	7.55	134.17	123.60
1	B	1	PCA	C-N-CA	7.49	140.43	121.70
1	B	41	ARG	CD-NE-CZ	7.45	134.02	123.60
1	A	199	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	358	ASP	CB-CG-OD2	7.24	124.82	118.30
1	B	332	MET	CG-SD-CE	7.24	111.78	100.20
1	A	30	TYR	CB-CG-CD2	7.22	125.33	121.00
1	A	254	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	261	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	B	62	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	254	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	B	334	ASP	CB-CG-OD1	6.97	124.58	118.30
1	B	173	ASP	CB-CG-OD1	6.95	124.55	118.30
1	B	27	GLN	N-CA-CB	6.94	123.09	110.60
1	A	76	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	93	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	148	GLU	OE1-CD-OE2	-6.82	115.11	123.30
1	A	334	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	261	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	352	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	346	VAL	N-CA-CB	6.71	126.27	111.50
1	A	245	ARG	NE-CZ-NH1	-6.69	116.96	120.30
1	B	346	VAL	N-CA-CB	6.63	126.09	111.50
1	A	1	PCA	C-N-CA	6.52	137.99	121.70
1	A	130	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	312	ASP	CB-CG-OD1	6.42	124.07	118.30
1	A	1	PCA	O-C-N	-6.31	112.60	122.70
1	A	199	ASP	OD1-CG-OD2	-6.20	111.51	123.30
1	A	383	GLU	OE1-CD-OE2	-6.17	115.89	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	352	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	41	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	199	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	76	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	145	TYR	CB-CG-CD1	5.84	124.50	121.00
1	B	254	ARG	CD-NE-CZ	5.76	131.66	123.60
1	B	208	THR	CB-CA-C	-5.68	96.25	111.60
1	A	261	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	334	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	93	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	235	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	208	THR	N-CA-CB	5.55	120.84	110.30
1	B	352	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	177	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	323	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	A	93	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	53	GLN	CB-CA-C	-5.39	99.63	110.40
1	A	282	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	B	305	PRO	N-CA-CB	5.34	109.71	103.30
1	A	358	ASP	OD1-CG-OD2	-5.34	113.15	123.30
1	B	208	THR	OG1-CB-CG2	5.29	122.16	110.00
1	B	279	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	323	TYR	CB-CG-CD2	5.27	124.16	121.00
1	B	27	GLN	CB-CA-C	-5.27	99.86	110.40
1	B	352	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	3	PRO	N-CA-CB	5.25	109.60	103.30
1	A	264	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	A	106	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	4	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	62	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	208	THR	CB-CA-C	-5.20	97.56	111.60
1	B	12	LYS	CA-CB-CG	5.17	124.78	113.40
1	A	393	GLU	CG-CD-OE1	5.15	128.59	118.30
1	A	206	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	285	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	27	GLN	N-CA-CB	5.02	119.63	110.60
1	A	271	GLN	CG-CD-NE2	5.02	128.74	116.70
1	B	240	GLY	CA-C-O	5.01	129.61	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PCA	Mainchain
1	B	1	PCA	Mainchain

## 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	3035	0	2919	52	0
1	B	3035	0	2919	49	0
2	A	28	0	26	2	0
2	B	28	0	26	1	0
3	A	227	0	0	7	0
3	B	195	0	0	6	0
All	All	6548	0	5890	100	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 8.

