



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:55 PM GMT

PDB ID : 1D7F
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.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

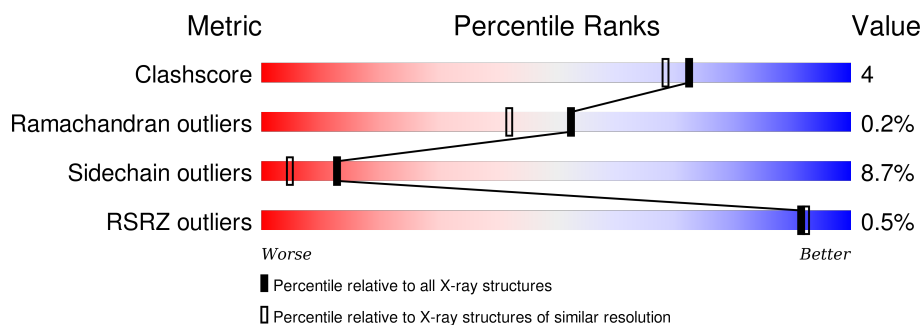
1 Overall quality at a glance

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 80% 16% ..
1	B	686	 81% 16% ..

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	UNP P05618
A	452	PRO	ARG	CONFLICT	UNP P05618
A	454	GLY	ALA	CONFLICT	UNP P05618
B	233	ASN	HIS	ENGINEERED	UNP P05618
B	452	PRO	ARG	CONFLICT	UNP P05618
B	454	GLY	ALA	CONFLICT	UNP P05618

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

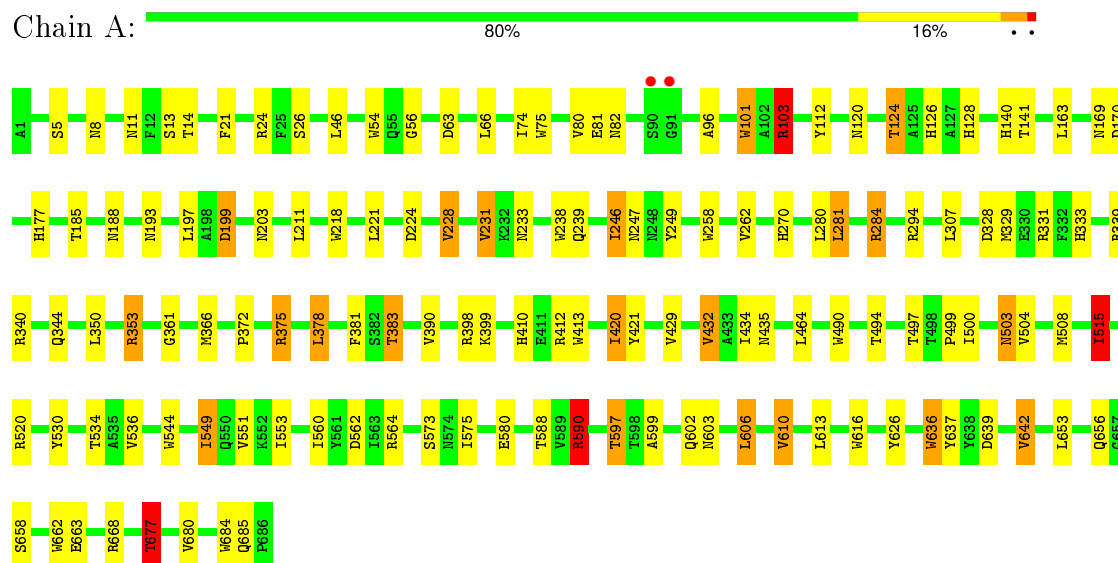
- Molecule 3 is water.

