



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:53 PM UTC

PDB ID : 1D7F / pdb_00001d7f
Title : CRYSTAL STRUCTURE OF ASPARAGINE 233-REPLACED CYCLODEX-
TRIN GLUCANOTRANSFERASE FROM ALKALOPHILIC BACILLUS SP.
1011 DETERMINED AT 1.9 Å RESOLUTION
Authors : Ishii, N.; Haga, K.; Yamane, K.; Harata, K.
Deposited on : 1999-10-18
Resolution : 1.90 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
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

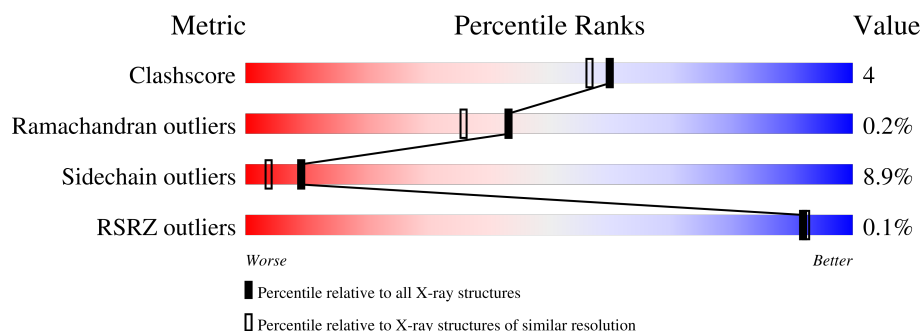
1 Overall quality at a glance

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))
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	686	 78% 16% 5% •
1	B	686	 77% 18% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11435 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
			5310	3352	905	1037	16			
1	B	686	Total	C	N	O	S	0	0	0
			5310	3352	905	1037	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	ASN	HIS	engineered mutation	UNP P05618
A	452	PRO	ARG	conflict	UNP P05618
A	454	GLY	ALA	conflict	UNP P05618
B	233	ASN	HIS	engineered mutation	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		

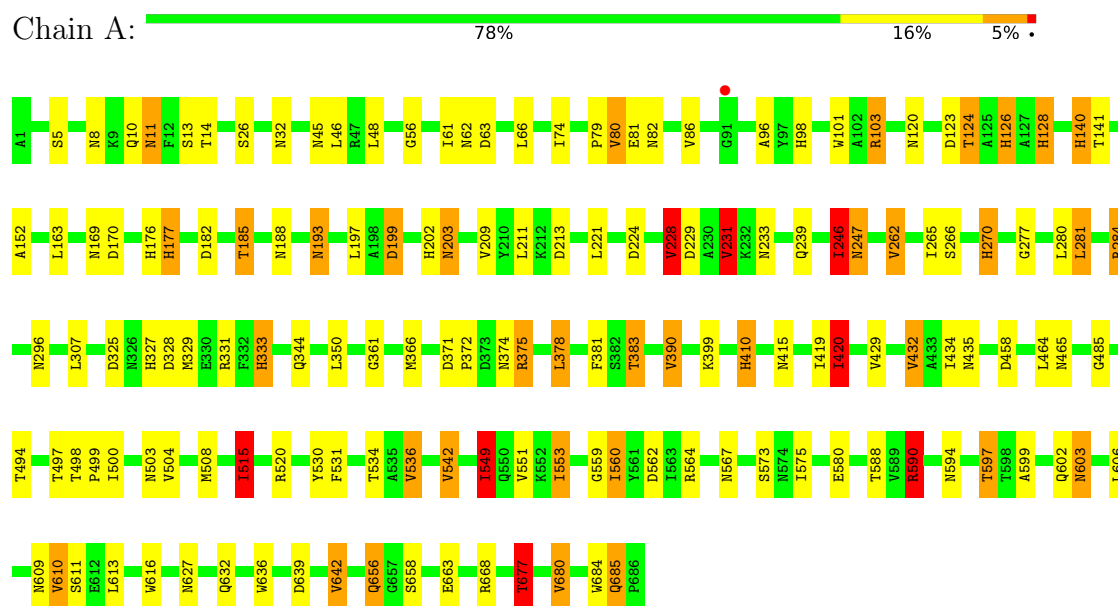
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	431	Total	O	0	0
			431	431		
3	B	380	Total	O	0	0
			380	380		

