



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:46 AM UTC

PDB ID : 1I75 / pdb_00001i75
Title : CRYSTAL STRUCTURE OF CYCLODEXTRIN GLUCANOTRANSFERASE FROM ALKALOPHILIC BACILLUS SP.#1011 COMPLEXED WITH 1-DEOXYNOJIRIMYCIN
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Deposited on : 2001-03-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

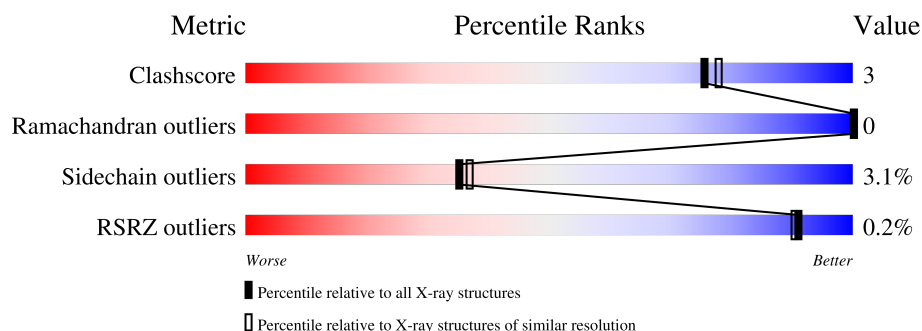
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	686	
1	B	686	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11262 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 CYCLODEXTRIN GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5312	3354	906	1036	16			
1	B	686	Total	C	N	O	S	0	0	0
			5312	3354	906	1036	16			

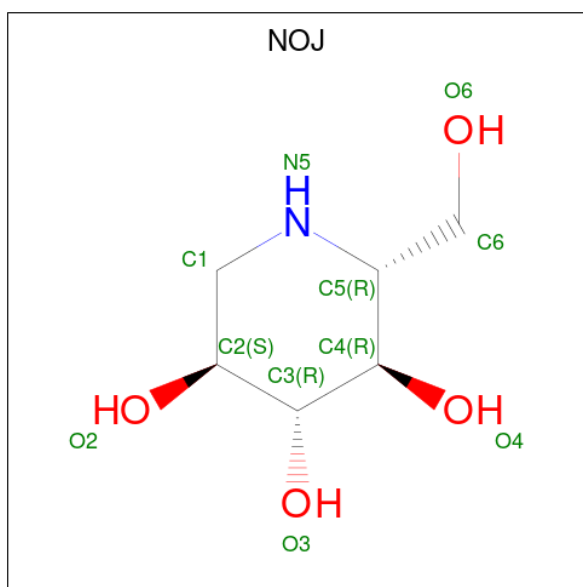
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	PRO	ARG	conflict	UNP P05618
A	454	GLY	ALA	conflict	UNP P05618
B	452	PRO	ARG	conflict	UNP P05618
B	454	GLY	ALA	conflict	UNP P05618

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 1-DEOXYNOJIRIMYCIN (CCD ID: NOJ) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		

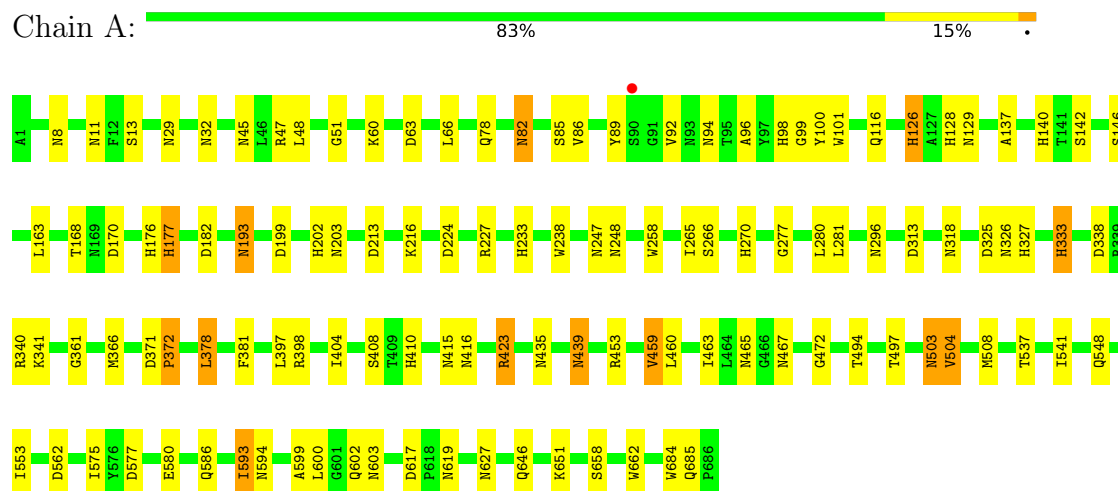
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	272	Total	O	0	0
			272	272		

