



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 1V3K / pdb_00001v3k
Title : Crystal structure of F283Y mutant cyclodextrin glycosyltransferase
Authors : Kanai, R.; Haga, K.; Akiba, T.; Yamane, K.; Harata, K.
Deposited on : 2003-11-03
Resolution : 2.00 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
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

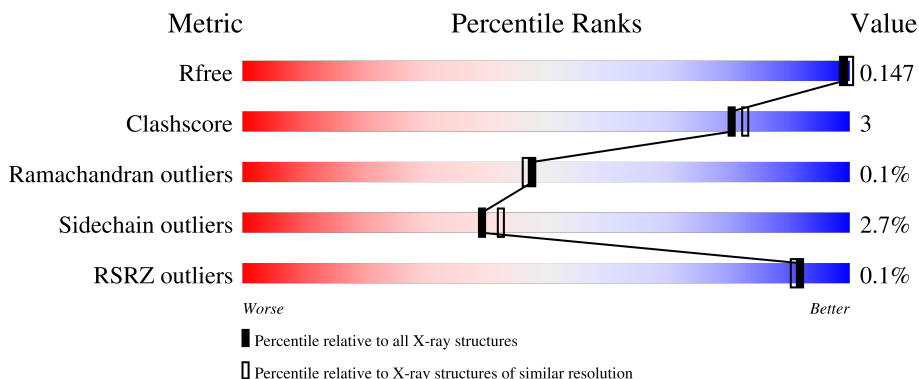
1 Overall quality at a glance

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))
R_{free}	180053	10052 (2.00-2.00)
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	 87% 11% .
1	B	686	 85% 12% .

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 Cyclomaltodextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5313	3354	906	1037	16			
1	B	686	Total	C	N	O	S	0	0	0
			5313	3354	906	1037	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	TYR	PHE	engineered mutation	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	283	TYR	PHE	engineered mutation	UNP P05618
B	452	PRO	ARG	SEE REMARK 999	UNP P05618
B	454	GLY	ALA	SEE REMARK 999	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		

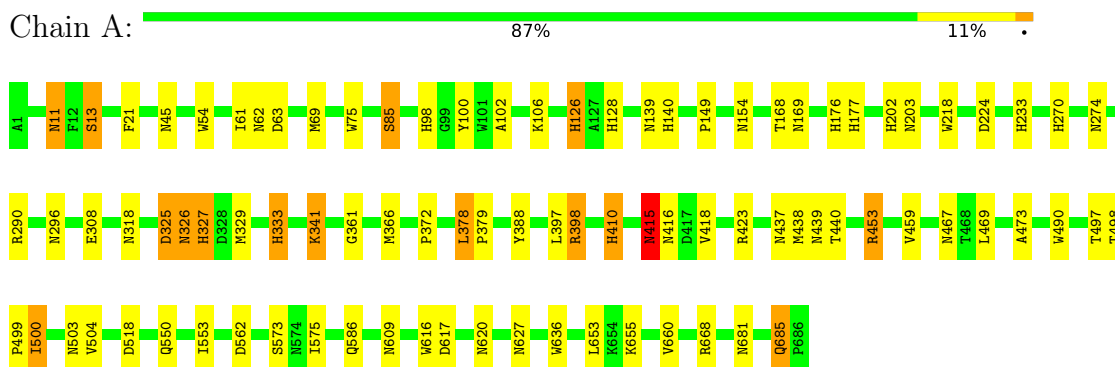
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	436	Total	O	0	0
			436	436		
3	B	369	Total	O	0	0
			369	369		