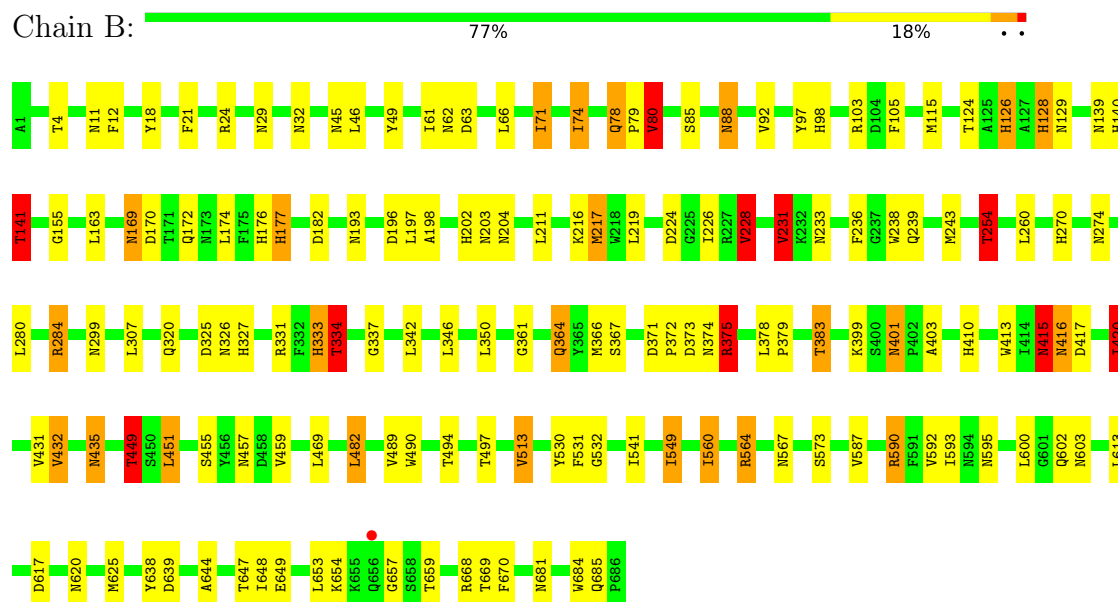
3 Residue-property plots

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	64.86Å 74.46Å 79.10Å 85.10° 105.00° 100.90°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	75.5 (10.00-1.90) 92.3 (10.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.86Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.156 , 0.203 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.6	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	0.96	EDS
Total number of atoms	11435	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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

5.1 Standard geometry

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

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	0.99	22/5443 (0.4%)	1.72	99/7425 (1.3%)
1	B	0.98	19/5443 (0.3%)	1.69	89/7425 (1.2%)
All	All	0.98	41/10886 (0.4%)	1.70	188/14850 (1.3%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	VAL	CA-CB	10.90	1.67	1.54
1	A	228	VAL	CA-CB	9.14	1.65	1.54
1	B	420	ILE	CA-CB	8.94	1.66	1.54
1	A	98	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	140	HIS	CD2-NE2	-7.32	1.29	1.37
1	A	420	ILE	CA-CB	7.32	1.63	1.54
1	B	140	HIS	CD2-NE2	-7.11	1.30	1.37
1	B	126	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	333	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	549	ILE	CA-CB	6.93	1.64	1.54
1	B	176	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	333	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	246	ILE	CA-CB	6.73	1.63	1.54
1	B	549	ILE	CA-CB	6.73	1.63	1.54
1	A	176	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	327	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	128	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	410	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	128	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	390	VAL	CA-CB	6.22	1.63	1.54
1	B	98	HIS	CD2-NE2	-6.16	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	HIS	CD2-NE2	-6.15	1.31	1.37
1	B	432	VAL	CA-CB	6.15	1.63	1.54
1	B	410	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	141	THR	CA-C	5.86	1.55	1.52
1	B	513	VAL	CA-CB	5.84	1.62	1.54
1	A	536	VAL	CA-CB	5.79	1.62	1.54
1	B	270	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	680	VAL	CA-CB	5.78	1.61	1.54
1	A	128	HIS	CG-ND1	-5.75	1.31	1.38
1	A	270	HIS	CD2-NE2	-5.57	1.31	1.37
1	B	202	HIS	CD2-NE2	-5.56	1.31	1.37
1	A	202	HIS	CD2-NE2	-5.51	1.31	1.37
1	B	254	THR	CA-CB	5.40	1.67	1.53
1	B	177	HIS	CG-ND1	-5.23	1.32	1.38
1	A	177	HIS	CG-ND1	-5.12	1.32	1.38
1	A	542	VAL	CA-CB	5.11	1.61	1.54
1	A	233	ASN	CA-CB	5.03	1.60	1.53