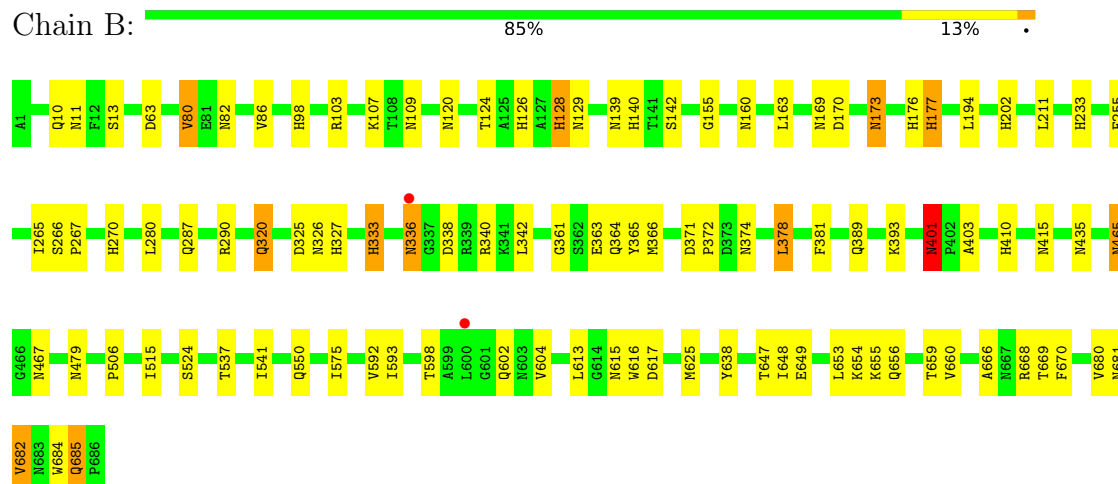
3 Residue-property plots

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: CYCLODEXTRIN GLUCANOTRANSFERASE



• Molecule 1: CYCLODEXTRIN GLUCANOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.78Å 74.24Å 79.03Å 85.03° 104.88° 101.02°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	81.5 (10.00-2.00) 95.6 (10.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 1.84Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.154 , 0.214 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11262	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: CA, NOJ

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	0.92	16/5446 (0.3%)	1.59	84/7429 (1.1%)
1	B	0.90	13/5446 (0.2%)	1.56	50/7429 (0.7%)
All	All	0.91	29/10892 (0.3%)	1.57	134/14858 (0.9%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	HIS	CD2-NE2	-8.93	1.28	1.37
1	B	128	HIS	CD2-NE2	-7.72	1.29	1.37
1	B	140	HIS	CD2-NE2	-7.45	1.29	1.37
1	A	140	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	176	HIS	CD2-NE2	-7.31	1.29	1.37
1	B	98	HIS	CD2-NE2	-6.97	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.86	1.30	1.37
1	A	327	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	128	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	333	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	176	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	333	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	126	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	202	HIS	CD2-NE2	-6.26	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	126	HIS	CG-ND1	-6.03	1.31	1.38
1	B	410	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	176	HIS	CG-ND1	-5.81	1.31	1.38
1	A	410	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	126	HIS	CD2-NE2	-5.53	1.31	1.37
1	B	270	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	233	HIS	CD2-NE2	-5.42	1.31	1.37
1	A	270	HIS	CD2-NE2	-5.34	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	233	HIS	CG-ND1	-5.10	1.32	1.38
1	B	202	HIS	CD2-NE2	-5.07	1.32	1.37
1	A	327	HIS	CG-ND1	-5.06	1.32	1.38
1	A	593	ILE	CA-CB	5.03	1.60	1.54

