



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:32 PM UTC

PDB ID : 1C7T / pdb_00001c7t
Title : BETA-N-ACETYLHEXOSAMINIDASE MUTANT E540D COMPLEXED
WITH DI-N ACETYL-D-GLUCOSAMINE (CHITOBIASE)
Authors : Prag, G.; Papanikolau, Y.; Tavlas, G.; Vorgias, C.E.; Petratos, K.; Oppenheim,
A.B.
Deposited on : 2000-03-17
Resolution : 1.90 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

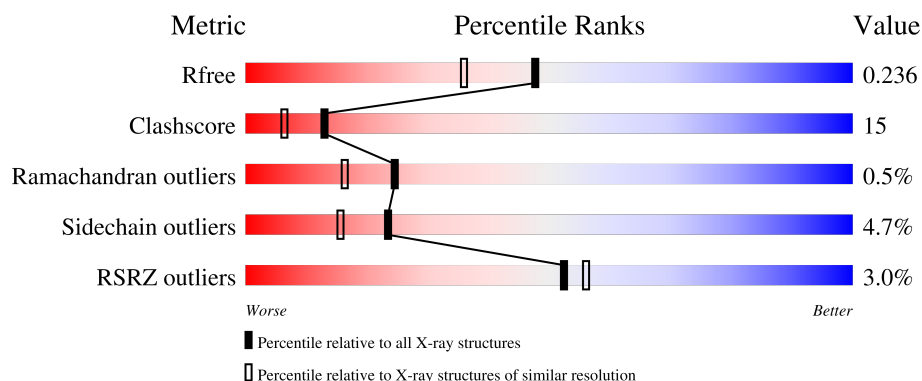
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	858	 3% 65% 28% 6%
2	B	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7657 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 BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	858	6776	4287	1185	1282	22	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	GLN	PRO	conflict	UNP Q54468
A	540	ASP	GLU	engineered mutation	UNP Q54468
A	828	GLY	ALA	conflict	UNP Q54468

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	29	16	2	11	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

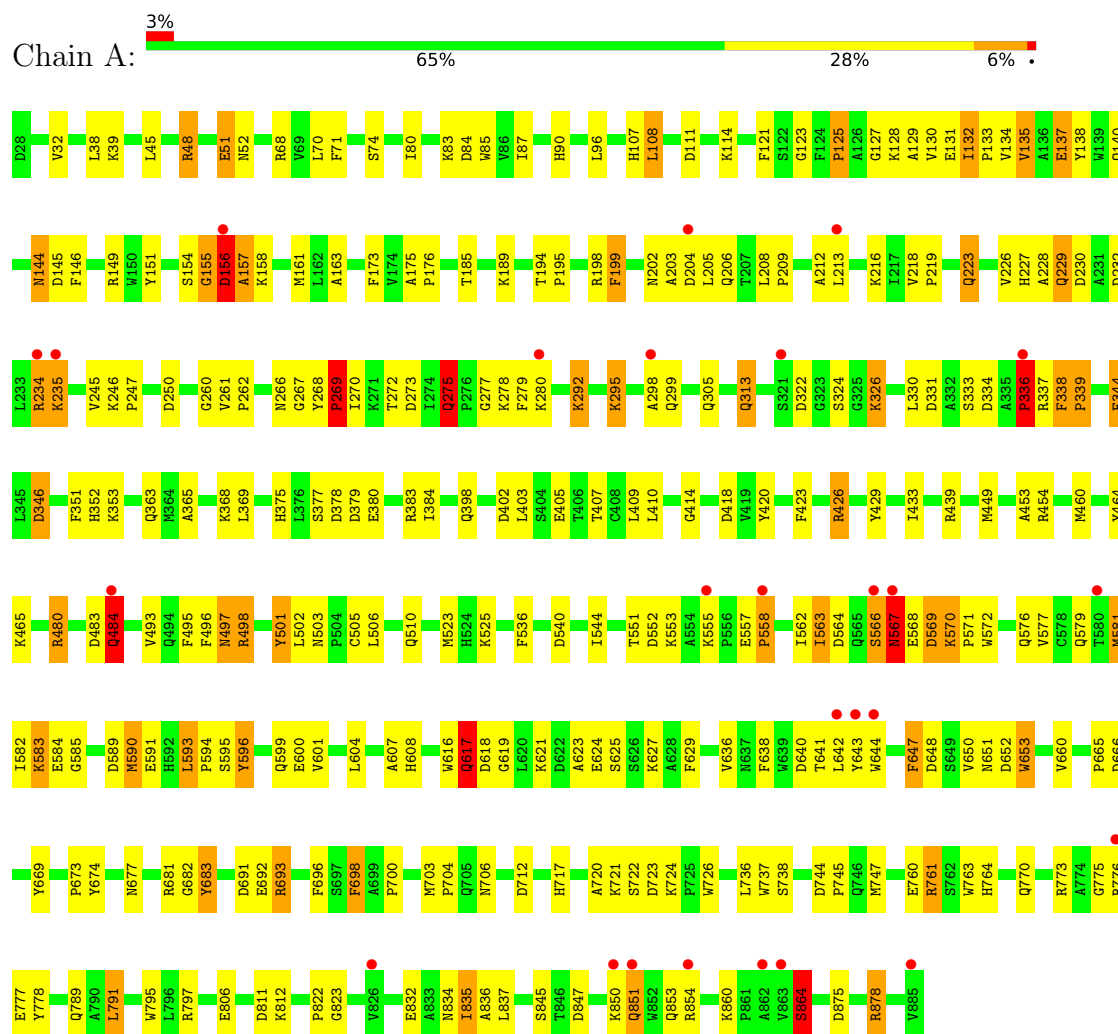
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	832	Total	O	0	0
			832	832		