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	VAL	N-CA-CB	-14.05	96.42	111.87
1	A	233	ASN	OD1-CG-ND2	-12.89	109.71	122.60
1	B	415	ASN	CA-CB-CG	11.02	123.62	112.60
1	A	642	VAL	CB-CA-C	10.55	121.28	109.89
1	A	677	THR	N-CA-CB	-10.39	94.91	111.43
1	A	685	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	A	668	ARG	NE-CZ-NH2	9.43	127.69	119.20
1	A	668	ARG	NE-CZ-NH1	-8.82	112.67	121.50
1	B	595	ASN	OD1-CG-ND2	-8.48	114.11	122.60
1	B	88	ASN	N-CA-C	8.44	122.08	111.69
1	B	325	ASP	CA-CB-CG	8.42	121.02	112.60
1	B	415	ASN	OD1-CG-ND2	-8.42	114.18	122.60
1	A	415	ASN	CA-CB-CG	8.41	121.01	112.60
1	B	11	ASN	OD1-CG-ND2	-8.11	114.49	122.60
1	B	141	THR	N-CA-CB	-8.10	95.36	111.15
1	A	231	VAL	N-CA-CB	-8.04	96.90	110.65
1	B	331	ARG	NE-CZ-NH2	-7.99	112.01	119.20
1	A	383	THR	N-CA-CB	-7.84	99.09	110.47
1	A	435	ASN	OD1-CG-ND2	-7.84	114.76	122.60
1	B	228	VAL	CA-C-O	7.83	128.95	120.57
1	A	685	GLN	CG-CD-NE2	7.79	128.09	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	656	GLN	OE1-CD-NE2	-7.72	114.88	122.60
1	A	325	ASP	CA-CB-CG	7.63	120.23	112.60
1	A	233	ASN	CB-CG-ND2	7.62	127.83	116.40
1	A	63	ASP	CA-CB-CG	7.60	120.20	112.60
1	A	98	HIS	CB-CG-CD2	-7.57	121.36	131.20
1	B	233	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	182	ASP	CA-CB-CG	7.38	119.97	112.60
1	A	32	ASN	CA-CB-CG	7.13	119.73	112.60
1	B	415	ASN	CB-CG-ND2	7.07	127.00	116.40
1	B	139	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	A	228	VAL	CA-C-O	7.02	128.08	120.57
1	A	80	VAL	N-CA-CB	-6.99	99.23	110.13
1	B	274	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	B	401	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	A	327	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	A	126	HIS	CB-CG-CD2	-6.88	122.26	131.20
1	A	45	ASN	OD1-CG-ND2	-6.83	115.78	122.60
1	B	383	THR	N-CA-CB	-6.81	100.41	110.49
1	B	11	ASN	CB-CG-ND2	6.71	126.47	116.40
1	B	176	HIS	CB-CG-CD2	-6.68	122.51	131.20
1	A	597	THR	N-CA-CB	-6.68	100.15	109.97
1	A	371	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	620	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	A	98	HIS	CB-CG-ND1	6.54	132.50	122.70
1	B	169	ASN	CA-CB-CG	-6.49	106.11	112.60
1	B	449	THR	N-CA-CB	-6.49	101.11	111.62
1	B	98	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	331	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	270	HIS	CA-CB-CG	-6.40	107.40	113.80
1	A	560	ILE	CB-CG1-CD1	-6.40	100.36	113.80
1	A	610	VAL	N-CA-CB	-6.39	99.98	111.92
1	B	602	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	A	61	ILE	N-CA-C	-6.33	104.68	110.82
1	B	617	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	609	ASN	N-CA-C	6.30	119.99	112.93
1	B	74	ILE	N-CA-CB	-6.30	101.10	111.44
1	A	296	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	172	GLN	N-CA-C	-6.30	99.01	109.46
1	B	126	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	A	627	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	465	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	A	458	ASP	CA-CB-CG	6.21	118.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	567	ASN	CA-CB-CG	6.20	118.80	112.60
1	A	277	GLY	N-CA-C	-6.17	106.90	114.92
1	A	594	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	B	685	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	B	684	TRP	CG-CD2-CE3	6.12	140.02	133.90
1	B	334	THR	N-CA-CB	-6.11	100.46	110.41
1	A	266	SER	CA-C-N	6.10	125.82	119.05
1	A	266	SER	C-N-CA	6.10	125.82	119.05
1	A	333	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	642	VAL	O-C-N	-6.09	117.46	121.72
1	A	515	ILE	CA-CB-CG2	6.08	120.84	110.50
1	A	329	MET	CG-SD-CE	-6.07	87.54	100.90
1	B	129	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	8	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	86	VAL	N-CA-C	-6.04	99.03	107.80
1	B	63	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	590	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	A	567	ASN	CA-CB-CG	5.99	118.59	112.60
1	A	247	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	373	ASP	N-CA-C	5.94	119.79	112.54
1	A	140	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	B	140	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	B	334	THR	CB-CA-C	5.92	119.64	109.51
1	B	320	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	A	531	PHE	N-CA-C	-5.89	97.56	107.99
1	B	80	VAL	N-CA-CB	-5.86	99.02	110.45
1	B	203	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	B	602	GLN	N-CA-C	-5.83	100.16	109.96
1	B	549	ILE	CB-CG1-CD1	-5.81	101.59	113.80
