



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:40 PM UTC

PDB ID : 3OVW / pdb_00003ovw
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

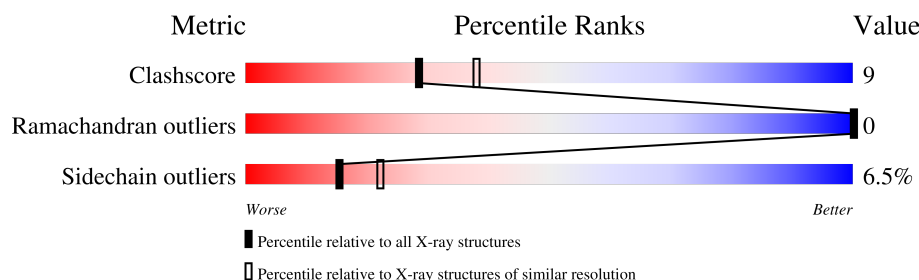
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	411	 72% 20% 5% . .
1	B	411	 70% 23% . . .

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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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.

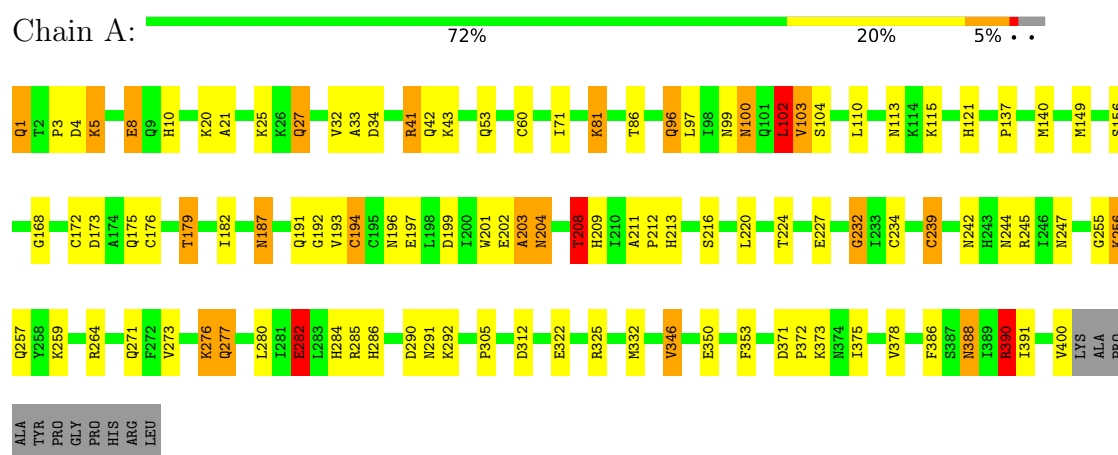
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	227	Total 227	O 227	0	0
3	B	195	Total 195	O 195	0	0

3 Residue-property plots [i](#)

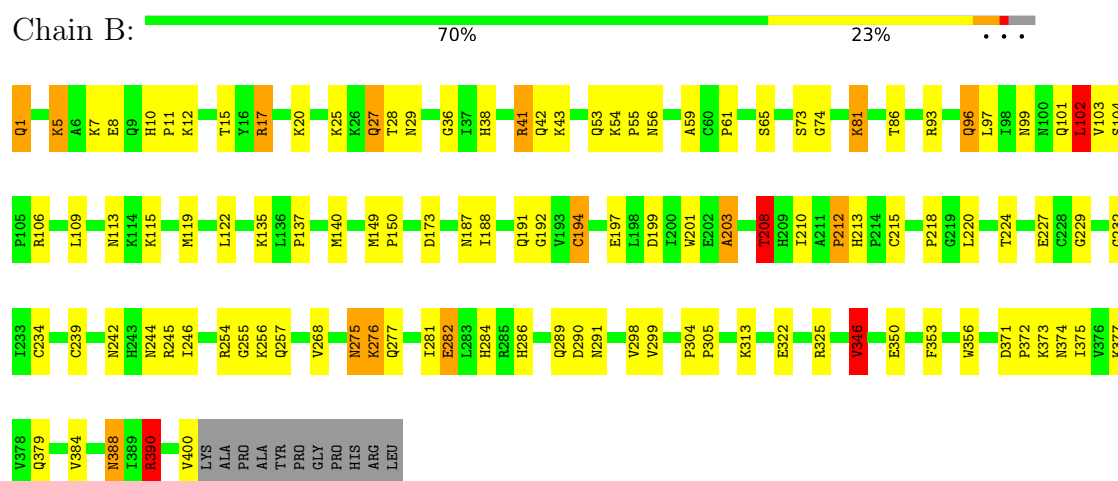
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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, α , β , γ	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 ²)	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	0.83	1/3089 (0.0%)	1.87	76/4173 (1.8%)
1	B	0.83	0/3089	1.87	68/4173 (1.6%)
All	All	0.83	1/6178 (0.0%)	1.87	144/8346 (1.7%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	C-N	5.84	1.41	1.33