All (100) 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:388:ASN:HD21	1:B:390:ARG:HH11	1.10	0.97
1:A:100:ASN:HB3	3:A:875:HOH:O	1.67	0.94
1:A:388:ASN:HD21	1:A:390:ARG:HH11	1.23	0.84
1:B:203:ALA:HB2	1:B:208:THR:HG23	1.67	0.77
1:A:81:LYS:HD3	1:A:86:THR:HG22	1.71	0.73
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.70	0.72
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.26	0.71
1:B:81:LYS:HD3	1:B:86:THR:HG22	1.73	0.70
1:A:187:ASN:HD21	1:A:191:GLN:H	1.37	0.70
1:B:276:LYS:H	1:B:276:LYS:HZ3	1.40	0.70
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.26	0.70
1:B:113:ASN:HD22	1:B:115:LYS:H	1.42	0.68
1:B:276:LYS:NZ	1:B:276:LYS:H	1.92	0.67
1:B:187:ASN:HD21	1:B:191:GLN:H	1.42	0.67
1:A:113:ASN:HD22	1:A:115:LYS:H	1.45	0.65
1:B:113:ASN:ND2	1:B:115:LYS:H	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:HD2	3:A:956:HOH:O	2.00	0.61
1:A:276:LYS:NZ	1:A:276:LYS:H	1.97	0.61
1:A:216:SER:O	1:B:99:ASN:HB3	2.00	0.61
1:B:284:HIS:HD2	3:B:866:HOH:O	1.83	0.61
1:B:97:LEU:HD23	1:B:102:LEU:HA	1.83	0.60
1:A:193:VAL:HG13	1:A:220:LEU:HD21	1.82	0.60
1:A:5:LYS:H	1:A:5:LYS:HZ2	1.49	0.60
1:B:290:ASP:O	1:B:291:ASN:HB2	2.02	0.59
1:A:97:LEU:HD23	1:A:102:LEU:HA	1.83	0.59
1:B:113:ASN:HD22	1:B:115:LYS:HB2	1.69	0.57
1:A:203:ALA:HB2	1:A:208:THR:CG2	2.35	0.57
1:A:256:LYS:HD3	3:A:959:HOH:O	2.05	0.56
1:A:388:ASN:HD21	1:A:390:ARG:NH1	2.00	0.56
1:B:291:ASN:HB3	3:B:975:HOH:O	2.06	0.55
1:B:203:ALA:HB2	1:B:208:THR:CG2	2.35	0.55
1:B:388:ASN:HD21	1:B:390:ARG:NH1	1.92	0.53
1:A:201:TRP:CH2	1:A:208:THR:HG21	2.44	0.53
1:B:322:GLU:OE1	1:B:325:ARG:NH2	2.39	0.52
1:A:113:ASN:HD22	1:A:115:LYS:HB2	1.76	0.50
1:B:137:PRO:HD2	1:B:140:MET:HG3	1.93	0.49
1:A:137:PRO:HD2	1:A:140:MET:CG	2.43	0.49
1:B:173:ASP:HB2	1:B:197:GLU:OE1	2.12	0.49
1:A:32:VAL:HB	1:A:110:LEU:HD11	1.95	0.49
1:A:322:GLU:OE1	1:A:325:ARG:NH2	2.41	0.48
1:B:212:PRO:HD2	1:B:239:CYS:O	2.12	0.48
1:A:290:ASP:O	1:A:291:ASN:HB2	2.13	0.48
1:B:203:ALA:CB	1:B:208:THR:HG23	2.40	0.48
1:B:388:ASN:ND2	1:B:390:ARG:HD3	2.28	0.48
1:B:17:ARG:HH22	1:B:29:ASN:HD21	1.62	0.48
1:B:54:LYS:HD3	1:B:188:ILE:O	2.13	0.48
1:B:96:GLN:HA	1:B:96:GLN:HE21	1.78	0.48
1:A:137:PRO:HD2	1:A:140:MET:HG3	1.95	0.48
1:A:182:ILE:HD12	1:A:193:VAL:HG22	1.96	0.47
1:B:8:GLU:HG2	1:B:10:HIS:CE1	2.48	0.47
1:A:81:LYS:HD3	1:A:86:THR:CG2	2.43	0.47
1:B:73:SER:HB3	3:B:899:HOH:O	2.14	0.47
1:B:20:LYS:HE3	3:B:987:HOH:O	2.13	0.47
1:A:173:ASP:HB2	1:A:197:GLU:OE1	2.15	0.47
1:B:7:LYS:HE3	3:B:948:HOH:O	2.14	0.47
1:A:372:PRO:HA	1:A:375:ILE:HD12	1.97	0.47
1:A:212:PRO:HD2	1:A:239:CYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASN:HD21	1:A:191:GLN:N	2.10	0.46