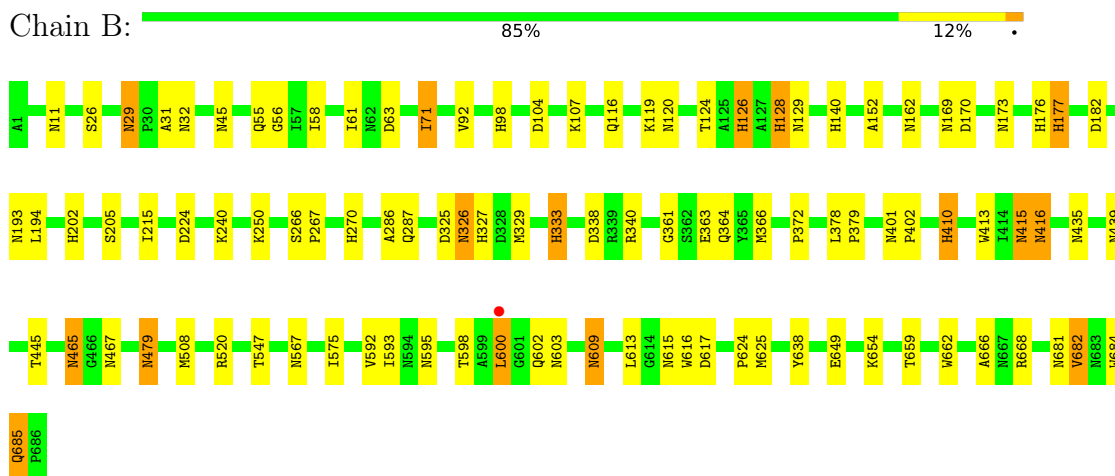
3 Residue-property plots

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: Cyclomaltodextrin glucanotransferase



• Molecule 1: Cyclomaltodextrin glucanotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.88Å 74.43Å 79.01Å 85.15° 105.05° 101.02°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.1 (10.00-2.00) 89.3 (10.00-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.155 , 0.200 0.148 , 0.147	Depositor DCC
R_{free} test set	5099 reflections (6.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	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)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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	0.89	13/5447 (0.2%)	1.55	67/7431 (0.9%)
1	B	0.89	11/5447 (0.2%)	1.57	70/7431 (0.9%)
All	All	0.89	24/10894 (0.2%)	1.56	137/14862 (0.9%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	HIS	CD2-NE2	-7.86	1.29	1.37
1	B	98	HIS	CD2-NE2	-7.25	1.29	1.37
1	B	140	HIS	CD2-NE2	-7.11	1.30	1.37
1	A	333	HIS	CD2-NE2	-6.95	1.30	1.37
1	A	128	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	176	HIS	CD2-NE2	-6.89	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	128	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	176	HIS	CD2-NE2	-6.40	1.30	1.37
1	B	410	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	140	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	233	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	410	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	126	HIS	CD2-NE2	-5.99	1.31	1.37
1	B	177	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	202	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	126	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	333	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	177	HIS	CG-ND1	-5.63	1.32	1.38
1	B	270	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	202	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	270	HIS	CD2-NE2	-5.14	1.32	1.37