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	VAL	CB-CA-C	-11.56	93.46	110.33
1	B	1	PCA	CA-C-N	10.41	140.43	121.70
1	B	1	PCA	C-N-CA	10.41	140.43	121.70
1	A	346	VAL	N-CA-CB	10.10	126.27	111.52
1	B	1	PCA	O-C-N	-9.37	108.00	123.00
1	A	1	PCA	CA-C-N	9.05	137.99	121.70
1	A	1	PCA	C-N-CA	9.05	137.99	121.70
1	B	346	VAL	N-CA-CB	8.96	126.09	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	VAL	CB-CA-C	-8.44	96.94	110.28
1	B	356	TRP	CA-C-O	8.41	129.66	119.49
1	A	271	GLN	CG-CD-NE2	8.22	128.74	116.40
1	A	277	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	A	100	ASN	CA-CB-CG	-7.87	104.73	112.60
1	A	209	HIS	CA-CB-CG	7.86	121.66	113.80
1	B	255	GLY	N-CA-C	7.49	119.68	112.04
1	A	271	GLN	OE1-CD-NE2	-7.42	115.18	122.60
1	A	102	LEU	CA-C-N	-7.39	113.48	121.84
1	A	102	LEU	C-N-CA	-7.39	113.48	121.84
1	B	305	PRO	N-CA-CB	7.32	109.71	103.35
1	A	204	ASN	CA-C-O	-7.29	112.72	121.32
1	A	203	ALA	N-CA-C	7.23	119.16	108.60
1	B	27	GLN	N-CA-CB	7.08	123.09	111.62
1	A	3	PRO	N-CA-CB	7.07	109.60	103.31
1	A	285	ARG	NE-CZ-NH2	7.05	125.55	119.20
1	A	41	ARG	CD-NE-CZ	6.98	134.17	124.40
1	B	282	GLU	CB-CG-CD	6.90	124.33	112.60
1	B	41	ARG	CD-NE-CZ	6.87	134.02	124.40
1	A	353	PHE	CA-CB-CG	6.71	120.51	113.80
1	A	53	GLN	N-CA-C	6.60	119.75	109.52
1	B	53	GLN	N-CA-C	6.60	119.75	109.52
1	B	353	PHE	CA-CB-CG	6.54	120.33	113.80
1	B	379	GLN	CA-C-O	6.54	127.79	120.34
1	B	242	ASN	CA-CB-CG	6.52	119.12	112.60
1	A	99	ASN	CA-CB-CG	-6.51	106.09	112.60
1	A	1	PCA	O-C-N	-6.50	112.60	123.00
1	A	213	HIS	CA-CB-CG	6.48	120.28	113.80
1	A	96	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	B	208	THR	OG1-CB-CG2	6.43	122.16	109.30
1	B	149	MET	CA-C-N	6.35	126.57	119.90
1	B	149	MET	C-N-CA	6.35	126.57	119.90
1	A	192	GLY	N-CA-C	-6.34	103.49	112.37
1	B	213	HIS	O-C-N	-6.33	115.56	121.32
1	B	122	LEU	CA-C-O	-6.32	111.94	119.15
1	B	210	ILE	CA-C-O	-6.31	113.28	120.67
1	A	255	GLY	N-CA-C	6.29	119.76	111.70
1	B	208	THR	CB-CA-C	-6.28	96.25	109.38
1	A	332	MET	CA-C-N	6.28	126.95	119.98
1	A	332	MET	C-N-CA	6.28	126.95	119.98
1	A	378	VAL	N-CA-C	-6.27	106.42	111.81
1	B	17	ARG	NE-CZ-NH2	-6.25	113.58	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	GLY	O-C-N	-6.25	115.62	122.24
1	A	305	PRO	N-CA-CB	6.20	108.74	103.35
1	B	28	THR	CA-CB-OG1	-6.16	100.36	109.60
1	A	373	LYS	CA-C-O	-6.14	112.91	119.97
1	B	27	GLN	OE1-CD-NE2	6.14	128.74	122.60
1	B	390	ARG	CA-C-O	6.13	127.13	120.32
1	A	100	ASN	OD1-CG-ND2	6.12	128.72	122.60
1	A	247	ASN	OD1-CG-ND2	6.12	128.72	122.60
1	A	204	ASN	OD1-CG-ND2	6.07	128.67	122.60
1	A	196	ASN	CA-CB-CG	-6.06	106.54	112.60
1	A	245	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	B	135	LYS	CA-C-N	-6.02	114.56	122.74
1	B	135	LYS	C-N-CA	-6.02	114.56	122.74
1	A	282	GLU	CB-CG-CD	5.98	122.77	112.60
1	B	194	CYS	N-CA-C	5.96	119.42	109.95
1	B	208	THR	CA-CB-OG1	5.96	118.53	109.60
1	A	179	THR	CA-C-N	5.95	125.82	119.28
1	A	179	THR	C-N-CA	5.95	125.82	119.28
1	B	245	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	168	GLY	O-C-N	-5.82	115.53	122.34
1	B	203	ALA	N-CA-C	5.78	117.03	108.60