1:B:374:ASN:HB3	3:B:978:HOH:O	2.14	0.46
1:A:282:GLU:OE1	1:A:284:HIS:HE1	1.97	0.46
1:A:284:HIS:HD2	3:A:945:HOH:O	1.99	0.46
1:A:42:GLN:NE2	2:A:800:NAG:O6	2.48	0.46
1:A:276:LYS:HZ2	1:A:276:LYS:H	1.65	0.46
1:B:42:GLN:NE2	2:B:800:NAG:O6	2.49	0.46
1:A:8:GLU:HG2	1:A:10:HIS:CE1	2.51	0.45
1:A:197:GLU:OE2	1:A:199:ASP:OD1	2.34	0.45
1:B:227:GLU:O	1:B:232:GLY:HA3	2.17	0.45
1:A:203:ALA:CB	1:A:208:THR:HG23	2.41	0.44
1:B:374:ASN:HA	1:B:377:LYS:HD2	1.98	0.44
1:A:113:ASN:ND2	1:A:115:LYS:H	2.14	0.44
1:A:4:ASP:HB2	1:A:5:LYS:HE3	2.00	0.44
1:A:179:THR:HB	3:A:893:HOH:O	2.18	0.43
1:B:197:GLU:OE2	1:B:199:ASP:OD1	2.36	0.43
1:B:194:CYS:HB3	1:B:234:CYS:SG	2.58	0.43
1:A:5:LYS:H	1:A:5:LYS:CE	2.32	0.43
1:B:372:PRO:HA	1:B:375:ILE:HD12	2.00	0.43
1:A:227:GLU:O	1:A:232:GLY:HA3	2.18	0.43
1:A:42:GLN:HE22	2:A:800:NAG:C6	2.32	0.42
1:A:140:MET:O	1:A:204:ASN:HB3	2.19	0.42
1:B:201:TRP:CE3	1:B:208:THR:HG21	2.55	0.42
1:B:276:LYS:HD3	1:B:276:LYS:N	2.35	0.42
1:B:15:THR:OG1	1:B:29:ASN:ND2	2.52	0.42
1:A:20:LYS:HE3	3:A:941:HOH:O	2.19	0.42
1:B:346:VAL:HG13	1:B:384:VAL:HG12	2.02	0.42
1:B:201:TRP:CH2	1:B:208:THR:HG21	2.55	0.41
1:B:275:ASN:HB2	1:B:276:LYS:NZ	2.35	0.41
1:B:371:ASP:OD1	1:B:372:PRO:HD2	2.20	0.41
1:A:194:CYS:HB3	1:A:234:CYS:SG	2.60	0.41
1:B:281:ILE:HG13	1:B:282:GLU:HG3	2.02	0.41
1:A:103:VAL:O	1:A:104:SER:C	2.58	0.41
1:A:137:PRO:HG2	1:A:375:ILE:HG23	2.02	0.41
1:A:276:LYS:HB2	3:A:1023:HOH:O	2.20	0.41
1:A:5:LYS:H	1:A:5:LYS:NZ	2.15	0.41
1:B:5:LYS:H	1:B:5:LYS:HZ2	1.68	0.41
1:B:61:PRO:HD2	1:B:65:SER:HB2	2.01	0.41
1:A:276:LYS:HZ3	1:A:276:LYS:H	1.66	0.41
1:B:81:LYS:HD3	1:B:86:THR:CG2	2.48	0.41
1:A:199:ASP:HB3	1:A:202:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HH11	1:A:264:ARG:HD2	1.66	0.40
1:B:113:ASN:ND2	1:B:115:LYS:HB2	2.33	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	398/411 (97%)	384 (96%)	14 (4%)	0	100	100
1	B	398/411 (97%)	384 (96%)	14 (4%)	0	100	100
All	All	796/822 (97%)	768 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	325/333 (98%)	302 (93%)	23 (7%)	17	22
1	B	325/333 (98%)	301 (93%)	24 (7%)	16	20
All	All	650/666 (98%)	603 (93%)	47 (7%)	17	21

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	25	LYS
1	A	27	GLN
1	A	41	ARG
1	A	43	LYS
1	A	81	LYS
1	A	96	GLN
1	A	102	LEU
1	A	156	SER
1	A	162	LYS
1	A	187	ASN
1	A	208	THR
1	A	224	THR
1	A	256	LYS
1	A	257	GLN
1	A	276	LYS
1	A	282	GLU
1	A	292	LYS
1	A	346	VAL
1	A	348	TRP
1	A	350	GLU
1	A	388	ASN
1	A	390	ARG
1	B	5	LYS
1	B	25	LYS
1	B	27	GLN
1	B	41	ARG
1	B	43	LYS
1	B	81	LYS
1	B	96	GLN
1	B	102	LEU
1	B	187	ASN
1	B	208	THR
1	B	224	THR
1	B	246	ILE
1	B	256	LYS
1	B	257	GLN