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	NE-CZ-NH2	-12.42	108.02	119.20
1	B	416	ASN	CA-CB-CG	10.51	123.11	112.60
1	A	415	ASN	CA-CB-CG	9.37	121.97	112.60
1	B	415	ASN	OD1-CG-ND2	-9.32	113.28	122.60
1	B	682	VAL	N-CA-CB	-9.23	98.60	112.35
1	B	415	ASN	CA-CB-CG	8.43	121.03	112.60
1	B	685	GLN	OE1-CD-NE2	-8.16	114.44	122.60
1	A	327	HIS	CB-CG-CD2	-8.07	120.71	131.20
1	B	325	ASP	CA-CB-CG	7.95	120.55	112.60
1	A	63	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	398	ARG	CG-CD-NE	-7.88	94.67	112.00
1	B	29	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	B	327	HIS	CB-CG-CD2	-7.75	121.13	131.20
1	B	609	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	A	98	HIS	CB-CG-CD2	-7.48	121.47	131.20
1	B	326	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	B	415	ASN	CB-CG-ND2	7.21	127.22	116.40
1	B	98	HIS	CB-CG-CD2	-7.18	121.87	131.20
1	A	550	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	A	415	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	B	410	HIS	CB-CG-CD2	-7.12	121.94	131.20
1	A	62	ASN	OD1-CG-ND2	-7.05	115.55	122.60
1	B	45	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	B	326	ASN	CA-CB-CG	6.87	119.47	112.60
1	B	415	ASN	O-C-N	-6.86	115.65	122.99
1	B	609	ASN	CB-CG-ND2	6.81	126.62	116.40
1	A	627	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	B	615	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	A	326	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	169	ASN	CA-CB-CG	-6.49	106.11	112.60
1	A	126	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	416	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	B	617	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	681	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	B	63	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	498	THR	CA-C-O	-6.31	114.89	120.19
1	B	182	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	326	ASN	CB-CG-ND2	6.24	125.76	116.40
1	A	98	HIS	CB-CG-ND1	6.24	132.06	122.70
1	A	45	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	61	ILE	N-CA-C	-6.18	104.82	110.82
1	B	609	ASN	N-CA-C	6.16	119.83	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	682	VAL	CB-CA-C	6.08	120.07	110.52
1	B	465	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	11	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	B	193	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	139	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	B	685	GLN	CG-CD-NE2	5.97	125.36	116.40
1	A	327	HIS	CB-CG-ND1	5.95	131.63	122.70
1	A	333	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	B	595	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	586	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	274	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	A	616	TRP	CG-CD2-CE3	5.90	139.80	133.90
1	B	32	ASN	CA-CB-CG	5.90	118.50	112.60
1	B	98	HIS	CB-CG-ND1	5.88	131.52	122.70
1	B	327	HIS	CB-CG-ND1	5.86	131.49	122.70
1	A	398	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	B	287	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	B	602	GLN	N-CA-C	-5.83	100.20	109.59
1	B	126	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	A	553	ILE	CA-C-N	5.82	125.79	120.03
1	A	553	ILE	C-N-CA	5.82	125.79	120.03
1	A	410	HIS	CA-CB-CG	5.81	119.61	113.80
1	B	286	ALA	N-CA-C	5.80	117.60	111.28
1	B	467	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	467	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	415	ASN	CB-CG-ND2	5.77	125.05	116.40
1	B	666	ALA	N-CA-C	-5.76	102.78	110.55
1	A	100	TYR	N-CA-C	5.75	120.14	113.18
1	A	177	HIS	CB-CG-CD2	-5.75	123.73	131.20
1	A	685	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	B	107	LYS	CB-CG-CD	-5.68	98.25	111.30
1	A	620	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	B	129	ASN	N-CA-C	5.67	119.25	111.54
1	A	106	LYS	CA-CB-CG	-5.67	102.77	114.10
1	B	333	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	102	ALA	N-CA-C	5.63	118.01	110.35
1	A	500	ILE	CB-CA-C	-5.62	102.13	110.33
1	B	11	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	B	140	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	416	ASN	CB-CG-ND2	5.55	124.72	116.40
1	A	416	ASN	N-CA-C	5.55	118.09	111.71
1	A	75	TRP	CG-CD2-CE3	5.51	139.41	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	435	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	B	363	GLU	CB-CG-CD	5.44	121.85	112.60
1	A	617	ASP	CA-C-N	5.40	125.48	119.32
1	A	617	ASP	C-N-CA	5.40	125.48	119.32
1	A	437	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	29	ASN	CA-C-N	5.39	124.90	119.19
1	B	29	ASN	C-N-CA	5.39	124.90	119.19
1	A	609	ASN	N-CA-C	5.38	118.95	112.93
1	A	440	THR	CA-C-N	5.38	125.32	119.78
1	A	440	THR	C-N-CA	5.38	125.32	119.78
1	B	410	HIS	CB-CG-ND1	5.37	130.75	122.70
1	A	140	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	A	203	ASN	N-CA-C	-5.37	106.69	113.18
1	A	218	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	B	338	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	154	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	685	GLN	CG-CD-NE2	5.31	124.36	116.40
1	B	128	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	54	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	A	325	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	270	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	61	ILE	N-CA-C	-5.24	105.29	111.00
1	A	318	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	423	ARG	N-CA-C	-5.22	100.89	109.40
1	B	120	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	B	205	SER	N-CA-C	5.21	116.96	111.28
1	A	202	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	B	684	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	B	29	ASN	CB-CG-ND2	5.18	124.18	116.40
1	B	176	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	A	85	SER	N-CA-C	5.16	117.51	110.24
1	B	416	ASN	N-CA-C	5.14	119.18	113.01
1	A	616	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	A	497	THR	N-CA-CB	-5.13	102.98	110.47
1	A	439	ASN	CA-CB-CG	5.12	117.72	112.60
1	B	71	ILE	CA-C-O	-5.11	115.77	121.23
1	B	173	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	A	518	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	55	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	B	104	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	413	TRP	CE2-CD2-CG	-5.06	101.12	107.20
1	A	296	ASN	OD1-CG-ND2	-5.06	117.54	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	616	TRP	CG-CD2-CE3	5.05	138.95	133.90
1	B	202	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	B	567	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	152	ALA	CB-CA-C	-5.03	110.75	116.54
1	B	662	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	410	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	A	636	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	B	128	HIS	CB-CG-ND1	5.01	130.21	122.70
1	B	240	LYS	CG-CD-CE	-5.01	99.78	111.30
1	A	326	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	B	162	ASN	OD1-CG-ND2	-5.01	117.59	122.60