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

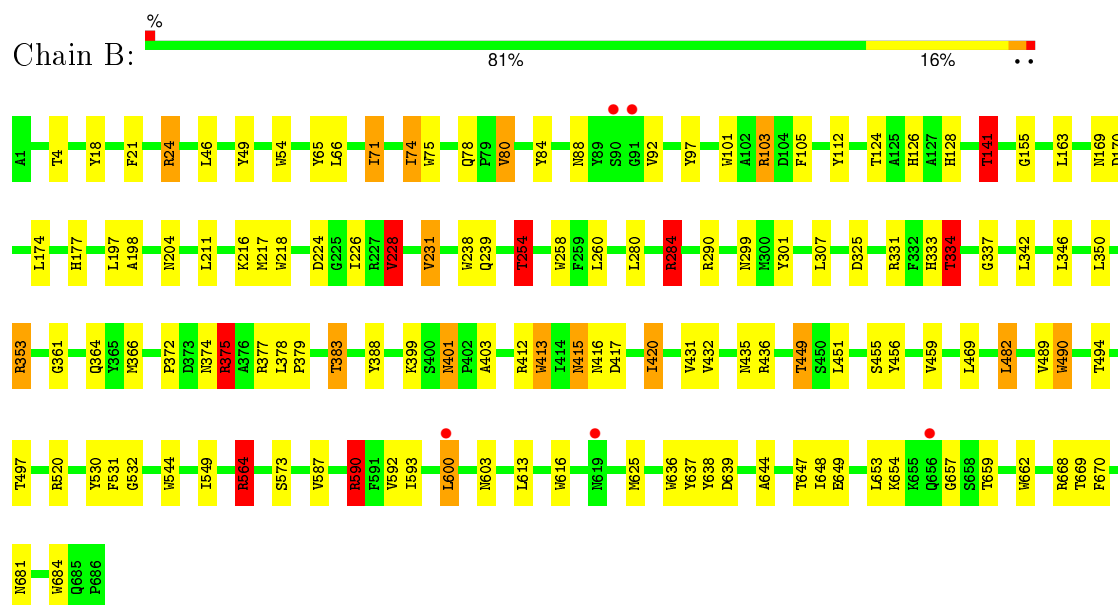
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	64.86 Å 74.46 Å 79.10 Å 85.10° 105.00° 100.90°	Depositor
Resolution (Å)	10.00 – 1.90 20.15 – 1.86	Depositor EDS
% Data completeness (in resolution range)	75.5 (10.00-1.90) 87.7 (20.15-1.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.86 Å)	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.	DCC
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 103616 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.80	0/5443	1.50	82/7425 (1.1%)
1	B	0.79	2/5443 (0.0%)	1.46	73/7425 (1.0%)
All	All	0.79	2/10886 (0.0%)	1.48	155/14850 (1.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	VAL	CA-CB	5.97	1.67	1.54
1	B	254	THR	CA-CB	5.34	1.67	1.53