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ASN	CA-CB-CG	9.94	122.53	112.60
1	B	415	ASN	CA-CB-CG	9.78	122.38	112.60
1	A	398	ARG	NE-CZ-NH2	-9.54	110.61	119.20
1	A	415	ASN	CA-CB-CG	9.15	121.75	112.60
1	A	325	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	435	ASN	OD1-CG-ND2	-8.30	114.30	122.60
1	B	685	GLN	OE1-CD-NE2	-7.93	114.67	122.60
1	A	32	ASN	CA-CB-CG	7.92	120.52	112.60
1	B	479	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	B	63	ASP	CA-CB-CG	7.71	120.31	112.60
1	B	338	ASP	CA-CB-CG	7.67	120.27	112.60
1	B	325	ASP	CA-CB-CG	7.65	120.25	112.60
1	B	326	ASN	CA-CB-CG	7.50	120.10	112.60
1	A	203	ASN	OD1-CG-ND2	-7.47	115.12	122.60
1	A	326	ASN	CA-CB-CG	7.40	120.00	112.60
1	B	467	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	A	627	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	A	603	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	A	503	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	98	HIS	CB-CG-CD2	-7.28	121.74	131.20
1	A	63	ASP	CA-CB-CG	7.21	119.81	112.60
1	B	336	ASN	CA-C-O	7.10	130.50	122.27
1	B	327	HIS	CB-CG-CD2	-6.93	122.19	131.20
1	A	193	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	B	410	HIS	CA-CB-CG	6.84	120.64	113.80
1	A	11	ASN	OD1-CG-ND2	-6.83	115.78	122.60
1	B	435	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	140	HIS	CB-CG-CD2	-6.72	122.46	131.20
1	A	467	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	A	371	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	685	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	B	682	VAL	N-CA-CB	-6.59	100.16	112.36
1	B	86	VAL	N-CA-C	-6.59	98.37	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	479	ASN	CB-CG-ND2	6.54	126.20	116.40
1	A	338	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	182	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	116	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	A	266	SER	CA-C-N	6.34	125.56	118.97
1	A	266	SER	C-N-CA	6.34	125.56	118.97
1	A	398	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	B	401	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	B	363	GLU	CB-CG-CD	6.31	123.33	112.60
1	A	142	SER	N-CA-C	6.26	115.34	108.14
1	A	503	ASN	CB-CG-ND2	6.25	125.78	116.40
1	A	86	VAL	N-CA-C	-6.23	98.90	107.99
1	A	247	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	398	ARG	CG-CD-NE	-6.17	98.44	112.00
1	A	216	LYS	CB-CG-CD	-6.10	97.27	111.30
1	B	98	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	A	333	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	B	685	GLN	CG-CD-NE2	6.05	125.47	116.40
1	B	287	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	B	374	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	416	ASN	N-CA-C	5.94	118.54	111.71
1	B	265	ILE	N-CA-C	-5.92	99.59	108.12
1	B	173	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	327	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	410	HIS	CA-CB-CG	5.85	119.65	113.80
1	A	258	TRP	N-CA-C	-5.84	97.62	108.02
1	A	548	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	A	594	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	439	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	586	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	A	617	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	126	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	51	GLY	CA-C-N	5.69	125.38	119.92
1	A	51	GLY	C-N-CA	5.69	125.38	119.92
1	B	666	ALA	N-CA-C	-5.67	102.89	110.55
