



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:34 AM UTC

PDB ID : 4OVW / pdb_00004ovw
Title : ENDOGLUCANASE I COMPLEXED WITH EPOXYBUTYL CELLULOSE
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

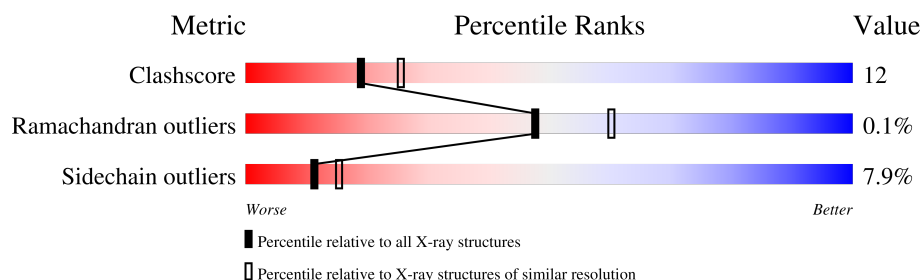
1 Overall quality at a glance

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	 64% 24% 8% . .
1	B	411	 62% 27% 6% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6833 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.

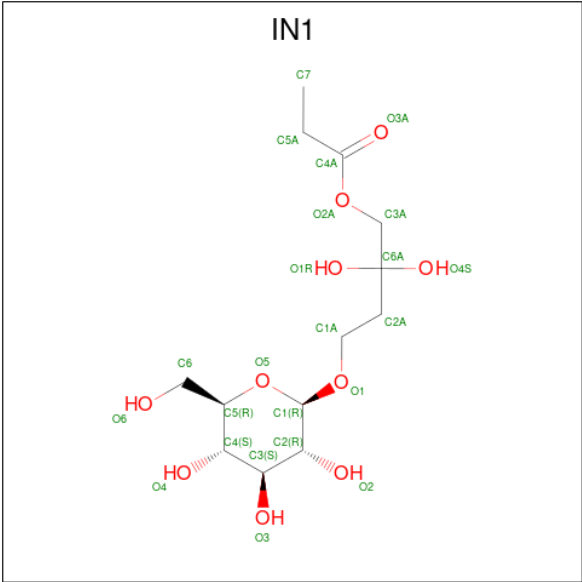
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3030	1875	536	590	29			
1	B	400	Total	C	N	O	S	0	0	0
			3030	1875	536	590	29			

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 4-(beta-D-glucopyranosyloxy)-2,2-dihydroxybutyl propanoate (CCD ID: IN1) (formula: $C_{13}H_{24}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	13	10		
3	B	1	Total	C	O	0	0
			23	13	10		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	356	Total	O	0	0
			356	356		
4	B	343	Total	O	0	0
			343	343		

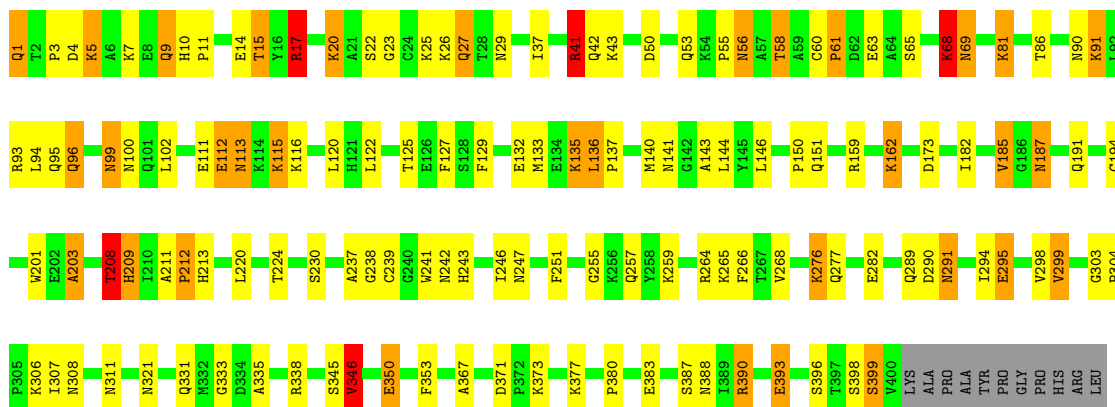
3 Residue-property plots

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.

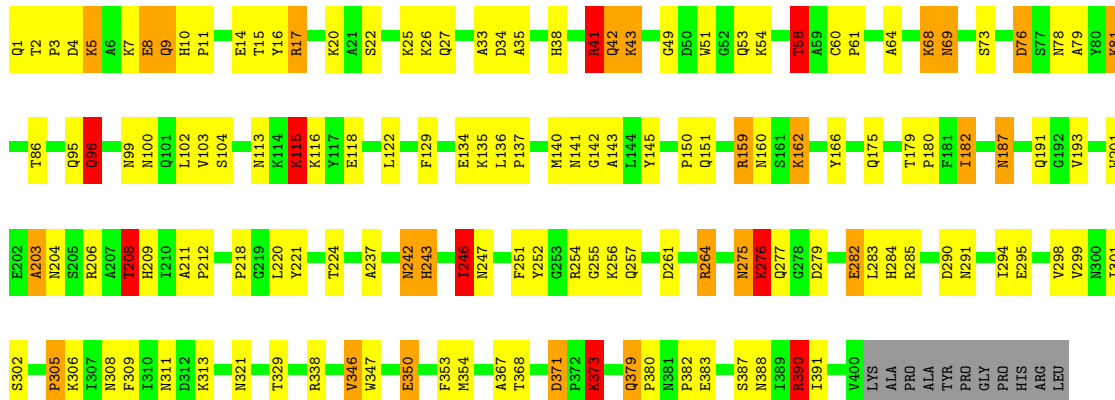
• Molecule 1: ENDOGLUCANASE I

Chain A: 