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	A	668	ARG	NE-CZ-NH1	-15.25	112.67	120.30
1	A	668	ARG	NE-CZ-NH2	14.77	127.69	120.30
1	A	331	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	A	590	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	A	590	ARG	NE-CZ-NH1	12.60	126.60	120.30
1	A	331	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	A	375	ARG	NE-CZ-NH1	12.33	126.46	120.30
1	A	375	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	B	331	ARG	NE-CZ-NH1	12.09	126.35	120.30
1	B	284	ARG	NE-CZ-NH1	11.61	126.10	120.30
1	B	590	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	B	24	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	A	284	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	B	590	ARG	NE-CZ-NH2	-9.53	115.54	120.30
1	B	353	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	112	TYR	CB-CG-CD2	-8.71	115.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	TRP	CD1-CG-CD2	8.63	113.21	106.30
1	B	413	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	B	662	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	A	490	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	103	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	616	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	564	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	B	101	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	B	375	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	B	636	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	A	677	THR	N-CA-CB	-8.10	94.91	110.30
1	B	564	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	B	218	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	A	284	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	329	MET	CG-SD-CE	-7.91	87.54	100.20
1	A	75	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	B	141	THR	N-CA-CB	-7.87	95.36	110.30
1	A	24	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	101	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	A	616	TRP	CE2-CD2-CG	-7.71	101.14	107.30
1	B	684	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	413	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	B	490	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	636	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	A	54	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	B	413	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	B	684	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	B	662	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	B	101	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	B	238	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	B	75	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	B	238	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	103	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	684	TRP	CE2-CD2-CG	-7.41	101.38	107.30
1	A	54	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	B	412	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	B	75	TRP	CE2-CD2-CG	-7.26	101.50	107.30
1	A	294	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	544	TRP	CD1-CG-CD2	7.18	112.05	106.30
1	A	684	TRP	CD1-CG-CD2	7.17	112.03	106.30
1	B	490	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	B	375	ARG	NE-CZ-NH1	7.14	123.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A	75	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	A	636	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	544	TRP	CE2-CD2-CG	-6.98	101.71	107.30
1	B	636	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	662	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	A	340	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	642	VAL	N-CA-CB	-6.86	96.42	111.50
1	B	616	TRP	CE2-CD2-CG	-6.86	101.82	107.30
1	A	339	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	B	544	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	A	413	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	B	684	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	A	258	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	A	339	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	B	218	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	24	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	231	VAL	N-CA-CB	-6.64	96.90	111.50
1	A	238	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	B	544	TRP	CD1-CG-CD2	6.56	111.55	106.30
1	A	353	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	218	TRP	CD1-CG-CD2	6.53	111.52	106.30
1	B	54	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	B	637	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	B	616	TRP	CD1-CG-CD2	6.40	111.42	106.30
1	A	112	TYR	CB-CG-CD1	6.36	124.82	121.00
1	A	238	TRP	CD1-CG-CD2	6.33	111.37	106.30
1	A	101	TRP	CE2-CD2-CG	-6.33	102.24	107.30
1	B	325	ASP	CB-CG-OD1	6.27	123.95	118.30
1	B	217	MET	CA-CB-CG	6.26	123.94	113.30
1	A	218	TRP	CE2-CD2-CG	-6.18	102.36	107.30
1	B	377	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	388	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	B	258	TRP	CD1-CG-CD2	6.16	111.22	106.30
1	B	258	TRP	CE2-CD2-CG	-6.12	102.41	107.30
1	B	112	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	A	642	VAL	CG1-CB-CG2	5.91	120.35	110.90
1	B	54	TRP	CD1-CG-CD2	5.91	111.02	106.30
1	A	383	THR	N-CA-CB	-5.90	99.09	110.30
1	B	238	TRP	CG-CD2-CE3	5.86	139.17	133.90
1	A	684	TRP	CG-CD2-CE3	5.85	139.16	133.90
1	A	258	TRP	CE2-CD2-CG	-5.83	102.64	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	A	637	TYR	CB-CG-CD2	-5.76	117.55	121.00
1	B	80	VAL	N-CA-CB	-5.67	99.02	111.50
1	A	412	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	413	TRP	CB-CG-CD1	-5.61	119.71	127.00
1	A	80	VAL	N-CA-CB	-5.58	99.23	111.50
1	B	103	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	65	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	421	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	A	490	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	B	684	TRP	CB-CG-CD1	-5.54	119.80	127.00
1	A	398	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	353	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	74	ILE	CA-CB-CG1	-5.49	100.56	111.00
1	A	606	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	249	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	B	413	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	B	24	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	301	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	B	662	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	A	340	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	662	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	A	101	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	B	218	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	B	490	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	A	597	THR	N-CA-CB	-5.34	100.15	110.30
1	A	75	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	B	284	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	233	ASN	OD1-CG-ND2	-5.30	109.71	121.90
1	A	616	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	B	662	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	B	101	TRP	CG-CD2-CE3	5.24	138.62	133.90
1	A	610	VAL	N-CA-CB	-5.24	99.98	111.50
1	A	616	TRP	CB-CG-CD1	-5.22	120.22	127.00
1	A	642	VAL	CB-CA-C	5.20	121.28	111.40
1	B	290	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	383	THR	N-CA-CB	-5.20	100.41	110.30
1	A	616	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	A	75	TRP	CG-CD2-CE3	5.18	138.57	133.90
1	B	334	THR	N-CA-CB	-5.18	100.46	110.30
1	B	531	PHE	N-CA-C	-5.18	97.02	111.00
1	B	413	TRP	CG-CD2-CE3	5.13	138.52	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	B	456	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	436	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	515	ILE	CA-CB-CG1	-5.12	101.28	111.00
1	A	281	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	413	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	A	63	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	54	TRP	CG-CD2-CE3	5.03	138.42	133.90
1	A	626	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	B	238	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	B	636	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	B	216	LYS	CB-CG-CD	-5.00	98.59	111.60