1	B	364	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	B	140	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	603	ASN	CB-CG-ND2	5.63	124.85	116.40
1	A	98	HIS	CB-CG-ND1	5.62	131.14	122.70
1	B	617	ASP	CA-C-N	5.62	125.46	119.28
1	B	617	ASP	C-N-CA	5.62	125.46	119.28
1	B	255	PHE	CA-CB-CG	5.61	119.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASN	CB-CG-ND2	5.61	124.82	116.40
1	B	139	ASN	OD1-CG-ND2	-5.61	117.00	122.60
1	A	238	TRP	CG-CD2-CE3	5.60	139.50	133.90
1	B	290	ARG	NE-CZ-NH2	5.56	124.21	119.20
1	A	213	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	586	GLN	CG-CD-NE2	5.54	124.71	116.40
1	A	423	ARG	N-CA-C	-5.53	100.39	109.40
1	B	616	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	233	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	177	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	270	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	176	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	B	109	ASN	CA-C-N	5.46	125.29	119.28
1	B	109	ASN	C-N-CA	5.46	125.29	119.28
1	A	8	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	341	LYS	CB-CG-CD	-5.46	98.74	111.30
1	A	29	ASN	CA-C-N	5.46	125.07	119.56
1	A	29	ASN	C-N-CA	5.46	125.07	119.56
1	A	553	ILE	CA-C-N	5.46	125.76	119.92
1	A	553	ILE	C-N-CA	5.46	125.76	119.92
1	B	327	HIS	CB-CG-ND1	5.42	130.84	122.70
1	A	202	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	265	ILE	N-CA-C	-5.39	100.56	108.11
1	A	128	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	B	129	ASN	N-CA-C	5.36	118.83	111.54
1	A	82	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	318	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	577	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	320	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	A	45	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	B	615	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	100	TYR	N-CA-C	5.28	119.57	113.18
1	A	277	GLY	N-CA-C	-5.25	108.09	114.92
1	B	617	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	202	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	313	ASP	N-CA-C	5.23	117.88	111.82
1	B	120	ASN	CB-CA-C	-5.19	102.17	110.79
1	A	248	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	281	LEU	N-CA-C	-5.18	102.19	109.96
1	A	504	VAL	N-CA-C	-5.16	100.82	108.45
1	A	435	ASN	CB-CG-ND2	5.15	124.13	116.40
1	A	129	ASN	N-CA-C	5.14	118.53	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	646	GLN	N-CA-C	5.13	116.98	109.24
1	A	459	VAL	O-C-N	-5.12	116.73	121.90
1	A	684	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	A	541	ILE	N-CA-C	-5.12	99.75	107.73
1	A	548	GLN	CG-CD-NE2	5.10	124.05	116.40
1	B	541	ILE	N-CA-C	-5.09	99.78	107.73
1	B	371	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	662	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	B	680	VAL	N-CA-C	-5.06	100.47	107.80
1	B	10	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	336	ASN	N-CA-CB	-5.03	104.06	111.71
1	B	465	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	B	103	ARG	N-CA-C	-5.02	107.83	114.31
1	A	404	ILE	N-CA-C	-5.02	105.81	110.53
1	A	617	ASP	CA-C-N	5.01	125.04	119.32
1	A	617	ASP	C-N-CA	5.01	125.04	119.32
1	A	684	TRP	CG-CD2-CE3	5.00	138.90	133.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5312	0	5050	30	0
1	B	5312	0	5050	33	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	22	0	26	0	0
3	B	22	0	26	0	0
4	A	318	0	0	4	0
4	B	272	0	0	3	0
All	All	11262	0	10152	63	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 3.