1	B	98	HIS	CB-CG-ND1	5.81	131.42	122.70
1	B	595	ASN	CB-CG-ND2	5.81	125.11	116.40
1	B	85	SER	N-CA-C	5.80	118.24	110.35
1	A	553	ILE	CA-C-N	5.79	125.77	120.21
1	A	553	ILE	C-N-CA	5.79	125.77	120.21
1	B	74	ILE	CA-CB-CG1	-5.79	100.56	110.40
1	A	632	GLN	OE1-CD-NE2	-5.75	116.86	122.60
1	B	620	ASN	CB-CG-ND2	5.73	125.00	116.40
1	B	61	ILE	N-CA-C	-5.71	104.78	111.00
1	A	262	VAL	CA-C-O	-5.68	113.68	120.78
1	B	193	ASN	CA-CB-CG	5.68	118.28	112.60
1	B	231	VAL	N-CA-CB	-5.68	100.94	110.65
1	A	610	VAL	CB-CA-C	5.67	120.86	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	PHE	CA-CB-CG	5.66	119.46	113.80
1	A	203	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	10	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	B	193	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	677	THR	CB-CA-C	5.63	121.45	110.30
1	B	326	ASN	CA-CB-CG	5.62	118.22	112.60
1	B	182	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	327	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	B	12	PHE	CA-CB-CG	5.59	119.39	113.80
1	A	8	ASN	CB-CG-ND2	5.59	124.79	116.40
1	A	62	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	265	ILE	N-CA-C	-5.57	100.31	108.11
1	A	374	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	435	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	B	32	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	375	ARG	NE-CZ-NH2	-5.55	114.21	119.20
1	B	541	ILE	N-CA-C	-5.54	99.08	107.73
1	A	498	THR	CA-C-O	-5.53	115.54	120.19
1	B	216	LYS	CB-CG-CD	-5.53	98.59	111.30
1	B	364	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	B	375	ARG	N-CA-C	5.48	117.02	110.44
1	A	193	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	603	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	B	21	PHE	N-CA-C	-5.44	98.42	107.99
1	A	383	THR	CA-CB-OG1	-5.42	101.47	109.60
1	B	560	ILE	CB-CG1-CD1	-5.42	102.42	113.80
1	B	219	LEU	N-CA-C	-5.40	105.47	111.36
1	B	141	THR	CB-CA-C	5.38	124.26	114.52
1	B	531	PHE	N-CA-C	-5.38	97.02	107.62
1	B	457	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	564	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	B	196	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	420	ILE	CA-C-O	5.37	125.69	120.27
1	A	123	ASP	CA-C-O	-5.37	114.86	120.55
1	A	515	ILE	CA-CB-CG1	-5.36	101.28	110.40
1	B	45	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	559	GLY	CA-C-N	-5.34	116.21	123.10
1	A	559	GLY	C-N-CA	-5.34	116.21	123.10
1	A	597	THR	CB-CA-C	5.33	118.76	109.65
1	B	74	ILE	CB-CA-C	5.31	118.68	110.50
1	A	202	HIS	CB-CG-CD2	-5.30	124.30	131.20
1	A	246	ILE	CB-CG1-CD1	-5.30	102.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	B	238	TRP	CG-CD2-CE3	5.27	139.17	133.90
1	A	281	LEU	N-CA-C	-5.27	101.84	109.59
1	A	684	TRP	CG-CD2-CE3	5.26	139.16	133.90
1	B	416	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	231	VAL	CB-CA-C	5.25	120.30	112.16
1	B	270	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	333	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	10	GLN	CG-CD-NE2	5.20	124.20	116.40
1	B	74	ILE	CA-CB-CG2	5.19	119.32	110.50
1	A	383	THR	CB-CA-C	5.17	119.58	110.37
1	B	451	LEU	CA-C-N	5.17	125.17	119.89
1	B	451	LEU	C-N-CA	5.17	125.17	119.89
1	B	457	ASN	N-CA-CB	5.16	117.60	110.17
1	A	229	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	79	PRO	CA-C-N	5.15	128.07	120.91
1	A	79	PRO	C-N-CA	5.15	128.07	120.91
1	A	270	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	A	419	ILE	CA-C-N	-5.14	116.41	123.14
1	A	419	ILE	C-N-CA	-5.14	116.41	123.14
1	B	233	ASN	CB-CG-ND2	5.13	124.10	116.40
1	B	62	ASN	N-CA-C	5.12	117.76	111.82
1	B	79	PRO	CA-C-N	5.11	128.21	120.75
1	B	79	PRO	C-N-CA	5.11	128.21	120.75
1	B	202	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	152	ALA	CB-CA-C	-5.10	110.67	116.54
1	A	590	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	B	78	GLN	CG-CD-NE2	5.08	124.03	116.40
1	A	262	VAL	CA-C-N	-5.08	115.01	122.83
1	A	262	VAL	C-N-CA	-5.08	115.01	122.83
1	B	29	ASN	O-C-N	-5.07	117.23	121.44
1	B	169	ASN	N-CA-C	5.06	118.23	111.24
1	A	485	GLY	CA-C-N	5.06	124.78	119.92
1	A	485	GLY	C-N-CA	5.06	124.78	119.92
1	B	129	ASN	N-CA-C	5.06	118.42	111.54
1	A	616	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	213	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	126	HIS	CB-CG-ND1	5.04	130.25	122.70
1	A	656	GLN	CG-CD-NE2	5.03	123.94	116.40
1	B	371	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	88	ASN	CA-CB-CG	-5.01	107.59	112.60