• Molecule 1: ENDOGLUCANASE I

Chain B: 



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	65.94Å 82.62Å 73.16Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6833	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: IN1, NAG, PCA

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	1.00	0/3084	2.18	127/4166 (3.0%)
1	B	1.03	2/3084 (0.1%)	2.25	121/4166 (2.9%)
All	All	1.02	2/6168 (0.0%)	2.21	248/8332 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PCA	C-N	5.51	1.41	1.33
1	B	141	ASN	C-N	-5.05	1.31	1.33

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ARG	CD-NE-CZ	29.29	165.41	124.40
1	A	159	ARG	CD-NE-CZ	24.71	158.99	124.40
1	B	9	GLN	OE1-CD-NE2	-16.86	105.74	122.60
1	B	264	ARG	NE-CZ-NH2	13.83	131.64	119.20
1	B	390	ARG	CD-NE-CZ	12.77	142.28	124.40
1	B	308	ASN	OD1-CG-ND2	-11.66	110.94	122.60
1	B	279	ASP	CA-CB-CG	11.44	124.04	112.60
1	B	1	PCA	CA-C-N	11.24	141.94	121.70
1	B	1	PCA	C-N-CA	11.24	141.94	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	ARG	CD-NE-CZ	11.15	140.02	124.40
1	B	242	ASN	CA-CB-CG	10.34	122.94	112.60
1	B	282	GLU	CB-CG-CD	10.24	130.00	112.60
1	B	9	GLN	CG-CD-OE1	10.19	141.18	120.80
1	A	95	GLN	OE1-CD-NE2	-10.02	112.58	122.60
1	A	187	ASN	OD1-CG-ND2	-9.89	112.71	122.60
1	B	209	HIS	CA-CB-CG	9.64	123.44	113.80
1	B	141	ASN	OD1-CG-ND2	-9.55	113.05	122.60
1	A	390	ARG	CD-NE-CZ	9.38	137.53	124.40
1	A	9	GLN	OE1-CD-NE2	-9.35	113.25	122.60
1	A	151	GLN	OE1-CD-NE2	-9.25	113.35	122.60
1	A	41	ARG	CA-C-O	-9.24	110.64	120.99
1	A	1	PCA	O-C-N	-9.18	108.31	123.00
1	A	68	LYS	CG-CD-CE	9.03	132.07	111.30
1	A	68	LYS	CB-CG-CD	8.66	131.21	111.30
1	B	346	VAL	CB-CA-C	-8.42	97.53	110.50
1	A	243	HIS	CA-C-O	-8.23	111.70	120.92
1	B	246	ILE	CA-C-O	8.22	129.30	120.26
1	A	346	VAL	CB-CA-C	-8.21	98.34	110.33
1	A	113	ASN	CB-CG-ND2	8.21	128.71	116.40
1	B	159	ARG	NE-CZ-NH1	8.11	129.61	121.50
1	A	264	ARG	CD-NE-CZ	8.07	135.69	124.40
1	A	111	GLU	CA-C-N	8.05	131.06	120.28
1	A	111	GLU	C-N-CA	8.05	131.06	120.28
1	B	41	ARG	N-CA-CB	-8.01	98.28	111.66
1	A	159	ARG	NE-CZ-NH2	7.96	126.37	119.20
1	A	282	GLU	CB-CG-CD	7.96	126.14	112.60
1	A	14	GLU	CA-C-O	-7.90	111.68	120.69
1	A	1	PCA	CA-C-N	7.69	135.55	121.70
1	A	1	PCA	C-N-CA	7.69	135.55	121.70
1	A	93	ARG	CD-NE-CZ	7.65	135.11	124.40
1	B	264	ARG	NE-CZ-NH1	-7.63	113.87	121.50
1	B	353	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	159	ARG	NE-CZ-NH1	-7.54	113.96	121.50
1	B	96	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	A	353	PHE	CA-CB-CG	7.48	121.28	113.80
1	B	95	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	A	151	GLN	CG-CD-NE2	7.41	127.51	116.40
1	B	134	GLU	N-CA-C	7.41	120.29	111.33
1	A	93	ARG	NE-CZ-NH2	7.41	125.87	119.20
1	A	41	ARG	O-C-N	7.35	131.63	123.33
1	B	308	ASN	CA-CB-CG	7.33	119.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	TRP	CA-C-O	-7.33	112.98	120.96
1	B	382	PRO	N-CA-CB	7.29	109.83	103.27
1	A	17	ARG	CD-NE-CZ	7.26	134.57	124.40
1	A	346	VAL	N-CA-CB	7.21	122.05	111.52
1	B	301	ILE	CA-C-O	-7.17	114.14	121.67
1	A	136	LEU	CA-C-O	7.13	126.32	119.62
1	A	41	ARG	N-CA-C	7.11	120.14	108.99
1	A	246	ILE	CA-C-O	7.09	127.23	120.14
1	B	261	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	329	THR	N-CA-C	7.01	119.82	111.33
1	B	53	GLN	CA-CB-CG	7.01	128.12	114.10
1	B	1	PCA	O-C-N	-6.97	111.85	123.00
1	B	43	LYS	O-C-N	-6.93	113.14	122.43
1	A	367	ALA	CA-C-O	-6.88	110.92	119.38
1	B	69	ASN	N-CA-C	6.82	121.60	113.28
1	A	10	HIS	CA-CB-CG	6.82	120.62	113.80
1	A	211	ALA	CA-C-N	6.74	126.98	119.90
1	A	211	ALA	C-N-CA	6.74	126.98	119.90
1	B	17	ARG	O-C-N	-6.71	115.31	123.30
1	A	100	ASN	CA-CB-CG	-6.68	105.92	112.60
1	B	58	THR	CA-CB-CG2	6.66	121.82	110.50
1	B	346	VAL	N-CA-CB	6.64	122.33	111.44
1	A	9	GLN	CG-CD-OE1	6.63	134.06	120.80