All (63) 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:340:ARG:HH12	1:B:465:ASN:HD22	1.29	0.79
1:A:340:ARG:HH12	1:A:465:ASN:HD22	1.33	0.74
1:A:82:ASN:HD22	1:A:96:ALA:HB1	1.56	0.70
1:B:333:HIS:HD2	4:B:779:HOH:O	1.85	0.59
1:B:124:THR:O	1:B:128:HIS:HD2	1.87	0.58
1:A:453:ARG:HH11	1:A:472:GLY:HA2	1.69	0.57
1:A:82:ASN:ND2	1:A:101:TRP:H	2.03	0.56
1:A:170:ASP:OD1	1:A:177:HIS:HE1	1.88	0.56
1:B:361:GLY:HA3	1:B:366:MET:SD	2.45	0.56
1:A:503:ASN:HD22	1:A:504:VAL:H	1.55	0.55
1:B:655:LYS:HG2	1:B:660:VAL:HG22	1.89	0.55
1:A:126:HIS:HE1	1:A:224:ASP:OD2	1.90	0.54
1:A:177:HIS:HD2	4:A:1147:HOH:O	1.90	0.54
1:B:401:ASN:HD22	1:B:403:ALA:H	1.56	0.53
1:B:11:ASN:ND2	4:B:1225:HOH:O	2.41	0.52
1:A:397:LEU:HD11	1:A:459:VAL:HG11	1.90	0.52
1:B:592:VAL:HB	1:B:681:ASN:HA	1.92	0.52
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.45	0.52
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.92	0.52
1:A:78:GLN:NE2	1:A:137:ALA:H	2.09	0.50
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.94	0.49
1:B:653:LEU:HD12	1:B:660:VAL:HG13	1.95	0.49
1:B:389:GLN:O	1:B:393:LYS:HG2	2.13	0.49
1:B:342:LEU:HD23	1:B:365:TYR:CD1	2.48	0.48
1:A:408:SER:O	1:A:423:ARG:HA	2.14	0.48
1:B:378:LEU:HD21	1:B:381:PHE:CZ	2.48	0.48
1:A:361:GLY:HA3	1:A:366:MET:SD	2.54	0.48
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.74	0.47
1:A:193:ASN:OD1	1:A:199:ASP:HB2	2.14	0.47
1:B:80:VAL:HA	1:B:107:LYS:O	2.15	0.47
1:A:599:ALA:H	1:A:602:GLN:HE21	1.62	0.46
1:B:649:GLU:HA	1:B:668:ARG:O	2.16	0.45
1:A:460:LEU:O	1:A:463:ILE:HG12	2.16	0.45
1:B:280:LEU:H	1:B:320:GLN:NE2	2.14	0.45
1:A:82:ASN:HD21	1:A:99:GLY:C	2.24	0.45
1:A:47:ARG:HH11	1:A:92:VAL:HG11	1.82	0.45
1:B:537:THR:HB	4:B:1068:HOH:O	2.16	0.45
1:B:506:PRO:HD2	1:B:515:ILE:HG22	2.00	0.44