1	A	21	ALA	N-CA-C	5.76	117.56	111.28
1	A	121	HIS	CA-CB-CG	-5.76	108.04	113.80
1	B	268	VAL	O-C-N	-5.74	116.38	123.10
1	B	122	LEU	O-C-N	5.71	129.91	122.42
1	B	106	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	A	208	THR	CB-CA-C	-5.66	97.56	109.38
1	A	390	ARG	CB-CG-CD	5.63	124.26	111.30
1	A	391	ILE	CA-C-O	-5.56	114.55	120.39
1	B	102	LEU	CA-C-O	-5.53	114.04	120.62
1	B	11	PRO	CA-C-N	5.52	131.52	122.07
1	B	11	PRO	C-N-CA	5.52	131.52	122.07
1	B	215	CYS	N-CA-C	-5.51	100.69	109.23
1	A	378	VAL	CB-CA-C	-5.51	105.21	111.55
1	B	27	GLN	CB-CG-CD	-5.51	103.24	112.60
1	A	103	VAL	N-CA-C	-5.48	107.48	112.96
1	B	229	GLY	CA-C-N	5.42	129.27	120.60
1	B	229	GLY	C-N-CA	5.42	129.27	120.60
1	A	27	GLN	CB-CG-CD	-5.42	103.39	112.60
1	B	244	ASN	CA-C-O	-5.42	114.81	120.55
1	B	379	GLN	OE1-CD-NE2	5.42	128.02	122.60
1	B	150	PRO	N-CA-CB	5.41	108.12	103.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	PRO	N-CA-CB	5.41	108.33	103.19
1	A	211	ALA	CA-C-N	5.37	125.13	119.76
1	A	211	ALA	C-N-CA	5.37	125.13	119.76
1	B	74	GLY	N-CA-C	-5.34	106.45	112.33
1	B	12	LYS	CA-CB-CG	5.34	124.78	114.10
1	A	196	ASN	CA-C-O	-5.33	115.69	121.44
1	A	213	HIS	CA-C-N	5.31	125.21	119.85
1	A	213	HIS	C-N-CA	5.31	125.21	119.85
1	B	109	LEU	CA-C-O	5.30	126.03	120.36
1	A	280	LEU	CA-C-O	-5.29	114.72	120.81
1	A	371	ASP	CA-C-N	5.27	126.43	119.84
1	A	371	ASP	C-N-CA	5.27	126.43	119.84
1	B	213	HIS	CA-C-N	5.25	125.15	119.85
1	B	213	HIS	C-N-CA	5.25	125.15	119.85
1	A	149	MET	CA-C-N	5.24	125.48	119.83
1	A	149	MET	C-N-CA	5.24	125.48	119.83
1	A	244	ASN	CA-C-O	-5.22	115.02	120.55
1	A	71	ILE	CB-CG1-CD1	5.21	124.73	113.80
1	B	192	GLY	N-CA-C	-5.21	105.08	112.37
1	A	208	THR	N-CA-CB	5.20	120.84	111.37
1	A	239	CYS	O-C-N	-5.19	116.88	123.05
1	B	254	ARG	CD-NE-CZ	5.18	131.66	124.40
1	A	172	CYS	CA-C-O	-5.18	115.69	121.23
1	B	388	ASN	N-CA-CB	-5.17	104.04	111.70
1	A	60	CYS	CA-C-N	5.16	124.66	119.19
1	A	60	CYS	C-N-CA	5.16	124.66	119.19
1	B	277	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	239	CYS	CA-C-N	5.15	126.91	121.45
1	A	239	CYS	C-N-CA	5.15	126.91	121.45
1	A	194	CYS	N-CA-C	5.13	118.11	109.95
1	B	289	GLN	OE1-CD-NE2	5.13	127.73	122.60
1	B	212	PRO	N-CA-CB	5.12	108.06	103.19
1	B	38	HIS	N-CA-C	-5.11	105.89	111.82
1	A	312	ASP	CA-CB-CG	-5.09	107.51	112.60
1	B	119	MET	O-C-N	-5.09	116.82	122.93
1	A	187	ASN	CA-C-N	5.09	127.70	120.53
1	A	187	ASN	C-N-CA	5.09	127.70	120.53
1	B	286	HIS	CA-CB-CG	5.08	118.88	113.80
1	A	8	GLU	CA-C-O	-5.08	114.80	120.54
1	A	388	ASN	N-CA-CB	-5.06	104.22	111.70
1	A	386	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	93	ARG	NE-CZ-NH2	5.04	123.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	GLY	CA-C-O	5.04	126.88	121.64
1	B	379	GLN	O-C-N	-5.04	117.26	121.44
1	A	273	VAL	N-CA-C	5.03	115.59	109.30
1	B	304	PRO	CA-C-N	5.02	124.95	119.78
1	B	304	PRO	C-N-CA	5.02	124.95	119.78
1	A	242	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	286	HIS	N-CA-CB	5.01	119.48	111.56
1	B	59	ALA	CA-C-N	-5.01	117.09	123.15
1	B	59	ALA	C-N-CA	-5.01	117.09	123.15
1	B	275	ASN	OD1-CG-ND2	-5.01	117.59	122.60