1	B	276	LYS
1	B	292	LYS
1	B	313	LYS
1	B	331	GLN
1	B	346	VAL
1	B	348	TRP

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Mol	Chain	Res	Type
1	B	350	GLU
1	B	373	LYS
1	B	388	ASN
1	B	390	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	29	ASN
1	A	42	GLN
1	A	69	ASN
1	A	95	GLN
1	A	96	GLN
1	A	113	ASN
1	A	151	GLN
1	A	175	GLN
1	A	187	ASN
1	A	284	HIS
1	A	331	GLN
1	A	388	ASN
1	B	9	GLN
1	B	29	ASN
1	B	42	GLN
1	B	69	ASN
1	B	96	GLN
1	B	113	ASN
1	B	175	GLN
1	B	187	ASN
1	B	277	GLN
1	B	284	HIS
1	B	331	GLN
1	B	388	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PCA	A	1	1	8,8,9	1.65	2 (25%)	9,10,12	1.46	1 (11%)
1	PCA	B	1	1	8,8,9	1.54	1 (12%)	9,10,12	1.63	2 (22%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	O-C	2.34	1.29	1.19
1	B	1	PCA	CA-C	2.97	1.54	1.50
1	A	1	PCA	CA-C	3.26	1.54	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	OE-CD-CG	-3.72	120.00	126.86
1	A	1	PCA	OE-CD-CG	-3.25	120.87	126.86
1	B	1	PCA	CA-N-CD	-2.26	105.83	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	800	1	14,14,15	1.23	1 (7%)	15,19,21	1.82	4 (26%)
2	NAG	A	801	1	14,14,15	1.09	1 (7%)	15,19,21	2.26	6 (40%)
2	NAG	B	800	1	14,14,15	1.25	1 (7%)	15,19,21	2.61	8 (53%)
2	NAG	B	801	1	14,14,15	1.22	1 (7%)	15,19,21	1.47	3 (20%)

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	800	1	-	0/6/23/26	0/1/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	800	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	NAG	O7-C7	-3.77	1.14	1.23
2	B	800	NAG	O7-C7	-3.56	1.14	1.23
2	A	801	NAG	O7-C7	-3.38	1.15	1.23
2	B	801	NAG	O7-C7	-3.31	1.15	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	NAG	O5-C1-C2	-4.46	105.26	111.47
2	A	801	NAG	C4-C3-C2	-4.23	104.83	111.02
2	B	800	NAG	C4-C3-C2	-4.05	105.09	111.02
2	A	800	NAG	O5-C1-C2	-3.42	106.72	111.47
2	A	800	NAG	C2-N2-C7	-3.40	117.99	122.94
2	A	801	NAG	C3-C4-C5	-3.32	104.36	110.22
2	B	800	NAG	C6-C5-C4	-3.11	105.73	113.00
2	B	800	NAG	O4-C4-C5	-2.78	102.28	109.28
2	A	800	NAG	C6-C5-C4	-2.74	106.58	113.00
2	A	800	NAG	O3-C3-C4	-2.68	104.52	110.36
2	B	801	NAG	O5-C1-C2	-2.62	107.83	111.47
2	B	801	NAG	C4-C3-C2	-2.42	107.47	111.02
2	B	800	NAG	C3-C4-C5	-2.18	106.38	110.22
2	B	800	NAG	C2-N2-C7	-2.11	119.87	122.94
2	A	801	NAG	O7-C7-N2	-2.02	118.03	121.92
2	B	800	NAG	O7-C7-C8	2.21	126.08	122.06
2	A	801	NAG	O3-C3-C2	2.24	114.19	109.39
2	A	801	NAG	O7-C7-C8	2.29	126.23	122.06
2	B	801	NAG	C1-O5-C5	3.10	116.44	112.17
2	B	800	NAG	O4-C4-C3	4.64	120.45	110.36
2	A	801	NAG	C1-O5-C5	5.39	119.59	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	NAG	2	0
2	B	800	NAG	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.