1:A:296:ASN:HB2	4:A:1030:HOH:O	2.17	0.44
1:B:340:ARG:HH22	1:B:465:ASN:ND2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:SER:HA	1:B:267:PRO:HD3	1.87	0.44
1:A:340:ARG:HH22	1:A:465:ASN:ND2	2.16	0.44
1:B:598:THR:HG22	1:B:654:LYS:HD2	2.00	0.44
1:B:648:ILE:O	1:B:669:THR:HA	2.18	0.44
1:B:647:THR:HA	1:B:670:PHE:O	2.17	0.43
1:B:598:THR:HB	1:B:602:GLN:HB3	2.00	0.43
1:A:92:VAL:HG13	1:A:94:ASN:HD21	1.84	0.42
1:A:82:ASN:HD21	1:A:101:TRP:H	1.68	0.42
1:B:515:ILE:O	1:B:550:GLN:HA	2.19	0.42
1:B:340:ARG:HH12	1:B:465:ASN:ND2	2.08	0.42
1:B:656:GLN:O	1:B:659:THR:HG22	2.19	0.42
1:A:47:ARG:HH21	1:A:372:PRO:HD3	1.84	0.42
1:B:142:SER:OG	1:B:155:GLY:HA2	2.20	0.42
1:B:593:ILE:HG21	1:B:604:VAL:HG11	2.02	0.41
1:A:89:TYR:O	1:A:92:VAL:HG12	2.19	0.41
1:B:340:ARG:NH1	1:B:465:ASN:HD22	2.06	0.41
1:B:401:ASN:HD22	1:B:401:ASN:C	2.28	0.41
1:B:593:ILE:HD11	1:B:684:TRP:HA	2.03	0.41
1:A:508:MET:HA	1:A:580:GLU:O	2.20	0.41
1:A:651:LYS:HG2	4:A:1002:HOH:O	2.21	0.41
1:A:333:HIS:HD2	4:A:803:HOH:O	2.04	0.41
1:A:146:SER:HA	1:A:168:THR:OG1	2.21	0.41
1:B:625:MET:HG2	1:B:638:TYR:HB2	2.02	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	684/686 (100%)	665 (97%)	19 (3%)	0	100	100
1	B	684/686 (100%)	661 (97%)	23 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1368/1372 (100%)	1326 (97%)	42 (3%)	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	564/564 (100%)	547 (97%)	17 (3%)	36	38
1	B	564/564 (100%)	546 (97%)	18 (3%)	34	35
All	All	1128/1128 (100%)	1093 (97%)	35 (3%)	35	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	48	LEU
1	A	66	LEU
1	A	85	SER
1	A	163	LEU
1	A	227	ARG
1	A	280	LEU
1	A	372	PRO
1	A	378	LEU
1	A	439	ASN
1	A	494	THR
1	A	497	THR
1	A	537	THR
1	A	593	ILE
1	A	600	LEU
1	A	619	ASN
1	A	658	SER
1	B	13	SER
1	B	80	VAL
1	B	82	ASN