1	B	208	THR	CA-CB-OG1	6.62	119.53	109.60
1	A	241	TRP	CA-C-O	6.61	127.47	120.33
1	A	95	GLN	CG-CD-NE2	6.58	126.27	116.40
1	A	27	GLN	N-CA-CB	6.49	122.49	111.66
1	A	295	GLU	CA-C-O	-6.46	114.04	121.47
1	A	338	ARG	NE-CZ-NH1	-6.46	115.04	121.50
1	B	99	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	B	22	SER	N-CA-C	6.42	120.04	112.72
1	A	100	ASN	OD1-CG-ND2	6.42	129.02	122.60
1	A	371	ASP	CA-C-N	6.42	126.64	119.32
1	A	371	ASP	C-N-CA	6.42	126.64	119.32
1	A	37	ILE	CA-C-O	6.36	127.33	120.47
1	B	203	ALA	N-CA-CB	-6.36	101.67	111.46
1	A	127	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	203	ALA	N-CA-C	6.33	118.48	108.79
1	B	100	ASN	OD1-CG-ND2	6.31	128.91	122.60
1	A	112	GLU	CB-CG-CD	6.31	123.33	112.60
1	B	142	GLY	O-C-N	-6.28	119.39	123.35
1	B	58	THR	N-CA-CB	6.27	119.54	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	THR	OG1-CB-CG2	6.26	121.83	109.30
1	A	26	LYS	CA-C-O	-6.26	114.73	121.56
1	A	56	ASN	OD1-CG-ND2	6.25	128.85	122.60
1	A	335	ALA	O-C-N	-6.22	115.53	122.12
1	B	42	GLN	O-C-N	-6.21	115.42	122.68
1	A	266	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	100	ASN	CB-CG-ND2	-6.20	107.10	116.40
1	A	237	ALA	CA-C-O	-6.20	112.84	119.97
1	A	143	ALA	N-CA-C	6.20	119.50	109.40
1	B	252	TYR	CA-C-O	-6.17	113.70	120.24
1	B	204	ASN	CA-C-O	-6.15	114.06	121.32
1	A	291	ASN	N-CA-C	6.13	120.71	113.23
1	A	247	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	B	143	ALA	N-CA-C	6.10	119.43	109.24
1	A	307	ILE	CA-C-N	6.10	132.37	122.67
1	A	307	ILE	C-N-CA	6.10	132.37	122.67
1	A	53	GLN	CA-CB-CG	6.08	126.26	114.10
1	A	10	HIS	CA-C-O	6.07	125.87	119.80
1	A	230	SER	CA-CB-OG	-6.03	99.04	111.10
1	B	129	PHE	CA-C-O	-6.03	114.26	120.89
1	A	255	GLY	N-CA-C	6.02	120.60	112.17
1	B	211	ALA	CA-C-N	6.02	125.78	119.76
1	B	211	ALA	C-N-CA	6.02	125.78	119.76
1	B	8	GLU	O-C-N	-6.01	116.18	123.16
1	B	208	THR	CB-CA-C	-5.99	98.04	109.66
1	B	206	ARG	CD-NE-CZ	5.97	132.76	124.40
1	B	53	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	A	294	ILE	N-CA-CB	5.95	119.37	111.64
1	A	22	SER	N-CA-C	5.92	119.81	112.59
1	A	291	ASN	CA-CB-CG	-5.91	106.69	112.60
1	B	367	ALA	CA-C-O	-5.91	111.98	119.31
1	B	151	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	209	HIS	CA-CB-CG	5.88	119.68	113.80
1	B	237	ALA	CA-C-O	-5.81	113.29	119.97
1	B	276	LYS	CA-C-O	-5.81	112.23	119.38
1	B	206	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	B	251	PHE	CA-CB-CG	-5.81	107.99	113.80
1	B	150	PRO	N-CA-CB	5.80	108.73	103.34
1	A	289	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	11	PRO	O-C-N	-5.76	116.07	123.03
1	A	371	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	159	ARG	CA-CB-CG	5.75	125.59	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	PRO	N-CA-CB	5.74	108.42	103.31
1	B	79	ALA	CA-C-O	-5.73	114.34	120.42
1	B	311	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	132	GLU	CA-C-N	5.70	131.32	122.49
1	A	132	GLU	C-N-CA	5.70	131.32	122.49
1	B	41	ARG	N-CA-C	5.70	117.73	109.07
1	A	393	GLU	O-C-N	5.70	129.84	122.89
1	B	212	PRO	N-CA-CB	5.68	108.62	103.34
1	A	295	GLU	CA-CB-CG	-5.67	102.75	114.10
1	B	118	GLU	CA-C-O	-5.67	114.85	120.98
1	B	255	GLY	N-CA-C	5.67	118.96	111.70
1	B	180	PRO	N-CA-CB	5.64	109.48	103.39
1	A	308	ASN	CA-CB-CG	5.64	118.24	112.60
1	A	113	ASN	CB-CG-OD1	-5.64	109.53	120.80
1	B	243	HIS	CA-C-O	-5.63	114.88	120.90
1	A	396	SER	N-CA-C	5.63	120.30	113.38
1	A	213	HIS	CA-C-N	5.62	125.60	120.03
1	A	213	HIS	C-N-CA	5.62	125.60	120.03
1	A	173	ASP	N-CA-CB	5.59	121.34	111.49
1	A	42	GLN	O-C-N	-5.59	115.78	122.65
1	B	60	CYS	CA-C-N	5.58	125.20	119.56
1	B	60	CYS	C-N-CA	5.58	125.20	119.56
1	A	23	GLY	O-C-N	-5.58	117.60	122.90
1	A	212	PRO	O-C-N	-5.57	116.86	123.10
1	B	285	ARG	O-C-N	-5.57	116.59	123.33
1	A	350	GLU	CB-CG-CD	5.57	122.06	112.60