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	54	0
1	B	3035	0	2919	53	0
2	A	28	0	26	2	0
2	B	28	0	26	1	0
3	A	227	0	0	8	0
3	B	195	0	0	6	0
All	All	6548	0	5890	106	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 (106) 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:H	1:B:276:LYS:NZ	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:A:276:LYS:H	1:A:276:LYS:HZ3	1.44	0.64
1:B:113:ASN:ND2	1:B:115:LYS:H	1.97	0.62
1:A:256:LYS:HD2	3:A:956:HOH:O	2.00	0.61
1:A:276:LYS:H	1:A:276:LYS:NZ	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:HZ2	1:A:5:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:290:ASP:O	1:A:291:ASN:HB2	2.13	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:HE21	1:B:96:GLN:HA	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
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:103:VAL:O	1:A:104:SER:C	2.58	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:B:103:VAL:O	1:B:104:SER:C	2.61	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:B:298:VAL:O	1:B:299:VAL:C	2.60	0.43
1:A:42:GLN:HE22	2:A:800:NAG:C6	2.32	0.42
1:A:259:LYS:NZ	3:A:988:HOH:O	2.32	0.42
1:A:140:MET:O	1:A:204:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TRP:CE3	1:B:208:THR:HG21	2.55	0.42
1:B:276:LYS:N	1:B:276:LYS:HD3	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:A:175:GLN:O	1:A:176:CYS:C	2.61	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:220:LEU:C	1:B:220:LEU:HD23	2.45	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:B:55:PRO:O	1:B:56:ASN:C	2.63	0.41
1:A:5:LYS:H	1:A:5:LYS:NZ	2.15	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:B:5:LYS:H	1:B:5:LYS:HZ2	1.67	0.41
1:B:61:PRO:HD2	1:B:65:SER:HB2	2.01	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
1:A:33:ALA:O	1:A:34:ASP:C	2.65	0.40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	796/822 (97%)	768 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	325/333 (98%)	304 (94%)	21 (6%)	15	22
1	B	325/333 (98%)	304 (94%)	21 (6%)	15	22
All	All	650/666 (98%)	608 (94%)	42 (6%)	15	22