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Mol	Chain	Res	Type
1	B	160	ASN
1	B	163	LEU
1	B	169	ASN
1	B	173	ASN
1	B	194	LEU
1	B	211	LEU
1	B	336	ASN
1	B	372	PRO
1	B	378	LEU
1	B	401	ASN
1	B	524	SER
1	B	575	ILE
1	B	613	LEU
1	B	682	VAL
1	B	685	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	55	GLN
1	A	78	GLN
1	A	82	ASN
1	A	94	ASN
1	A	116	GLN
1	A	126	HIS
1	A	128	HIS
1	A	129	ASN
1	A	177	HIS
1	A	203	ASN
1	A	247	ASN
1	A	316	GLN
1	A	333	HIS
1	A	370	ASN
1	A	392	GLN
1	A	435	ASN
1	A	439	ASN
1	A	465	ASN
1	A	503	ASN
1	A	550	GLN
1	A	578	ASN
1	A	594	ASN

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Mol	Chain	Res	Type
1	A	602	GLN
1	A	619	ASN
1	A	685	GLN
1	B	11	ASN
1	B	55	GLN
1	B	59	ASN
1	B	129	ASN
1	B	177	HIS
1	B	320	GLN
1	B	333	HIS
1	B	401	ASN
1	B	416	ASN
1	B	465	ASN
1	B	467	ASN
1	B	548	GLN
1	B	550	GLN
1	B	619	ASN
1	B	620	ASN
1	B	646	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	NOJ	B	2693	-	11,11,11	1.92	3 (27%)	13,15,15	2.98	7 (53%)
3	NOJ	B	2694	-	11,11,11	1.89	3 (27%)	13,15,15	1.73	4 (30%)
3	NOJ	A	2691	-	11,11,11	1.67	3 (27%)	13,15,15	1.64	3 (23%)
3	NOJ	A	2692	-	11,11,11	2.44	3 (27%)	13,15,15	1.84	5 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NOJ	B	2693	-	-	0/2/19/19	0/1/1/1
3	NOJ	B	2694	-	-	2/2/19/19	0/1/1/1
3	NOJ	A	2691	-	-	2/2/19/19	0/1/1/1
3	NOJ	A	2692	-	-	2/2/19/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2692	NOJ	C1-C2	6.78	1.58	1.52
3	B	2693	NOJ	C4-C5	4.07	1.61	1.52
3	A	2692	NOJ	C4-C5	3.54	1.59	1.52
3	A	2691	NOJ	C1-C2	3.30	1.55	1.52
3	B	2693	NOJ	C1-C2	3.29	1.55	1.52
3	B	2694	NOJ	C4-C5	3.25	1.59	1.52
3	B	2694	NOJ	C1-C2	3.22	1.55	1.52
3	A	2691	NOJ	C4-C5	3.17	1.59	1.52
3	B	2694	NOJ	C6-C5	2.76	1.57	1.52
3	A	2691	NOJ	C6-C5	2.31	1.57	1.52
3	B	2693	NOJ	C4-C3	2.26	1.58	1.52
3	A	2692	NOJ	C6-C5	2.10	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2693	NOJ	C3-C4-C5	-4.59	104.29	111.02
3	B	2693	NOJ	O2-C2-C1	4.18	117.75	109.65
3	B	2693	NOJ	O2-C2-C3	-4.08	101.70	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2693	NOJ	C1-C2-C3	3.95	115.07	110.25
3	B	2693	NOJ	O3-C3-C2	-3.91	102.08	110.05
3	B	2694	NOJ	C1-N5-C5	3.86	118.18	109.71
3	A	2692	NOJ	C1-N5-C5	3.58	117.57	109.71
3	A	2691	NOJ	C1-N5-C5	3.28	116.91	109.71
3	A	2692	NOJ	C1-C2-C3	3.04	113.97	110.25
3	B	2693	NOJ	O4-C4-C5	3.01	115.66	109.40
3	B	2693	NOJ	C6-C5-C4	2.89	122.44	112.03
3	A	2691	NOJ	C3-C4-C5	-2.75	106.98	111.02
3	A	2692	NOJ	O2-C2-C3	-2.61	104.75	110.15
3	A	2691	NOJ	O4-C4-C5	2.52	114.63	109.40
3	A	2692	NOJ	C4-C5-N5	2.39	113.95	109.12
3	B	2694	NOJ	C2-C3-C4	-2.33	106.77	110.86
3	B	2694	NOJ	O2-C2-C3	-2.06	105.89	110.15
3	B	2694	NOJ	O2-C2-C1	2.05	113.63	109.65
3	A	2692	NOJ	O4-C4-C3	-2.04	105.57	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2691	NOJ	N5-C5-C6-O6
3	A	2692	NOJ	C4-C5-C6-O6
3	A	2692	NOJ	N5-C5-C6-O6
3	B	2694	NOJ	C4-C5-C6-O6
3	B	2694	NOJ	N5-C5-C6-O6
3	A	2691	NOJ	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	686/686 (100%)	-0.74	1 (0%) 92 91	4, 11, 25, 46	0
1	B	686/686 (100%)	-0.55	2 (0%) 90 89	6, 14, 32, 53	0
All	All	1372/1372 (100%)	-0.64	3 (0%) 91 90	4, 12, 30, 53	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	4.0
1	B	336	ASN	3.1
1	A	90	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	NOJ	A	2691	11/11	0.34	0.31	6,15,19,25	0
3	NOJ	B	2693	11/11	0.54	0.30	8,15,18,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NOJ	A	2692	11/11	0.57	0.31	7,11,17,18	0
3	NOJ	B	2694	11/11	0.71	0.23	8,13,21,24	0
2	CA	B	1690	1/1	0.91	0.05	12,12,12,12	0
2	CA	A	1688	1/1	0.95	0.04	10,10,10,10	0
2	CA	B	1689	1/1	0.97	0.05	11,11,11,11	0
2	CA	A	1687	1/1	0.98	0.05	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.