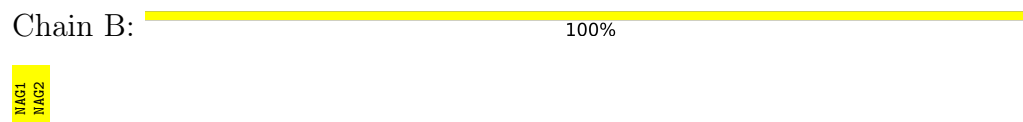
3 Residue-property plots

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 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: BETA-N-ACETYLHEXOSAMINIDASE



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.17Å 99.42Å 86.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (10.00-1.90) 96.2 (10.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 1.90Å)	Xtriage
Refinement program	REFMAC / ARP	Depositor
R, R_{free}	0.191 , 0.246 0.190 , 0.236	Depositor DCC
R_{free} test set	3772 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7657	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	1.03	2/6959 (0.0%)	1.83	156/9423 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	PRO	N-CA	5.62	1.55	1.47
1	A	229	GLN	CA-C	-5.08	1.46	1.53

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	TRP	N-CA-C	-14.47	91.20	112.04
1	A	576	GLN	OE1-CD-NE2	-10.67	111.93	122.60
1	A	229	GLN	OE1-CD-NE2	-10.60	112.00	122.60
1	A	540	ASP	CA-CB-CG	10.48	123.08	112.60
1	A	617	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	A	579	GLN	OE1-CD-NE2	-10.42	112.18	122.60
1	A	593	LEU	CA-C-O	10.37	128.40	118.34
1	A	313	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	484	GLN	OE1-CD-NE2	-9.46	113.14	122.60
1	A	338	PHE	CA-CB-CG	9.02	122.82	113.80
1	A	878	ARG	CD-NE-CZ	8.80	136.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	HIS	CA-CB-CG	-8.52	105.28	113.80
1	A	223	GLN	OE1-CD-NE2	-8.35	114.25	122.60
1	A	590	MET	CA-C-O	8.33	129.38	120.55
1	A	114	LYS	CA-C-O	8.26	129.62	120.70
1	A	557	GLU	CB-CA-C	8.17	122.36	109.37
1	A	199	PHE	CA-CB-CG	-8.02	105.78	113.80
1	A	681	ARG	CD-NE-CZ	8.02	135.62	124.40
1	A	235	LYS	N-CA-C	-7.98	103.03	114.12
1	A	761	ARG	CD-NE-CZ	7.89	135.45	124.40
1	A	653	TRP	N-CA-CB	7.86	122.38	110.19
1	A	583	LYS	CA-C-O	-7.56	113.06	121.00
1	A	706	ASN	CA-CB-CG	-7.49	105.11	112.60
1	A	418	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	146	PHE	CA-CB-CG	-7.41	106.39	113.80
1	A	698	PHE	CA-CB-CG	7.38	121.19	113.80
1	A	334	ASP	CA-CB-CG	7.36	119.95	112.60
1	A	156	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	576	GLN	CG-CD-NE2	7.22	127.22	116.40
1	A	640	ASP	CA-C-O	-7.17	113.69	121.94
1	A	552	ASP	CA-CB-CG	-6.99	105.61	112.60
1	A	51	GLU	CA-C-O	6.83	127.31	119.18
1	A	570	LYS	CA-C-N	6.83	126.79	119.76
1	A	570	LYS	C-N-CA	6.83	126.79	119.76
1	A	496	PHE	CA-C-O	-6.81	113.58	121.82
1	A	484	GLN	CG-CD-NE2	6.75	126.53	116.40
1	A	811	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	351	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	617	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	878	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	A	339	PRO	CA-N-CD	-6.64	102.70	112.00
1	A	503	ASN	CA-C-N	6.60	127.17	120.04
1	A	503	ASN	C-N-CA	6.60	127.17	120.04
1	A	495	PHE	CA-CB-CG	-6.58	107.22	113.80
1	A	854	ARG	CD-NE-CZ	6.58	133.62	124.40
1	A	346	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	409	LEU	CA-C-O	-6.52	114.03	121.72
1	A	558	PRO	CA-N-CD	-6.51	102.89	112.00
1	A	579	GLN	CG-CD-NE2	6.51	126.17	116.40
1	A	223	GLN	CG-CD-NE2	6.48	126.13	116.40
1	A	693	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	A	368	LYS	CA-C-O	6.41	127.49	120.12
1	A	647	PHE	CA-CB-CG	-6.40	107.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASN	CA-C-O	-6.40	112.78	120.65
1	A	229	GLN	CG-CD-NE2	6.32	125.89	116.40
1	A	52	ASN	N-CA-C	6.32	120.78	111.87
1	A	426	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	A	163	ALA	N-CA-C	6.21	118.84	111.33
1	A	584	GLU	CA-C-O	6.21	126.92	119.10
1	A	640	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	764	HIS	N-CA-C	6.17	119.01	109.07
1	A	51	GLU	N-CA-C	-6.15	105.78	113.28
1	A	398	GLN	CA-C-O	6.15	128.19	121.06
1	A	144	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	596	TYR	N-CA-C	-6.11	104.53	111.07
1	A	269	PRO	CA-N-CD	-6.11	103.45	112.00
1	A	313	GLN	CG-CD-NE2	6.10	125.55	116.40
1	A	629	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	738	SER	N-CA-C	6.04	120.26	112.41