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	45	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	87	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 (87) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:124:THR:O	1:B:128:HIS:HD2	1.86	0.58
1:A:284:ARG:HD2	3:A:5370:HOH:O	2.04	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:333:HIS:HD2	3:B:5362:HOH:O	1.89	0.54
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.91	0.54
1:A:515:ILE:HD13	1:A:553:ILE:HD11	1.90	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:603:ASN:HD22	1:A:636:TRP:HH2	1.65	0.45
1:A:361:GLY:HA3	1:A:366:MET:SD	2.57	0.45
1:A:185:THR:HG22	1:A:188:ASN:H	1.82	0.45
1:B:24:ARG:HD3	1:B:24:ARG:HA	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:B:455:SER:HA	1:B:469:LEU:O	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:A:520:ARG:HH21	1.68	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%)	664 (97%)	19 (3%)	1 (0%)	56	46
1	B	684/686 (100%)	663 (97%)	19 (3%)	2 (0%)	46	35
All	All	1368/1372 (100%)	1327 (97%)	38 (3%)	3 (0%)	52	42

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 [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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	564/564 (100%)	511 (91%)	53 (9%)	11 4
1	B	564/564 (100%)	519 (92%)	45 (8%)	15 6
All	All	1128/1128 (100%)	1030 (91%)	98 (9%)	13 5

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	8	ASN
1	A	13	SER
1	A	21	PHE
1	A	46	LEU
1	A	66	LEU
1	A	74	ILE
1	A	103	ARG
1	A	124	THR
1	A	163	LEU
1	A	169	ASN
1	A	197	LEU
1	A	199	ASP
1	A	211	LEU
1	A	221	LEU
1	A	228	VAL
1	A	246	ILE
1	A	280	LEU
1	A	281	LEU
1	A	307	LEU
1	A	328	ASP
1	A	350	LEU
1	A	353	ARG
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	435	ASN

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Mol	Chain	Res	Type
1	A	464	LEU
1	A	494	THR
1	A	497	THR
1	A	500	ILE
1	A	503	ASN
1	A	515	ILE
1	A	536	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	613	LEU
1	A	642	VAL
1	A	653	LEU
1	A	656	GLN
1	A	658	SER
1	A	677	THR
1	A	680	VAL
1	B	21	PHE
1	B	46	LEU
1	B	66	LEU
1	B	71	ILE
1	B	74	ILE
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	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

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Mol	Chain	Res	Type
1	B	342	LEU
1	B	346	LEU
1	B	350	LEU
1	B	353	ARG
1	B	372	PRO
1	B	375	ARG
1	B	383	THR
1	B	401	ASN
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	520	ARG
1	B	549	ILE
1	B	564	ARG
1	B	590	ARG
1	B	593	ILE
1	B	600	LEU
1	B	613	LEU
1	B	653	LEU
1	B	659	THR

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	11	ASN
1	A	78	GLN
1	A	82	ASN
1	A	126	HIS
1	A	177	HIS
1	A	239	GLN
1	A	296	ASN
1	A	333	HIS
1	A	435	ASN
1	A	503	ASN
1	A	594	ASN
1	A	602	GLN
1	A	603	ASN

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Mol	Chain	Res	Type
1	B	126	HIS
1	B	128	HIS
1	B	177	HIS
1	B	204	ASN
1	B	239	GLN
1	B	270	HIS
1	B	333	HIS
1	B	364	GLN
1	B	401	ASN
1	B	410	HIS
1	B	415	ASN
1	B	548	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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%)	-0.55	2 (0%) 94 94	8, 17, 30, 54	0
1	B	686/686 (100%)	-0.40	5 (0%) 89 90	10, 19, 40, 67	0
All	All	1372/1372 (100%)	-0.47	7 (0%) 91 92	8, 18, 35, 67	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	4.6
1	B	90	SER	2.8
1	A	91	GLY	2.7
1	B	656	GLN	2.4
1	A	90	SER	2.4
1	B	619	ASN	2.3
1	B	91	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	5003	1/1	0.92	0.07	-0.62	30,30,30,30	0
2	CA	B	5002	1/1	0.97	0.06	-0.85	19,19,19,19	0
2	CA	B	5004	1/1	0.91	0.06	-1.36	29,29,29,29	0
2	CA	A	5001	1/1	0.99	0.04	-6.52	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.