1	A	321	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	B	159	ARG	NH1-CZ-NH2	-5.55	112.09	119.30
1	B	321	ASN	N-CA-C	5.54	118.09	111.71
1	A	185	VAL	O-C-N	-5.54	117.07	123.00
1	B	73	SER	CA-C-N	5.53	125.23	119.92
1	B	73	SER	C-N-CA	5.53	125.23	119.92
1	A	53	GLN	N-CA-C	5.53	117.58	109.24
1	A	331	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	B	383	GLU	CA-C-O	-5.51	115.56	121.45
1	A	41	ARG	CB-CA-C	-5.51	98.21	109.94
1	A	345	SER	CA-C-N	5.49	130.62	122.99
1	A	345	SER	C-N-CA	5.49	130.62	122.99
1	A	3	PRO	N-CA-CB	5.49	108.19	103.31
1	B	305	PRO	N-CA-CB	5.48	108.12	103.35
1	B	294	ILE	N-CA-CB	5.48	119.11	112.10
1	A	251	PHE	CA-CB-CG	-5.47	108.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	CYS	CA-C-N	5.45	125.06	119.56
1	A	60	CYS	C-N-CA	5.45	125.06	119.56
1	B	95	GLN	O-C-N	-5.45	116.29	123.21
1	A	346	VAL	CA-CB-CG2	5.45	119.66	110.40
1	A	69	ASN	N-CA-CB	-5.45	101.26	110.41
1	B	76	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	17	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	A	15	THR	O-C-N	-5.40	115.15	122.81
1	A	60	CYS	O-C-N	-5.39	116.54	121.34
1	A	135	LYS	N-CA-C	5.38	118.67	112.97
1	B	49	GLY	CA-C-O	-5.38	116.92	121.66
1	A	393	GLU	CB-CG-CD	5.37	121.74	112.60
1	A	141	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	299	VAL	CA-CB-CG1	5.37	119.52	110.40
1	B	371	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	134	GLU	CA-CB-CG	-5.36	103.39	114.10
1	B	309	PHE	N-CA-CB	-5.35	103.11	111.56
1	B	346	VAL	CG1-CB-CG2	5.35	122.57	110.80
1	A	99	ASN	CA-C-N	5.33	131.41	123.05
1	A	99	ASN	C-N-CA	5.33	131.41	123.05
1	A	242	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	379	GLN	O-C-N	5.30	124.45	121.27
1	B	203	ALA	N-CA-C	5.30	116.34	108.60
1	B	254	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	B	373	LYS	CG-CD-CE	5.30	123.48	111.30
1	B	160	ASN	CA-CB-CG	-5.28	107.32	112.60
1	A	238	GLY	O-C-N	-5.27	117.07	122.60
1	A	194	CYS	N-CA-C	5.27	118.33	109.95
1	B	61	PRO	N-CA-CB	5.27	108.57	103.51
1	B	15	THR	O-C-N	-5.27	115.47	122.74
1	B	17	ARG	CD-NE-CZ	5.26	131.76	124.40
1	B	99	ASN	O-C-N	-5.25	115.38	122.41
1	B	175	GLN	CA-C-O	5.23	125.41	119.18
1	A	282	GLU	CG-CD-OE1	5.23	130.42	118.40
1	B	11	PRO	N-CA-CB	5.21	107.96	103.27
1	B	247	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	268	VAL	O-C-N	-5.20	117.02	123.10
1	B	122	LEU	CA-C-O	-5.20	113.19	119.27
1	A	303	GLY	CA-C-N	5.20	125.73	120.38
1	A	303	GLY	C-N-CA	5.20	125.73	120.38
1	B	387	SER	N-CA-C	5.20	115.91	108.74
1	A	311	ASN	OD1-CG-ND2	5.19	127.79	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	PRO	N-CA-CB	5.17	107.91	103.36
1	A	291	ASN	CB-CA-C	-5.16	102.65	111.26
1	B	145	TYR	CA-C-N	-5.12	114.64	122.62
1	B	145	TYR	C-N-CA	-5.12	114.64	122.62
1	A	282	GLU	CB-CA-C	5.11	120.83	109.94
1	A	61	PRO	N-CA-C	-5.10	107.49	113.86
1	B	211	ALA	CA-C-O	5.09	127.14	120.16
1	B	302	SER	CB-CA-C	-5.09	100.09	109.46
1	A	50	ASP	CA-CB-CG	-5.08	107.52	112.60
1	B	115	LYS	CA-C-O	5.08	124.94	119.15
1	A	304	PRO	N-CA-CB	5.07	108.00	103.08
1	B	187	ASN	CA-C-O	5.07	129.23	122.44
1	B	275	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	B	42	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	135	LYS	CA-CB-CG	-5.06	103.98	114.10
1	B	179	THR	CA-C-N	5.06	124.85	119.28
1	B	179	THR	C-N-CA	5.06	124.85	119.28
1	B	338	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	B	166	TYR	O-C-N	-5.06	116.76	122.12
1	A	208	THR	CB-CA-C	-5.05	99.43	109.79
1	A	333	GLY	O-C-N	5.05	127.78	122.28
1	B	136	LEU	CA-C-N	5.05	126.15	119.84
1	B	136	LEU	C-N-CA	5.05	126.15	119.84
1	A	380	PRO	N-CA-CB	5.03	109.00	103.26
1	B	53	GLN	CB-CG-CD	5.03	121.14	112.60
1	A	63	GLU	CA-C-O	-5.01	115.11	120.42
1	B	368	THR	CA-CB-CG2	5.01	119.01	110.50
1	A	265	LYS	O-C-N	-5.00	116.41	122.82
1	B	218	PRO	CA-C-O	-5.00	115.56	121.67