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	5310	0	5049	42	0
1	B	5310	0	5049	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	431	0	0	4	0
3	B	380	0	0	3	0
All	All	11435	0	10098	90	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 4.

All (90) 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:82:ASN:HD22	1:A:96:ALA:HB1	1.40	0.85
1:B:431:VAL:HG23	1:B:490:TRP:HE3	1.52	0.74
1:B:18:TYR:HB2	1:B:71:ILE:HG12	1.70	0.71
1:B:231:VAL:HG22	1:B:239:GLN:HE22	1.56	0.70
1:B:141:THR:HG22	1:B:198:ALA:HB3	1.74	0.68
1:A:203:ASN:O	1:A:677:THR:HG21	1.94	0.68
1:B:115:MET:HE1	1:B:217:MET:HE1	1.79	0.64
1:B:378:LEU:HD12	1:B:379:PRO:HD2	1.80	0.62
1:A:82:ASN:ND2	1:A:101:TRP:H	1.98	0.62
1:A:82:ASN:HD21	1:A:101:TRP:H	1.47	0.62
1:B:449:THR:HG23	1:B:451:LEU:H	1.64	0.62
1:B:226:ILE:HB	1:B:254:THR:HB	1.80	0.61
1:A:231:VAL:HG22	1:A:239:GLN:HE22	1.64	0.60
1:B:459:VAL:HG22	1:B:489:VAL:HB	1.82	0.60
1:A:344:GLN:HB3	1:A:434:ILE:HD11	1.84	0.60
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.83	0.60
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.37	0.60
1:A:503:ASN:HD22	1:A:504:VAL:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HD3	1:A:639:ASP:OD2	2.03	0.59
1:B:590:ARG:HD3	1:B:639:ASP:OD2	2.02	0.59
1:A:11:ASN:ND2	3:A:5376:HOH:O	2.35	0.59
1:A:599:ALA:H	1:A:602:GLN:HE21	1.50	0.59
1:A:120:ASN:O	1:A:124:THR:HG23	2.04	0.58
1:A:284:ARG:HD2	3:A:5370:HOH:O	2.04	0.58
1:B:124:THR:O	1:B:128:HIS:HD2	1.86	0.58
1:A:170:ASP:OD1	1:A:177:HIS:HE1	1.89	0.56
1:B:564:ARG:HD3	1:B:573:SER:O	2.06	0.56
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.89	0.55
1:B:334:THR:HG22	1:B:337:GLY:HA3	1.88	0.55
1:B:231:VAL:HG22	1:B:239:GLN:NE2	2.21	0.55
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.89	0.54
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.91	0.54
1:B:333:HIS:HD2	3:B:5362:HOH:O	1.89	0.54
1:A:515:ILE:HD13	1:A:553:ILE:HD11	1.90	0.54
1:B:243:MET:HE1	1:B:254:THR:HG23	1.91	0.53
1:B:401:ASN:HD22	1:B:403:ALA:H	1.57	0.53
1:B:364:GLN:HG3	1:B:378:LEU:HD11	1.91	0.52
1:B:415:ASN:ND2	1:B:417:ASP:H	2.08	0.52
1:A:81:GLU:OE2	1:A:103:ARG:HD2	2.11	0.50
1:B:415:ASN:HD22	1:B:417:ASP:H	1.58	0.50
1:A:124:THR:O	1:A:128:HIS:HD2	1.94	0.49
1:A:599:ALA:H	1:A:602:GLN:NE2	2.11	0.49
1:A:228:VAL:HG22	1:A:231:VAL:HG23	1.94	0.49