1	A	619	GLY	CA-C-O	-6.02	112.39	119.50
1	A	563	ILE	CA-CB-CG1	6.00	120.60	110.40
1	A	71	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	480	ARG	CD-NE-CZ	5.94	132.71	124.40
1	A	717	HIS	CA-C-O	-5.94	115.09	121.56
1	A	601	VAL	CA-C-O	-5.89	114.61	120.85
1	A	403	LEU	CA-C-O	-5.88	111.41	119.05
1	A	566	SER	CA-C-O	-5.87	114.62	120.90
1	A	510	GLN	CA-C-O	-5.87	114.33	120.55
1	A	567	ASN	CA-CB-CG	-5.86	106.74	112.60
1	A	336	PRO	CA-N-CD	-5.86	103.80	112.00
1	A	379	ASP	CA-C-N	-5.85	113.28	122.65
1	A	379	ASP	C-N-CA	-5.85	113.28	122.65
1	A	627	LYS	CA-C-O	5.82	126.68	120.10
1	A	638	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	875	ASP	CA-C-O	5.81	126.31	119.28
1	A	683	TYR	N-CA-C	-5.79	103.06	110.53
1	A	228	ALA	CA-C-N	-5.76	112.70	122.67
1	A	228	ALA	C-N-CA	-5.76	112.70	122.67
1	A	268	TYR	O-C-N	5.73	126.30	121.31
1	A	135	VAL	CA-C-O	-5.71	114.43	120.48
1	A	571	PRO	CA-C-O	-5.64	114.91	121.34
1	A	660	VAL	N-CA-C	5.64	116.49	107.98
1	A	383	ARG	CA-C-O	-5.59	113.35	119.95
1	A	423	PHE	CA-C-O	-5.59	114.95	121.10
1	A	623	ALA	N-CA-CB	-5.58	102.39	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	GLN	CA-C-N	-5.55	114.61	122.94
1	A	229	GLN	C-N-CA	-5.55	114.61	122.94
1	A	134	VAL	CA-C-O	-5.55	116.14	121.63
1	A	677	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	696	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	130	VAL	CA-C-O	-5.51	114.45	120.84
1	A	453	ALA	CA-C-O	5.50	126.15	119.78
1	A	616	TRP	N-CA-C	-5.49	101.72	109.96
1	A	581	MET	CA-C-O	5.47	126.35	120.55
1	A	806	GLU	N-CA-C	5.46	117.32	111.36
1	A	206	GLN	CA-C-O	-5.46	115.59	121.38
1	A	864	SER	CA-C-O	-5.45	114.89	120.99
1	A	133	PRO	N-CA-CB	5.45	108.41	103.34
1	A	353	LYS	N-CA-C	5.45	117.72	110.53
1	A	368	LYS	N-CA-C	5.44	119.87	113.23
1	A	368	LYS	CA-C-N	-5.43	113.66	121.42
1	A	368	LYS	C-N-CA	-5.43	113.66	121.42
1	A	48	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	339	PRO	O-C-N	5.41	128.72	122.23
1	A	536	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	700	PRO	CA-C-O	-5.39	111.69	118.86
1	A	726	TRP	CA-C-N	5.39	124.91	119.19
1	A	726	TRP	C-N-CA	5.39	124.91	119.19
1	A	158	LYS	CA-C-O	-5.36	115.69	120.19
1	A	202	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	A	737	TRP	N-CA-C	-5.35	102.96	110.50
1	A	127	GLY	O-C-N	5.32	128.15	122.41
1	A	693	ARG	CD-NE-CZ	5.29	131.80	124.40
1	A	498	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	A	137	GLU	CA-C-O	5.25	127.28	121.56
1	A	563	ILE	CA-C-O	-5.24	115.46	121.44
1	A	369	LEU	N-CA-C	-5.24	101.92	110.20
1	A	501	TYR	CA-C-O	-5.23	115.10	120.54
1	A	380	GLU	CA-C-O	-5.22	113.45	119.56
1	A	593	LEU	O-C-N	-5.21	115.81	120.71
1	A	198	ARG	CA-C-O	5.17	125.90	120.42
1	A	627	LYS	O-C-N	-5.17	116.17	122.22
1	A	363	GLN	CA-C-O	-5.17	114.03	119.97
1	A	426	ARG	NH1-CZ-NH2	5.16	126.00	119.30
1	A	125	PRO	N-CA-CB	5.15	107.83	103.35
1	A	232	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	590	MET	CA-C-N	5.14	127.69	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	MET	C-N-CA	5.14	127.69	120.28
1	A	275	GLN	O-C-N	-5.14	117.63	121.23
1	A	607	ALA	CA-C-O	5.14	125.91	120.10
1	A	720	ALA	O-C-N	5.13	129.33	123.48
1	A	266	ASN	CA-C-O	5.12	125.64	119.59
1	A	568	GLU	CA-C-N	-5.12	114.56	122.59
1	A	568	GLU	C-N-CA	-5.12	114.56	122.59
1	A	497	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	449	MET	N-CA-CB	-5.10	105.75	111.10
1	A	823	GLY	N-CA-C	-5.09	103.43	112.54
1	A	84	ASP	CA-C-N	-5.09	113.97	122.21
1	A	84	ASP	C-N-CA	-5.09	113.97	122.21
1	A	203	ALA	N-CA-C	5.08	118.74	112.54
1	A	835	ILE	O-C-N	-5.07	118.56	122.97
1	A	454	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	A	132	ILE	N-CA-CB	5.06	118.29	111.21
1	A	568	GLU	CB-CA-C	-5.05	101.51	109.80
1	A	173	PHE	O-C-N	5.02	127.56	122.09
1	A	653	TRP	CA-CB-CG	-5.01	104.08	113.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ILE	Mainchain
1	A	96	LEU	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6776	0	6571	201	2
2	B	29	0	26	0	0
3	A	20	0	0	2	0
4	A	832	0	0	20	2
All	All	7657	0	6597	201	4

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 15.