All (42) 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	208	THR
1	A	224	THR
1	A	256	LYS
1	A	257	GLN
1	A	276	LYS
1	A	277	GLN
1	A	282	GLU
1	A	292	LYS
1	A	346	VAL
1	A	350	GLU
1	A	390	ARG

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Mol	Chain	Res	Type
1	A	400	VAL
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	101	GLN
1	B	102	LEU
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	313	LYS
1	B	346	VAL
1	B	350	GLU
1	B	373	LYS
1	B	390	ARG
1	B	400	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) 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	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

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Mol	Chain	Res	Type
1	B	113	ASN
1	B	175	GLN
1	B	187	ASN
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	7,8,9	1.36	1 (14%)	9,10,12	1.48	1 (11%)
1	PCA	B	1	1	7,8,9	1.32	2 (28%)	9,10,12	1.65	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	2.59	1.29	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	O-C	2.12	1.28	1.20
1	B	1	PCA	CG-CD	2.04	1.55	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	-3.76	120.00	126.72
1	A	1	PCA	OE-CD-CG	-3.28	120.87	126.72
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 oligosaccharides 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	1.29	1 (7%)	17,19,21	1.69	4 (23%)
2	NAG	B	800	1	14,14,15	1.30	1 (7%)	17,19,21	2.52	10 (58%)
2	NAG	A	801	1	14,14,15	1.14	1 (7%)	17,19,21	2.21	6 (35%)
2	NAG	B	801	1	14,14,15	1.28	1 (7%)	17,19,21	1.41	3 (17%)

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	B	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	801	1	-	2/6/23/26	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	-3.95	1.14	1.23
2	B	800	NAG	O7-C7	-3.73	1.14	1.23
2	A	801	NAG	O7-C7	-3.54	1.15	1.23
2	B	801	NAG	O7-C7	-3.46	1.15	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAG	C1-O5-C5	5.53	119.59	112.19
2	B	800	NAG	O4-C4-C3	4.27	120.45	110.38
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	B	800	NAG	O5-C1-C2	-3.90	105.26	111.29
2	A	800	NAG	C2-N2-C7	-3.67	117.99	122.90
2	A	801	NAG	C3-C4-C5	-3.24	104.36	110.23
2	B	801	NAG	C1-O5-C5	3.17	116.44	112.19
2	B	800	NAG	C6-C5-C4	-2.97	105.73	113.02
2	A	800	NAG	O5-C1-C2	-2.96	106.72	111.29
2	B	800	NAG	O4-C4-C5	-2.86	102.28	109.32
2	B	800	NAG	O5-C5-C6	2.85	113.22	107.66
2	A	800	NAG	C6-C5-C4	-2.62	106.58	113.02
2	A	800	NAG	O3-C3-C4	-2.48	104.52	110.38
2	B	801	NAG	C4-C3-C2	-2.42	107.47	111.02
2	A	801	NAG	O7-C7-C8	2.34	126.23	122.05
2	A	801	NAG	O3-C3-C2	2.30	114.19	109.40
2	B	800	NAG	C2-N2-C7	-2.26	119.87	122.90
2	B	800	NAG	O7-C7-C8	2.26	126.08	122.05
2	A	801	NAG	O7-C7-N2	-2.24	118.03	121.98
2	B	801	NAG	O5-C1-C2	-2.23	107.83	111.29
2	B	800	NAG	O5-C5-C4	-2.23	105.39	110.83
2	B	800	NAG	C3-C4-C5	-2.13	106.38	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAG	O5-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6

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.