1:B:649:GLU:HA	1:B:668:ARG:O	2.12	0.48
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.96	0.47
1:B:141:THR:HG21	1:B:155:GLY:O	2.15	0.47
1:A:549:ILE:HD11	1:A:551:VAL:HB	1.96	0.47
1:B:592:VAL:HB	1:B:681:ASN:HA	1.96	0.46
1:B:228:VAL:HG22	1:B:231:VAL:HG23	1.96	0.46
1:B:413:TRP:HB3	1:B:420:ILE:HG23	1.97	0.46
1:B:243:MET:HE1	1:B:254:THR:CG2	2.46	0.46
1:B:361:GLY:HA3	1:B:366:MET:SD	2.56	0.45
1:A:333:HIS:HD2	3:A:5087:HOH:O	2.00	0.45
1:A:503:ASN:HD22	1:A:504:VAL:N	2.14	0.45
1:A:231:VAL:HG22	1:A:239:GLN:NE2	2.31	0.45
1:A:663:GLU:HB2	1:A:685:GLN:O	2.17	0.45
1:A:185:THR:HG22	1:A:188:ASN:H	1.82	0.45
1:A:361:GLY:HA3	1:A:366:MET:SD	2.57	0.45
1:A:603:ASN:HD22	1:A:636:TRP:HH2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:HA	1:B:24:ARG:HD3	1.89	0.45
1:A:410:HIS:HB2	3:A:5412:HOH:O	2.16	0.44
1:A:82:ASN:ND2	1:A:96:ALA:HB1	2.22	0.44
1:B:603:ASN:O	1:B:654:LYS:HA	2.18	0.44
1:A:420:ILE:HA	1:A:432:VAL:O	2.17	0.43
1:B:4:THR:HB	1:B:399:LYS:HD2	2.00	0.43
1:A:193:ASN:OD1	1:A:199:ASP:HB2	2.18	0.43
1:B:49:TYR:CE1	1:B:97:TYR:HA	2.53	0.43
1:A:508:MET:HA	1:A:580:GLU:O	2.18	0.43
1:B:284:ARG:HB3	3:B:5126:HOH:O	2.18	0.43
1:B:374:ASN:OD1	1:B:375:ARG:HD3	2.19	0.42
1:B:587:VAL:HG13	1:B:644:ALA:HB2	2.00	0.42
1:B:648:ILE:O	1:B:669:THR:HA	2.20	0.42
1:A:26:SER:O	1:A:56:GLY:HA3	2.19	0.42
1:B:78:GLN:HG2	1:B:80:VAL:HB	2.01	0.42
1:B:284:ARG:HD3	3:B:5112:HOH:O	2.19	0.42
1:A:270:HIS:CE1	1:A:284:ARG:HH21	2.38	0.42
1:B:80:VAL:HG13	1:B:105:PHE:HA	2.02	0.41
1:A:530:TYR:HA	1:A:534:THR:O	2.20	0.41
1:B:530:TYR:HB3	1:B:532:GLY:O	2.20	0.41
1:B:647:THR:HA	1:B:670:PHE:O	2.20	0.41
1:A:246:ILE:HG13	1:A:247:ASN:N	2.35	0.41
1:A:14:THR:HB	1:A:399:LYS:HD3	2.03	0.41
1:A:126:HIS:HE1	1:A:224:ASP:OD2	2.03	0.41
1:B:455:SER:HA	1:B:469:LEU:O	2.21	0.41
1:B:435:ASN:HB2	1:B:482:LEU:HD13	2.03	0.41
1:B:647:THR:HG23	1:B:669:THR:HG23	2.03	0.40
1:A:140:HIS:HD2	1:A:141:THR:O	2.05	0.40
1:B:88:ASN:O	1:B:92:VAL:O	2.40	0.40
1:B:299:ASN:HB2	1:B:416:ASN:O	2.21	0.40
1:A:520:ARG:HH21	1:A:520:ARG:HD2	1.68	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	684/686 (100%)	664 (97%)	19 (3%)	1 (0%)	48	40
1	B	684/686 (100%)	663 (97%)	19 (3%)	2 (0%)	36	29
All	All	1368/1372 (100%)	1327 (97%)	38 (3%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	VAL
1	B	600	LEU
1	B	657	GLY