All (201) 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:336:PRO:HD3	1:A:763:TRP:CH2	1.84	1.10
1:A:336:PRO:HD3	1:A:763:TRP:CZ2	1.94	1.02
1:A:525:LYS:HE2	4:A:2674:HOH:O	1.62	0.98
1:A:336:PRO:HG3	1:A:763:TRP:CZ3	2.00	0.96
1:A:267:GLY:O	1:A:269:PRO:HD3	1.75	0.86
1:A:567:ASN:N	1:A:567:ASN:HD22	1.73	0.85
1:A:407:THR:HG21	4:A:2318:HOH:O	1.76	0.85
1:A:273:ASP:HB3	1:A:275:GLN:NE2	1.93	0.84
1:A:234:ARG:HA	1:A:234:ARG:NE	1.92	0.83
1:A:567:ASN:HD22	1:A:567:ASN:H	1.26	0.82
1:A:234:ARG:NE	1:A:234:ARG:CA	2.41	0.82
1:A:227:HIS:NE2	1:A:331:ASP:OD2	2.14	0.80
1:A:617:GLN:HB2	1:A:636:VAL:HG21	1.64	0.79
1:A:234:ARG:HA	1:A:234:ARG:CZ	2.13	0.79
1:A:336:PRO:CD	1:A:763:TRP:CH2	2.66	0.78
1:A:326:LYS:HB3	1:A:326:LYS:NZ	1.97	0.78
1:A:864:SER:HA	4:A:2648:HOH:O	1.84	0.77
1:A:229:GLN:HB2	1:A:295:LYS:NZ	1.99	0.77
1:A:212:ALA:C	1:A:213:LEU:HD22	2.10	0.76
1:A:213:LEU:HD22	1:A:213:LEU:N	2.02	0.74
1:A:480:ARG:NH1	1:A:484:GLN:HG2	2.03	0.74
1:A:570:LYS:HE2	1:A:591:GLU:OE1	1.89	0.72
1:A:567:ASN:H	1:A:567:ASN:ND2	1.87	0.72
1:A:230:ASP:O	1:A:295:LYS:NZ	2.23	0.70
1:A:229:GLN:CD	1:A:295:LYS:HE3	2.17	0.69
1:A:460:MET:HA	1:A:460:MET:HE2	1.73	0.69
1:A:480:ARG:HH12	1:A:484:GLN:HG2	1.58	0.68
1:A:405:GLU:CD	1:A:410:LEU:HG	2.20	0.67
1:A:617:GLN:CB	1:A:636:VAL:HG21	2.24	0.67
1:A:595:SER:O	1:A:599:GLN:HG3	1.93	0.67
1:A:273:ASP:HB3	1:A:275:GLN:HE21	1.58	0.67
1:A:189:LYS:HE2	4:A:2583:HOH:O	1.93	0.67
1:A:270:ILE:HG12	1:A:298:ALA:HB3	1.74	0.67
1:A:878:ARG:HD3	4:A:2250:HOH:O	1.94	0.67
1:A:617:GLN:HA	1:A:636:VAL:CG2	2.25	0.67
1:A:295:LYS:HA	1:A:295:LYS:HE2	1.78	0.66
1:A:229:GLN:HB2	1:A:295:LYS:HZ2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HE	1:A:234:ARG:C	2.04	0.65
1:A:245:VAL:HG23	1:A:305:GLN:OE1	1.96	0.65
1:A:234:ARG:NH2	1:A:261:VAL:HA	2.12	0.64
1:A:365:ALA:HB2	1:A:439:ARG:HB3	1.78	0.64
1:A:38:LEU:HD21	1:A:80:ILE:HD12	1.79	0.64
1:A:330:LEU:HD12	1:A:330:LEU:C	2.23	0.63
1:A:85:TRP:CZ3	1:A:87:ILE:HD12	2.34	0.62
1:A:593:LEU:N	1:A:594:PRO:CD	2.63	0.62
1:A:617:GLN:CA	1:A:636:VAL:CG2	2.77	0.62
1:A:48:ARG:HD3	1:A:185:THR:CA	2.30	0.61
1:A:199:PHE:C	1:A:199:PHE:CD1	2.78	0.61
1:A:832:GLU:HG3	1:A:860:LYS:HE3	1.83	0.60
1:A:208:LEU:CB	1:A:213:LEU:HD21	2.31	0.60
1:A:617:GLN:CB	1:A:636:VAL:CG2	2.78	0.60
1:A:48:ARG:HD3	1:A:185:THR:HA	1.84	0.60
1:A:497:ASN:HB3	3:A:2001:SO4:O3	2.02	0.59
1:A:70:LEU:HD11	1:A:131:GLU:HB3	1.85	0.58
1:A:212:ALA:O	1:A:213:LEU:HD13	2.02	0.58
1:A:246:LYS:HE3	1:A:250:ASP:OD1	2.04	0.58
1:A:156:ASP:O	1:A:157:ALA:C	2.45	0.57
1:A:642:LEU:HD22	1:A:647:PHE:HB3	1.87	0.57
1:A:498:ARG:HG3	4:A:2416:HOH:O	2.04	0.57
1:A:209:PRO:O	1:A:213:LEU:HD23	2.05	0.57
1:A:208:LEU:HB2	1:A:213:LEU:HD21	1.86	0.56
1:A:295:LYS:HE2	1:A:295:LYS:CA	2.29	0.56
1:A:429:TYR:CE2	1:A:433:ILE:HD11	2.40	0.56
1:A:812:LYS:HE3	4:A:2500:HOH:O	2.04	0.56
1:A:326:LYS:HB3	1:A:326:LYS:HZ2	1.68	0.56
1:A:234:ARG:HH22	1:A:261:VAL:HA	1.71	0.56
1:A:589:ASP:OD1	1:A:591:GLU:HB3	2.06	0.55
1:A:213:LEU:N	1:A:213:LEU:CD2	2.70	0.55