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	3030	0	2915	59	0
1	B	3030	0	2915	83	0
2	A	14	0	12	0	0
2	B	14	0	13	1	0
3	A	23	0	4	0	0
3	B	23	0	4	0	0
4	A	356	0	0	20	0
4	B	343	0	0	28	0
All	All	6833	0	5863	142	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 12.

All (142) 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:182:ILE:HD11	1:B:220:LEU:HD21	1.50	0.91
1:B:5:LYS:H	1:B:5:LYS:HZ2	1.19	0.89
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.57	0.85
1:B:113:ASN:HD22	1:B:115:LYS:H	1.27	0.83
1:B:350:GLU:HG3	4:B:975:HOH:O	1.80	0.80
1:A:7:LYS:HD2	1:A:9:GLN:HE21	1.49	0.78
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.19	0.78
1:A:257:GLN:HB3	4:A:989:HOH:O	1.85	0.76
1:A:350:GLU:HG3	4:A:1084:HOH:O	1.86	0.76
1:B:2:THR:HA	4:B:1058:HOH:O	1.87	0.74
1:B:81:LYS:HG2	4:B:1059:HOH:O	1.86	0.73
1:A:81:LYS:HD3	1:A:86:THR:HG22	1.70	0.73
1:A:120:LEU:HD12	1:A:146:LEU:HD21	1.69	0.73
1:A:4:ASP:HB2	1:A:5:LYS:HE3	1.71	0.72
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.25	0.71
1:B:182:ILE:HD11	1:B:220:LEU:CD2	2.21	0.71
1:B:182:ILE:HD13	4:B:955:HOH:O	1.92	0.69
1:B:81:LYS:HD3	1:B:86:THR:HG22	1.74	0.69
1:B:4:ASP:HB2	1:B:5:LYS:NZ	2.07	0.69
1:B:5:LYS:H	1:B:5:LYS:NZ	1.91	0.69
1:B:182:ILE:CD1	4:B:955:HOH:O	2.41	0.69
1:B:295:GLU:HG3	4:B:817:HOH:O	1.92	0.68
1:A:113:ASN:HD22	1:A:115:LYS:H	1.40	0.67
1:B:388:ASN:HD21	1:B:390:ARG:HH11	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LYS:HZ2	1:B:5:LYS:N	1.93	0.66
1:B:162:LYS:HD3	4:B:1087:HOH:O	1.95	0.66
1:B:257:GLN:HB3	4:B:1072:HOH:O	1.96	0.66
1:A:7:LYS:HD2	1:A:9:GLN:NE2	2.10	0.65
1:A:398:SER:O	1:A:399:SER:HB3	1.96	0.65
1:B:162:LYS:HB2	4:B:1058:HOH:O	1.95	0.65
1:B:187:ASN:HD21	1:B:191:GLN:H	1.46	0.64
1:A:99:ASN:HB3	4:A:956:HOH:O	1.98	0.63
1:B:26:LYS:HE2	4:B:1022:HOH:O	1.97	0.63
1:A:220:LEU:C	1:A:220:LEU:HD23	2.24	0.63
1:A:116:LYS:NZ	4:A:1142:HOH:O	2.32	0.62
1:A:68:LYS:HD2	4:A:991:HOH:O	2.00	0.62
1:A:135:LYS:HE2	1:A:383:GLU:HG2	1.82	0.62
1:B:391:ILE:HG22	4:B:1112:HOH:O	2.00	0.62
1:B:298:VAL:HG12	1:B:299:VAL:O	2.00	0.61
1:B:78:ASN:HB3	4:B:1099:HOH:O	1.99	0.61
1:A:187:ASN:HD21	1:A:191:GLN:H	1.49	0.60
1:B:4:ASP:HB2	1:B:5:LYS:CE	2.32	0.59
1:A:298:VAL:HG12	1:A:299:VAL:O	2.03	0.58
1:A:295:GLU:HG3	4:A:932:HOH:O	2.02	0.58
1:A:96:GLN:HE21	1:A:96:GLN:HA	1.69	0.58
1:B:4:ASP:HB2	1:B:5:LYS:HE3	1.85	0.57
1:B:182:ILE:HD12	1:B:193:VAL:HG13	1.86	0.57
1:A:58:THR:HG22	4:A:959:HOH:O	2.05	0.56
1:B:182:ILE:HG12	4:B:955:HOH:O	2.05	0.56
1:A:41:ARG:NH1	4:A:945:HOH:O	2.39	0.56
1:B:8:GLU:HG2	1:B:10:HIS:CE1	2.40	0.56
1:A:137:PRO:HD2	1:A:140:MET:HG3	1.90	0.54
1:A:81:LYS:HD3	1:A:86:THR:CG2	2.37	0.54
1:B:182:ILE:CG1	4:B:955:HOH:O	2.56	0.54
1:B:290:ASP:O	1:B:291:ASN:HB2	2.07	0.53
1:B:182:ILE:CD1	1:B:220:LEU:HD21	2.30	0.53
1:A:290:ASP:O	1:A:291:ASN:HB2	2.09	0.53
1:B:305:PRO:HG3	1:B:313:LYS:HD3	1.91	0.53
1:B:162:LYS:HG3	4:B:1058:HOH:O	2.09	0.52
1:B:203:ALA:HB2	1:B:208:THR:HG23	1.91	0.52
1:B:264:ARG:NH1	1:B:290:ASP:OD1	2.39	0.52
1:B:276:LYS:H	1:B:276:LYS:NZ	2.08	0.52
1:A:277:GLN:HG3	4:A:826:HOH:O	2.10	0.51
1:B:7:LYS:HG3	1:B:9:GLN:HE21	1.76	0.51
1:B:64:ALA:O	1:B:68:LYS:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TRP:CH2	1:A:208:THR:HG21	2.46	0.50
1:A:7:LYS:HE3	4:A:912:HOH:O	2.12	0.50
1:A:15:THR:OG1	1:A:29:ASN:ND2	2.44	0.50
1:A:135:LYS:HE2	1:A:383:GLU:CG	2.41	0.50
1:B:54:LYS:HE3	4:B:1031:HOH:O	2.12	0.50
1:B:81:LYS:HD3	1:B:86:THR:CG2	2.42	0.50
1:B:113:ASN:ND2	1:B:115:LYS:H	2.05	0.49