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	5313	0	5050	28	0
1	B	5313	0	5050	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	436	0	0	4	0
3	B	369	0	0	1	0
All	All	11435	0	10100	53	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 (53) 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:325:ASP:HA	1:A:329:MET:HE2	1.56	0.86
1:B:378:LEU:HD12	1:B:379:PRO:HD2	1.70	0.72
1:A:325:ASP:HA	1:A:329:MET:CE	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.82	0.61
1:A:11:ASN:ND2	3:A:1743:HOH:O	2.36	0.58
1:B:361:GLY:HA3	1:B:366:MET:SD	2.44	0.58
1:B:340:ARG:HH12	1:B:465:ASN:ND2	2.02	0.57
1:B:592:VAL:HB	1:B:681:ASN:HA	1.88	0.56
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.89	0.56
1:A:378:LEU:HD23	1:A:379:PRO:HD2	1.87	0.55
1:A:503:ASN:HD22	1:A:504:VAL:H	1.55	0.55
1:A:149:PRO:HG3	1:A:168:THR:HG21	1.89	0.54
1:A:453:ARG:HH22	1:A:473:ALA:HB2	1.73	0.54
1:A:126:HIS:HE1	1:A:224:ASP:OD2	1.93	0.52
1:A:653:LEU:HD12	1:A:660:VAL:HG13	1.90	0.52
1:B:124:THR:O	1:B:128:HIS:HD2	1.92	0.51
1:B:340:ARG:HH12	1:B:465:ASN:HD22	1.58	0.51
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.93	0.50
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.94	0.50
1:A:21:PHE:HE2	1:A:327:HIS:HB3	1.77	0.49
1:A:453:ARG:HH12	1:A:473:ALA:HA	1.78	0.49
1:B:29:ASN:HD21	1:B:31:ALA:HB3	1.77	0.49
1:A:333:HIS:HD2	3:A:1769:HOH:O	1.95	0.49
1:B:598:THR:HG22	1:B:654:LYS:HD2	1.95	0.49
1:A:655:LYS:HG2	1:A:660:VAL:HG22	1.94	0.48
1:B:58:ILE:HG23	1:B:124:THR:HG21	1.97	0.47
1:B:508:MET:HB3	1:B:508:MET:HE2	1.65	0.47
1:A:341:LYS:HG2	1:A:438:MET:HE3	1.98	0.45
1:B:603:ASN:HB3	1:B:624:PRO:HB3	1.98	0.45
1:A:126:HIS:HD2	3:A:1755:HOH:O	1.99	0.45
1:A:13:SER:O	1:A:398:ARG:HD3	2.17	0.44
1:B:333:HIS:HD2	3:B:1795:HOH:O	2.00	0.43
1:A:290:ARG:HD2	1:A:329:MET:HE1	2.00	0.43
1:A:410:HIS:HB2	3:A:1392:HOH:O	2.18	0.43
1:B:625:MET:HG2	1:B:638:TYR:HB2	2.01	0.43
1:B:361:GLY:HA2	1:B:378:LEU:HD13	2.01	0.42
1:A:361:GLY:HA3	1:A:366:MET:SD	2.59	0.42
1:B:445:THR:HG22	1:B:479:ASN:OD1	2.18	0.42
1:B:364:GLN:HG3	1:B:378:LEU:HD11	2.00	0.42
1:B:26:SER:O	1:B:56:GLY:HA3	2.19	0.42
1:B:215:ILE:HD12	1:B:215:ILE:HA	1.89	0.42
1:B:401:ASN:HA	1:B:402:PRO:HD2	1.91	0.42
1:B:520:ARG:HD3	1:B:547:THR:HG22	2.01	0.42
1:B:266:SER:HA	1:B:267:PRO:HD2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:OE2	1:B:410:HIS:HE1	2.04	0.41
1:A:397:LEU:HD11	1:A:459:VAL:HG11	2.03	0.41
1:B:668:ARG:NH1	1:B:685:GLN:HG3	2.35	0.41
1:A:69:MET:HG3	1:A:388:TYR:CE1	2.56	0.41
1:A:503:ASN:HD22	1:A:504:VAL:N	2.19	0.41
1:A:415:ASN:HD22	1:A:418:VAL:H	1.68	0.41
1:A:469:LEU:HB2	1:A:490:TRP:CE2	2.56	0.41
1:B:649:GLU:HA	1:B:668:ARG:O	2.22	0.40
1:A:668:ARG:NH1	1:A:685:GLN:HG3	2.36	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%)	669 (98%)	15 (2%)	0	100	100
1	B	684/686 (100%)	668 (98%)	15 (2%)	1 (0%)	48	46
All	All	1368/1372 (100%)	1337 (98%)	30 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	LEU