1:A:497:ASN:OD1	1:A:498:ARG:N	2.40	0.55
1:A:643:TYR:HE1	1:A:644:TRP:CE2	2.25	0.54
1:A:648:ASP:OD1	1:A:724:LYS:HE3	2.07	0.54
1:A:773:ARG:HD2	1:A:776:ARG:NE	2.22	0.54
1:A:744:ASP:N	1:A:745:PRO:CD	2.71	0.54
1:A:156:ASP:C	1:A:157:ALA:O	2.49	0.54
1:A:229:GLN:HG3	1:A:295:LYS:CE	2.38	0.54
1:A:525:LYS:HE3	4:A:2535:HOH:O	2.06	0.54
1:A:326:LYS:HB3	1:A:326:LYS:HZ3	1.73	0.53
1:A:272:THR:O	1:A:273:ASP:OD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HD3	4:A:2170:HOH:O	2.08	0.52
1:A:812:LYS:CE	4:A:2500:HOH:O	2.58	0.52
1:A:465:LYS:HE3	4:A:2438:HOH:O	2.09	0.52
1:A:583:LYS:C	1:A:585:GLY:H	2.18	0.52
1:A:591:GLU:HB2	4:A:2715:HOH:O	2.09	0.52
1:A:665:PRO:HA	1:A:669:TYR:CD1	2.44	0.52
1:A:121:PHE:CZ	1:A:123:GLY:HA2	2.45	0.52
1:A:108:LEU:HB3	4:A:2719:HOH:O	2.09	0.51
1:A:229:GLN:HB2	1:A:295:LYS:HZ1	1.75	0.51
1:A:770:GLN:OE1	1:A:778:TYR:OH	2.18	0.51
1:A:267:GLY:O	1:A:269:PRO:CD	2.54	0.51
1:A:234:ARG:HH21	1:A:262:PRO:HD2	1.75	0.51
1:A:336:PRO:CG	1:A:763:TRP:CZ3	2.84	0.51
1:A:484:GLN:NE2	4:A:2833:HOH:O	2.44	0.50
1:A:204:ASP:OD2	1:A:693:ARG:NH2	2.39	0.50
1:A:234:ARG:NH2	1:A:260:GLY:O	2.45	0.50
1:A:377:SER:O	1:A:378:ASP:HB2	2.12	0.50
1:A:292:LYS:HG3	1:A:331:ASP:OD1	2.12	0.50
1:A:497:ASN:CG	1:A:498:ARG:H	2.16	0.50
1:A:234:ARG:HH21	1:A:262:PRO:CD	2.25	0.50
1:A:493:VAL:HA	1:A:544:ILE:HG21	1.93	0.50
1:A:246:LYS:HB3	1:A:247:PRO:HD3	1.93	0.49
1:A:501:TYR:CD1	1:A:501:TYR:N	2.79	0.49
1:A:209:PRO:O	1:A:213:LEU:CD2	2.60	0.49
1:A:223:GLN:HB2	1:A:333:SER:HB3	1.94	0.49
1:A:218:VAL:HA	1:A:219:PRO:C	2.36	0.49
1:A:234:ARG:NE	1:A:234:ARG:C	2.67	0.49
1:A:582:ILE:HD12	1:A:590:MET:HE2	1.94	0.49
1:A:692:GLU:HB3	1:A:795:TRP:HH2	1.78	0.49
1:A:208:LEU:HB3	1:A:213:LEU:HD21	1.95	0.49
1:A:337:ARG:HG3	1:A:338:PHE:CD2	2.48	0.49
1:A:339:PRO:HD3	4:A:2288:HOH:O	2.13	0.48
1:A:834:ASN:HB2	4:A:2514:HOH:O	2.13	0.48
1:A:624:GLU:CD	1:A:625:SER:HB3	2.39	0.48
1:A:234:ARG:CA	1:A:234:ARG:HE	2.23	0.48
1:A:460:MET:HE2	1:A:460:MET:CA	2.42	0.47
1:A:39:LYS:HE3	4:A:2325:HOH:O	2.14	0.47
1:A:108:LEU:N	1:A:108:LEU:HD23	2.30	0.47
1:A:194:THR:HB	1:A:195:PRO:CD	2.44	0.47
1:A:722:SER:OG	1:A:724:LYS:HG3	2.14	0.47
1:A:154:SER:O	1:A:155:GLY:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:LEU:O	1:A:608:HIS:HD2	1.98	0.47
1:A:674:TYR:O	1:A:691:ASP:HB3	2.15	0.47
1:A:643:TYR:HE1	1:A:644:TRP:CZ2	2.34	0.46
1:A:847:ASP:CG	1:A:851:GLN:H	2.23	0.46
1:A:797:ARG:HH11	1:A:797:ARG:HD3	1.52	0.46
1:A:45:LEU:HD11	1:A:70:LEU:HB2	1.98	0.45
1:A:204:ASP:CG	1:A:693:ARG:HH22	2.22	0.45
1:A:137:GLU:HG2	1:A:138:TYR:CD2	2.51	0.45
1:A:144:ASN:ND2	1:A:682:GLY:H	2.14	0.45
1:A:483:ASP:OD1	1:A:483:ASP:C	2.60	0.45
1:A:673:PRO:HD3	1:A:683:TYR:O	2.17	0.45
1:A:464:TYR:CD2	1:A:464:TYR:C	2.94	0.45
1:A:551:THR:HG22	1:A:562:ILE:HA	1.99	0.45
1:A:723:ASP:OD1	1:A:775:GLY:HA2	2.16	0.45
1:A:32:VAL:HG23	1:A:154:SER:HB3	1.99	0.45
1:A:569:ASP:HB3	4:A:2391:HOH:O	2.16	0.45
1:A:847:ASP:OD2	1:A:851:GLN:N	2.50	0.45
1:A:641:THR:OG1	1:A:644:TRP:CE3	2.68	0.45