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%)	509 (90%)	55 (10%)	7	3
1	B	564/564 (100%)	519 (92%)	45 (8%)	11	5
All	All	1128/1128 (100%)	1028 (91%)	100 (9%)	9	4

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	13	SER
1	A	46	LEU
1	A	48	LEU
1	A	66	LEU
1	A	74	ILE
1	A	80	VAL
1	A	103	ARG
1	A	124	THR
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	185	THR
1	A	197	LEU
1	A	199	ASP
1	A	209	VAL
1	A	211	LEU
1	A	221	LEU
1	A	228	VAL
1	A	231	VAL
1	A	246	ILE
1	A	280	LEU
1	A	281	LEU
1	A	284	ARG
1	A	307	LEU
1	A	328	ASP
1	A	350	LEU
1	A	372	PRO
1	A	375	ARG
1	A	378	LEU
1	A	383	THR
1	A	390	VAL
1	A	420	ILE
1	A	429	VAL
1	A	432	VAL
1	A	464	LEU
1	A	494	THR
1	A	497	THR
1	A	500	ILE
1	A	515	ILE
1	A	536	VAL
1	A	542	VAL
1	A	549	ILE
1	A	560	ILE
1	A	588	THR
1	A	590	ARG
1	A	597	THR
1	A	606	LEU
1	A	610	VAL
1	A	611	SER
1	A	613	LEU
1	A	642	VAL
1	A	656	GLN