1:A:5:LYS:HD3	4:A:1085:HOH:O	2.12	0.49
1:A:61:PRO:HD2	1:A:65:SER:HB2	1.95	0.49
1:A:162:LYS:HE2	4:A:1011:HOH:O	2.12	0.49
1:B:81:LYS:CD	1:B:86:THR:HG22	2.42	0.49
1:B:282:GLU:HG3	1:B:284:HIS:CE1	2.48	0.48
1:B:16:TYR:HB2	1:B:390:ARG:HB3	1.96	0.48
1:B:41:ARG:NH2	4:B:956:HOH:O	2.45	0.48
1:A:133:MET:CE	1:A:136:LEU:HD12	2.43	0.48
1:B:182:ILE:CD1	1:B:193:VAL:HG13	2.43	0.48
1:A:276:LYS:N	1:A:276:LYS:HD3	2.29	0.48
1:A:112:GLU:HG2	4:A:1054:HOH:O	2.14	0.47
1:B:371:ASP:OD2	1:B:373:LYS:NZ	2.34	0.47
1:B:5:LYS:H	1:B:5:LYS:CE	2.27	0.46
1:B:220:LEU:C	1:B:220:LEU:HD23	2.40	0.46
1:B:283:LEU:HD12	1:B:283:LEU:N	2.30	0.46
1:B:291:ASN:HB3	4:B:915:HOH:O	2.14	0.46
1:A:201:TRP:CE3	1:A:208:THR:HG21	2.50	0.46
1:A:350:GLU:OE2	4:A:1084:HOH:O	2.21	0.46
1:A:182:ILE:O	1:A:185:VAL:HG22	2.16	0.45
1:B:282:GLU:HG3	1:B:284:HIS:HE1	1.81	0.45
1:A:4:ASP:HB2	1:A:5:LYS:CE	2.43	0.45
1:A:69:ASN:ND2	4:A:999:HOH:O	2.49	0.45
1:B:275:ASN:OD1	1:B:275:ASN:C	2.59	0.45
1:B:277:GLN:HB3	4:B:973:HOH:O	2.16	0.45
1:B:5:LYS:H	1:B:5:LYS:CD	2.30	0.44
1:B:96:GLN:HE21	1:B:96:GLN:HA	1.81	0.44
1:A:90:ASN:OD1	1:A:387:SER:HB2	2.17	0.44
1:B:137:PRO:HD2	1:B:140:MET:HG3	2.00	0.44
1:A:129:PHE:CE2	1:A:144:LEU:HD13	2.52	0.44
1:B:242:ASN:O	1:B:243:HIS:C	2.60	0.44
1:B:276:LYS:N	1:B:276:LYS:HD3	2.33	0.44
1:B:78:ASN:CG	4:B:1099:HOH:O	2.60	0.44
1:A:5:LYS:H	1:A:5:LYS:CD	2.30	0.44
1:B:58:THR:HG22	4:B:1101:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NH2	4:A:880:HOH:O	2.51	0.43
1:B:4:ASP:HB2	1:B:5:LYS:HZ1	1.80	0.43
1:A:91:LYS:HE3	4:A:985:HOH:O	2.18	0.43
1:B:9:GLN:NE2	1:B:76:ASP:HB2	2.34	0.43
1:A:129:PHE:CD2	1:A:144:LEU:HD13	2.54	0.43
1:B:42:GLN:NE2	4:B:904:HOH:O	2.48	0.43
1:A:212:PRO:HD2	1:A:239:CYS:O	2.18	0.43
1:B:14:GLU:HB3	1:B:26:LYS:HD2	2.00	0.43
1:B:35:ALA:O	1:B:38:HIS:HB2	2.19	0.43
1:B:116:LYS:HE3	4:B:1094:HOH:O	2.18	0.42
1:A:20:LYS:NZ	1:A:393:GLU:OE1	2.47	0.42
1:B:182:ILE:HD12	1:B:193:VAL:CG1	2.47	0.42
1:A:81:LYS:CD	1:A:86:THR:HG22	2.47	0.42
1:A:208:THR:HG22	1:A:209:HIS:H	1.83	0.42
1:B:78:ASN:CB	4:B:1099:HOH:O	2.61	0.42
1:B:103:VAL:O	1:B:104:SER:C	2.62	0.42
1:B:246:ILE:H	1:B:246:ILE:HG13	1.75	0.42
1:B:291:ASN:CG	4:B:915:HOH:O	2.62	0.42
1:B:379:GLN:HA	1:B:380:PRO:HD2	1.93	0.42
1:A:257:GLN:OE1	4:A:1034:HOH:O	2.21	0.42
1:B:284:HIS:HD2	4:B:1131:HOH:O	2.02	0.41
1:A:295:GLU:CD	4:A:824:HOH:O	2.63	0.41
1:A:203:ALA:CB	1:A:208:THR:HG23	2.39	0.41
1:A:259:LYS:HD2	4:A:858:HOH:O	2.20	0.41
1:B:313:LYS:HB2	4:B:1048:HOH:O	2.21	0.41
1:A:55:PRO:O	1:A:56:ASN:C	2.63	0.41
1:A:122:LEU:HA	1:A:125:THR:OG1	2.20	0.41
1:B:220:LEU:HD23	1:B:221:TYR:N	2.35	0.41
1:B:69:ASN:ND2	4:B:893:HOH:O	2.49	0.41
1:A:94:LEU:HB3	1:A:346:VAL:HG22	2.03	0.41
1:B:58:THR:HG23	2:B:800:NAG:H5	2.03	0.41
1:B:137:PRO:HD2	1:B:140:MET:CG	2.51	0.40
1:A:17:ARG:HA	1:A:17:ARG:HD3	1.83	0.40
1:B:33:ALA:O	1:B:34:ASP:C	2.64	0.40
1:B:305:PRO:HG3	1:B:313:LYS:CD	2.50	0.40
1:B:347:TRP:CE3	1:B:354:MET:HE1	2.56	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	398/411 (97%)	381 (96%)	16 (4%)	1 (0%)	36	46
1	B	398/411 (97%)	385 (97%)	13 (3%)	0	100	100
All	All	796/822 (97%)	766 (96%)	29 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	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	324/333 (97%)	300 (93%)	24 (7%)	13	17
1	B	324/333 (97%)	297 (92%)	27 (8%)	10	14
All	All	648/666 (97%)	597 (92%)	51 (8%)	11	15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	17	ARG
1	A	20	LYS
1	A	25	LYS
1	A	27	GLN