1:A:107:HIS:ND1	3:A:2004:SO4:O4	2.33	0.44
1:A:229:GLN:CG	1:A:295:LYS:CE	2.95	0.44
1:A:847:ASP:O	1:A:850:LYS:HG2	2.18	0.44
1:A:74:SER:HA	1:A:129:ALA:HA	1.99	0.44
1:A:156:ASP:O	1:A:157:ALA:O	2.35	0.44
1:A:596:TYR:CZ	1:A:600:GLU:HG3	2.53	0.44
1:A:149:ARG:HG3	1:A:414:GLY:O	2.17	0.44
1:A:650:VAL:O	1:A:651:ASN:C	2.60	0.44
1:A:617:GLN:HA	1:A:636:VAL:HG23	1.98	0.44
1:A:773:ARG:HD2	1:A:776:ARG:CZ	2.48	0.44
1:A:501:TYR:HB3	1:A:572:TRP:CZ2	2.53	0.44
1:A:583:LYS:C	1:A:585:GLY:N	2.74	0.44
1:A:68:ARG:HD3	4:A:2136:HOH:O	2.17	0.44
1:A:205:LEU:HD21	1:A:693:ARG:HH12	1.83	0.44
1:A:234:ARG:NE	1:A:234:ARG:O	2.51	0.44
1:A:822:PRO:HA	1:A:835:ILE:HD12	1.98	0.44
1:A:420:TYR:CD2	1:A:420:TYR:C	2.96	0.44
1:A:647:PHE:C	1:A:647:PHE:CD1	2.96	0.43
1:A:712:ASP:OD1	1:A:712:ASP:C	2.60	0.43
1:A:140:GLN:HA	1:A:145:ASP:OD2	2.17	0.43
1:A:617:GLN:HG3	1:A:653:TRP:CE2	2.53	0.43
1:A:405:GLU:OE2	1:A:410:LEU:HG	2.18	0.43
1:A:483:ASP:OD2	1:A:577:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:LEU:HD23	1:A:593:LEU:HA	1.89	0.43
1:A:277:GLY:C	1:A:279:PHE:H	2.26	0.43
1:A:426:ARG:HG3	1:A:523:MET:HG2	2.00	0.43
1:A:698:PHE:O	1:A:761:ARG:HD2	2.19	0.43
1:A:151:TYR:HA	1:A:161:MET:HA	2.01	0.43
1:A:245:VAL:HG23	1:A:305:GLN:CD	2.44	0.43
1:A:591:GLU:OE1	1:A:591:GLU:HA	2.19	0.43
1:A:212:ALA:HB3	1:A:213:LEU:HD22	2.00	0.43
1:A:339:PRO:HG3	4:A:2434:HOH:O	2.18	0.43
1:A:402:ASP:OD2	1:A:407:THR:HG22	2.18	0.43
1:A:736:LEU:CD2	1:A:747:MET:HG3	2.49	0.42
1:A:344:PHE:C	1:A:344:PHE:CD1	2.96	0.42
1:A:229:GLN:CG	1:A:295:LYS:HE3	2.49	0.42
1:A:48:ARG:HD2	1:A:51:GLU:CD	2.44	0.42
1:A:484:GLN:HE21	1:A:484:GLN:CA	2.32	0.42
1:A:277:GLY:C	1:A:279:PHE:N	2.75	0.42
1:A:483:ASP:HB2	1:A:506:LEU:HD21	2.01	0.42
1:A:48:ARG:HD2	1:A:51:GLU:OE1	2.19	0.42
1:A:123:GLY:O	1:A:125:PRO:HD3	2.19	0.42
1:A:219:PRO:HB3	1:A:760:GLU:HA	2.02	0.42
1:A:703:MET:N	1:A:704:PRO:CD	2.82	0.42
1:A:346:ASP:HA	1:A:375:HIS:HB3	2.00	0.42
1:A:791:LEU:HD12	1:A:791:LEU:C	2.45	0.42
1:A:564:ASP:OD1	1:A:566:SER:OG	2.38	0.42
1:A:68:ARG:HG2	1:A:135:VAL:HG22	2.02	0.42
1:A:505:CYS:SG	1:A:581:MET:HE2	2.59	0.41
1:A:567:ASN:ND2	1:A:567:ASN:C	2.75	0.41
1:A:90:HIS:HA	1:A:111:ASP:O	2.20	0.41
1:A:175:ALA:HA	1:A:176:PRO:HD3	1.87	0.41
1:A:245:VAL:CG2	1:A:305:GLN:HE22	2.33	0.41
1:A:845:SER:OG	1:A:847:ASP:OD1	2.38	0.41
1:A:617:GLN:HG3	1:A:653:TRP:CZ2	2.56	0.41
1:A:832:GLU:HG3	1:A:860:LYS:CE	2.50	0.41
1:A:322:ASP:OD1	1:A:324:SER:HB3	2.21	0.41
1:A:618:ASP:OD1	1:A:618:ASP:N	2.54	0.41
1:A:563:ILE:HD13	1:A:563:ILE:HG21	1.70	0.41
1:A:836:ALA:O	1:A:837:LEU:HD23	2.20	0.41
1:A:593:LEU:HB2	1:A:594:PRO:HD3	2.03	0.40
1:A:721:LYS:HB3	1:A:777:GLU:HG3	2.03	0.40
1:A:505:CYS:SG	1:A:581:MET:CE	3.09	0.40
1:A:847:ASP:OD2	1:A:850:LYS:HB2	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2137:HOH:O	4:A:2137:HOH:O[2_565]	1.59	0.61
1:A:776:ARG:NH2	1:A:851:GLN:NE2[4_556]	1.76	0.44
1:A:776:ARG:NH2	1:A:851:GLN:CD[4_556]	1.83	0.37
4:A:2740:HOH:O	4:A:2740:HOH:O[2_565]	2.14	0.06