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Mol	Chain	Res	Type
1	A	658	SER
1	A	677	THR
1	A	680	VAL
1	B	46	LEU
1	B	66	LEU
1	B	71	ILE
1	B	74	ILE
1	B	80	VAL
1	B	103	ARG
1	B	141	THR
1	B	163	LEU
1	B	169	ASN
1	B	174	LEU
1	B	197	LEU
1	B	204	ASN
1	B	211	LEU
1	B	217	MET
1	B	228	VAL
1	B	231	VAL
1	B	254	THR
1	B	260	LEU
1	B	280	LEU
1	B	284	ARG
1	B	307	LEU
1	B	334	THR
1	B	342	LEU
1	B	346	LEU
1	B	350	LEU
1	B	367	SER
1	B	372	PRO
1	B	375	ARG
1	B	383	THR
1	B	415	ASN
1	B	420	ILE
1	B	432	VAL
1	B	449	THR
1	B	482	LEU
1	B	494	THR
1	B	497	THR
1	B	513	VAL
1	B	549	ILE
1	B	560	ILE

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Mol	Chain	Res	Type
1	B	564	ARG
1	B	590	ARG
1	B	593	ILE
1	B	613	LEU
1	B	653	LEU
1	B	659	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	55	GLN
1	A	78	GLN
1	A	82	ASN
1	A	116	GLN
1	A	126	HIS
1	A	140	HIS
1	A	172	GLN
1	A	177	HIS
1	A	239	GLN
1	A	247	ASN
1	A	263	ASN
1	A	316	GLN
1	A	333	HIS
1	A	392	GLN
1	A	435	ASN
1	A	479	ASN
1	A	503	ASN
1	A	578	ASN
1	A	602	GLN
1	A	603	ASN
1	A	615	ASN
1	A	632	GLN
1	B	10	GLN
1	B	19	GLN
1	B	55	GLN
1	B	126	HIS
1	B	128	HIS
1	B	177	HIS
1	B	203	ASN
1	B	204	ASN
1	B	233	ASN

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Mol	Chain	Res	Type
1	B	239	GLN
1	B	270	HIS
1	B	333	HIS
1	B	401	ASN
1	B	410	HIS
1	B	415	ASN
1	B	465	ASN
1	B	467	ASN
1	B	479	ASN
1	B	550	GLN
1	B	603	ASN
1	B	619	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

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%)	-0.62	1 (0%) 92 92	8, 17, 30, 54	0
1	B	686/686 (100%)	-0.46	1 (0%) 92 92	10, 19, 40, 67	0
All	All	1372/1372 (100%)	-0.54	2 (0%) 92 92	8, 18, 35, 67	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	GLY	2.2
1	B	656	GLN	2.2

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
2	CA	A	5003	1/1	0.92	0.07	30,30,30,30	0
2	CA	B	5004	1/1	0.92	0.06	29,29,29,29	0
2	CA	B	5002	1/1	0.95	0.06	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	5001	1/1	0.97	0.04	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.