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Mol	Chain	Res	Type
1	A	41	ARG
1	A	43	LYS
1	A	58	THR
1	A	68	LYS
1	A	81	LYS
1	A	91	LYS
1	A	96	GLN
1	A	102	LEU
1	A	115	LYS
1	A	162	LYS
1	A	208	THR
1	A	224	THR
1	A	276	LYS
1	A	306	LYS
1	A	346	VAL
1	A	373	LYS
1	A	377	LYS
1	A	388	ASN
1	A	390	ARG
1	B	5	LYS
1	B	17	ARG
1	B	20	LYS
1	B	25	LYS
1	B	27	GLN
1	B	41	ARG
1	B	43	LYS
1	B	58	THR
1	B	68	LYS
1	B	81	LYS
1	B	96	GLN
1	B	102	LEU
1	B	115	LYS
1	B	135	LYS
1	B	159	ARG
1	B	162	LYS
1	B	182	ILE
1	B	208	THR
1	B	224	THR
1	B	246	ILE
1	B	256	LYS
1	B	276	LYS
1	B	306	LYS

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Mol	Chain	Res	Type
1	B	346	VAL
1	B	350	GLU
1	B	373	LYS
1	B	390	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	42	GLN
1	A	53	GLN
1	A	69	ASN
1	A	96	GLN
1	A	113	ASN
1	A	175	GLN
1	A	187	ASN
1	A	247	ASN
1	A	284	HIS
1	A	308	ASN
1	A	331	GLN
1	A	388	ASN
1	B	9	GLN
1	B	27	GLN
1	B	29	ASN
1	B	42	GLN
1	B	69	ASN
1	B	96	GLN
1	B	113	ASN
1	B	187	ASN
1	B	277	GLN
1	B	284	HIS
1	B	308	ASN
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	B	1	1	7,8,9	1.53	2 (28%)	9,10,12	1.39	1 (11%)
1	PCA	A	1	1	7,8,9	1.44	2 (28%)	9,10,12	2.05	4 (44%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CG-CD	2.55	1.57	1.50
1	A	1	PCA	O-C	2.41	1.29	1.20
1	B	1	PCA	O-C	2.27	1.28	1.20
1	B	1	PCA	CG-CD	2.26	1.56	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-CG	-3.40	120.66	126.72
1	A	1	PCA	CB-CG-CD	-2.94	99.86	104.41
1	A	1	PCA	CA-N-CD	-2.45	105.20	113.58
1	A	1	PCA	CG-CD-N	2.23	113.85	108.39
1	B	1	PCA	OE-CD-CG	-2.01	123.14	126.72

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	1.41	1 (7%)	17,19,21	2.42	7 (41%)
3	IN1	B	801	-	22,23,23	1.18	3 (13%)	28,32,32	1.53	3 (10%)
2	NAG	B	800	1	14,14,15	1.50	1 (7%)	17,19,21	1.77	4 (23%)
3	IN1	A	801	-	22,23,23	1.31	3 (13%)	28,32,32	1.93	5 (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
3	IN1	B	801	-	-	6/17/37/37	0/1/1/1
2	NAG	B	800	1	-	0/6/23/26	0/1/1/1
3	IN1	A	801	-	-	7/17/37/37	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	NAG	O7-C7	-4.19	1.13	1.23
2	A	800	NAG	O7-C7	-3.74	1.14	1.23
3	B	801	IN1	O5-C1	3.12	1.49	1.41
3	B	801	IN1	O2A-C4A	3.10	1.42	1.33
3	A	801	IN1	O1-C1	3.02	1.45	1.40
3	A	801	IN1	O2A-C4A	2.56	1.40	1.33
3	A	801	IN1	O2A-C3A	-2.52	1.40	1.44
3	B	801	IN1	O1-C1	2.16	1.43	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	IN1	C1A-O1-C1	-5.82	103.74	113.68
3	B	801	IN1	C1A-O1-C1	-5.41	104.44	113.68
3	A	801	IN1	C3A-O2A-C4A	5.18	125.93	116.71
2	A	800	NAG	O3-C3-C2	5.08	119.95	109.40
2	A	800	NAG	O6-C6-C5	5.07	128.59	111.33
2	A	800	NAG	O3-C3-C4	-3.51	102.11	110.38
2	B	800	NAG	C8-C7-N2	-3.36	110.55	116.12
2	B	800	NAG	O5-C1-C2	-3.28	106.22	111.29
2	A	800	NAG	C2-N2-C7	-2.94	118.96	122.90
2	A	800	NAG	C8-C7-N2	-2.60	111.81	116.12
3	A	801	IN1	O6-C6-C5	-2.50	102.82	111.33
2	B	800	NAG	C4-C3-C2	-2.42	107.47	111.02
2	A	800	NAG	O5-C1-C2	-2.34	107.67	111.29
3	B	801	IN1	O1-C1A-C2A	2.33	113.33	108.81
3	A	801	IN1	O5-C1-O1	-2.33	104.55	110.04
2	A	800	NAG	O7-C7-C8	2.19	125.95	122.05
2	B	800	NAG	C2-N2-C7	-2.12	120.05	122.90
3	B	801	IN1	O2A-C4A-C5A	-2.05	104.92	111.15
3	A	801	IN1	O1-C1A-C2A	2.04	112.77	108.81