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	859/858 (100%)	824 (96%)	31 (4%)	4 (0%)	24 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ASP
1	A	155	GLY
1	A	157	ALA
1	A	652	ASP

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	709/706 (100%)	676 (95%)	33 (5%)	23 15

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	128	LYS
1	A	216	LYS
1	A	226	VAL
1	A	234	ARG
1	A	235	LYS
1	A	269	PRO
1	A	275	GLN
1	A	278	LYS
1	A	280	LYS
1	A	292	LYS
1	A	295	LYS
1	A	299	GLN
1	A	313	GLN
1	A	326	LYS
1	A	336	PRO
1	A	344	PHE
1	A	384	ILE
1	A	484	GLN
1	A	502	LEU
1	A	553	LYS
1	A	555	LYS
1	A	558	PRO
1	A	567	ASN
1	A	569	ASP
1	A	617	GLN
1	A	621	LYS
1	A	666	ASP
1	A	789	GLN
1	A	791	LEU
1	A	851	GLN
1	A	853	GLN
1	A	864	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	275	GLN
1	A	363	GLN
1	A	484	GLN

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Mol	Chain	Res	Type
1	A	510	GLN
1	A	567	ASN
1	A	716	ASN
1	A	717	HIS
1	A	784	HIS
1	A	853	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 ⓘ

2 monosaccharides 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	B	1	2	15,15,15	1.84	3 (20%)	21,21,21	2.04	4 (19%)
2	NAG	B	2	2	14,14,15	1.37	2 (14%)	17,19,21	2.59	6 (35%)

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	B	1	2	-	0/6/26/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O1-C1	-5.61	1.22	1.39
2	B	2	NAG	O7-C7	-2.87	1.16	1.23
2	B	1	NAG	O7-C7	-2.53	1.17	1.23
2	B	2	NAG	C1-C2	-2.48	1.49	1.52
2	B	1	NAG	C2-N2	2.28	1.49	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O1-C1-C2	6.83	123.40	109.22
2	B	2	NAG	C1-O5-C5	5.93	120.14	112.19
2	B	2	NAG	O5-C1-C2	5.59	119.94	111.29
2	B	1	NAG	O1-C1-O5	-3.75	99.29	110.41
2	B	2	NAG	C1-C2-N2	3.01	115.18	110.43
2	B	1	NAG	O5-C1-C2	-2.99	106.51	109.52
2	B	2	NAG	O7-C7-C8	2.92	127.25	122.05
2	B	2	NAG	C3-C4-C5	-2.37	105.93	110.23
2	B	1	NAG	O7-C7-N2	2.15	125.78	121.98
2	B	2	NAG	C8-C7-N2	-2.07	112.68	116.12

There are no chirality outliers.

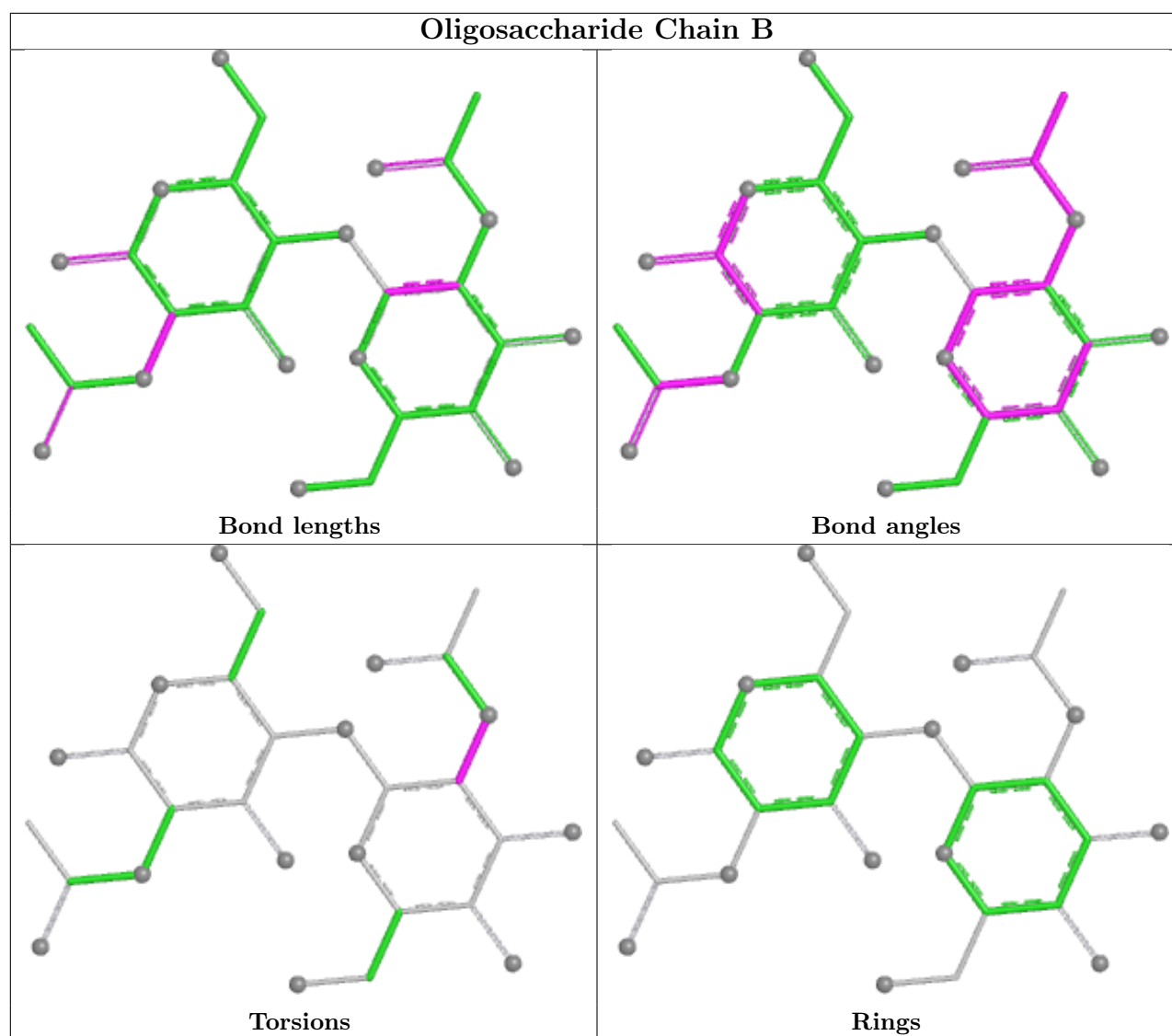
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