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	IN1	C1A-C2A-C6A-C3A
3	A	801	IN1	C1A-C2A-C6A-O4S
3	A	801	IN1	O2A-C3A-C6A-C2A
3	A	801	IN1	O2A-C3A-C6A-O4S
3	B	801	IN1	C1A-C2A-C6A-C3A
3	B	801	IN1	C1A-C2A-C6A-O4S

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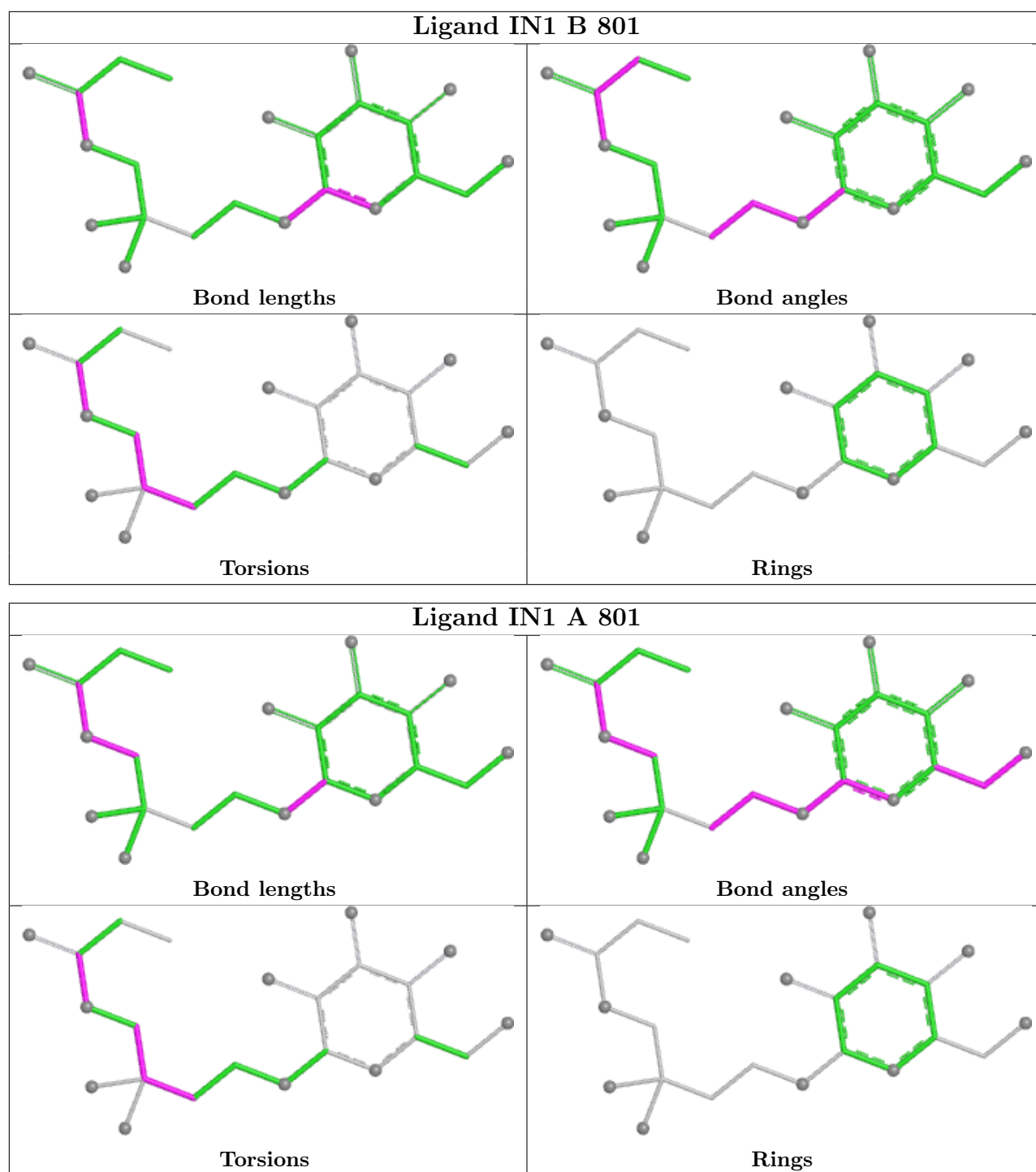
Mol	Chain	Res	Type	Atoms
3	B	801	IN1	O2A-C3A-C6A-C2A
3	A	801	IN1	C1A-C2A-C6A-O1R
3	B	801	IN1	C1A-C2A-C6A-O1R
3	B	801	IN1	C5A-C4A-O2A-C3A
3	A	801	IN1	C5A-C4A-O2A-C3A
3	A	801	IN1	O2A-C3A-C6A-O1R
3	B	801	IN1	O2A-C3A-C6A-O4S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.