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	$\# Z > 2$
3	SO4	A	2001	-	4,4,4	0.84	0	6,6,6	0.39	0
3	SO4	A	2002	-	4,4,4	0.69	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	2003	-	4,4,4	0.62	0	6,6,6	0.28	0
3	SO4	A	2004	-	4,4,4	0.75	0	6,6,6	0.21	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	SO4	1	0
3	A	2004	SO4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	858/858 (100%)	-0.11	26 (3%) 52 56	14, 24, 44, 62	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	TRP	9.2
1	A	484	GLN	6.3
1	A	156	ASP	4.7
1	A	851	GLN	4.7
1	A	642	LEU	4.5
1	A	234	ARG	4.2
1	A	885	VAL	3.8
1	A	213	LEU	3.3
1	A	336	PRO	3.2
1	A	298	ALA	3.1
1	A	643	TYR	2.9
1	A	863	VAL	2.9
1	A	235	LYS	2.9
1	A	850	LYS	2.7
1	A	204	ASP	2.5
1	A	280	LYS	2.5
1	A	566	SER	2.4
1	A	862	ALA	2.3
1	A	580	THR	2.3
1	A	826	VAL	2.2
1	A	567	ASN	2.2
1	A	854	ARG	2.2
1	A	558	PRO	2.2
1	A	776	ARG	2.1
1	A	555	LYS	2.0
1	A	321	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

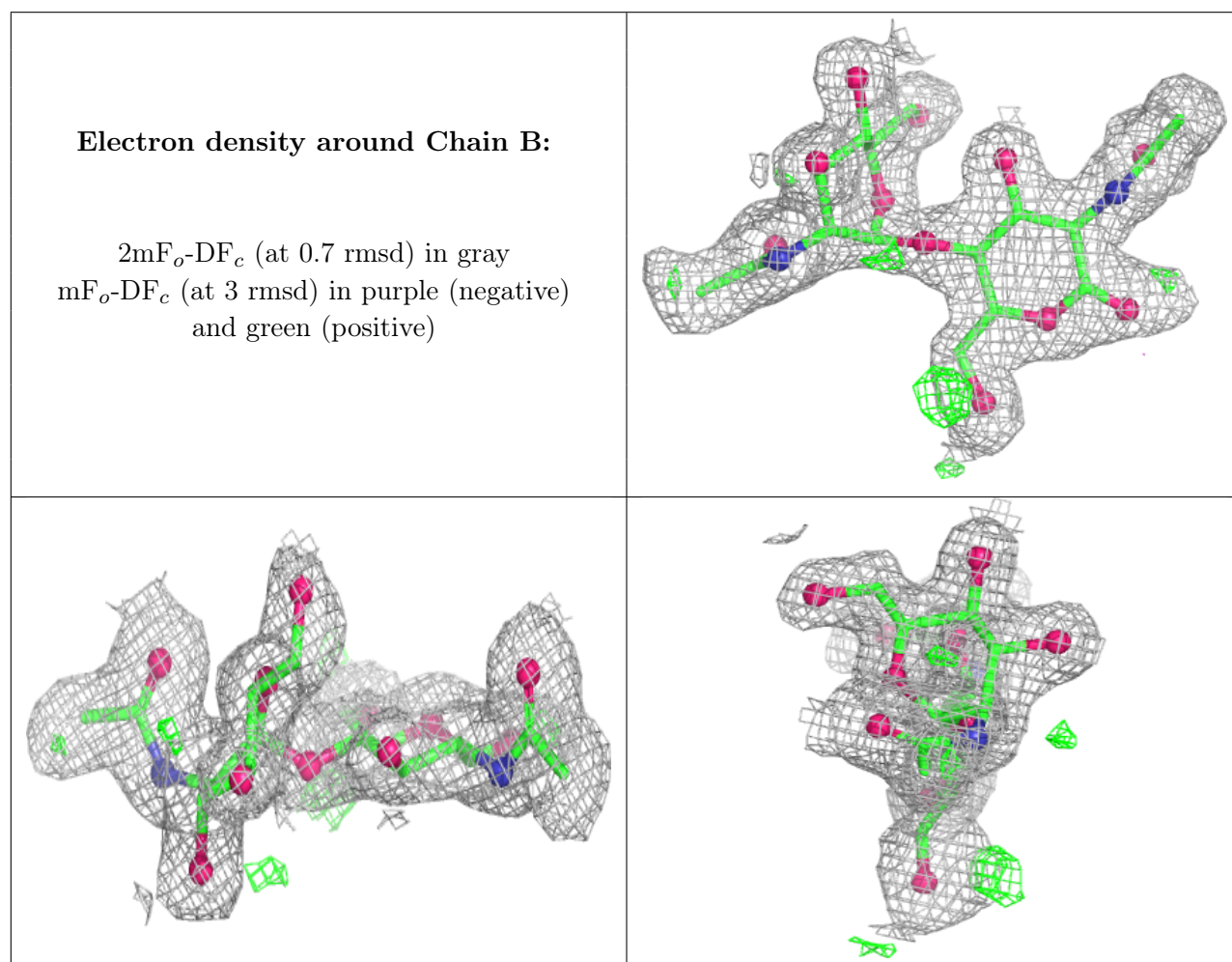
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.92	0.07	20,24,25,26	0
2	NAG	B	1	15/15	0.93	0.07	20,23,30,32	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	2004	5/5	0.80	0.13	67,68,68,69	0
3	SO4	A	2003	5/5	0.84	0.11	53,54,54,54	0
3	SO4	A	2001	5/5	0.96	0.07	21,23,24,26	0
3	SO4	A	2002	5/5	0.96	0.10	41,43,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.