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	564/564 (100%)	555 (98%)	9 (2%)	55	62
1	B	564/564 (100%)	543 (96%)	21 (4%)	30	30
All	All	1128/1128 (100%)	1098 (97%)	30 (3%)	39	42

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	85	SER
1	A	326	ASN
1	A	341	LYS
1	A	372	PRO
1	A	378	LEU
1	A	415	ASN
1	A	453	ARG
1	A	500	ILE
1	B	71	ILE
1	B	92	VAL
1	B	116	GLN
1	B	119	LYS
1	B	169	ASN
1	B	194	LEU
1	B	250	LYS
1	B	326	ASN
1	B	329	MET
1	B	372	PRO
1	B	415	ASN
1	B	416	ASN
1	B	439	ASN
1	B	479	ASN
1	B	575	ILE
1	B	593	ILE
1	B	600	LEU
1	B	609	ASN
1	B	613	LEU
1	B	659	THR
1	B	682	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	62	ASN
1	A	116	GLN
1	A	120	ASN
1	A	126	HIS
1	A	129	ASN
1	A	326	ASN
1	A	333	HIS
1	A	415	ASN
1	A	503	ASN
1	A	656	GLN
1	A	667	ASN
1	B	19	GLN
1	B	29	ASN
1	B	62	ASN
1	B	88	ASN
1	B	93	ASN
1	B	126	HIS
1	B	128	HIS
1	B	129	ASN
1	B	177	HIS
1	B	316	GLN
1	B	326	ASN
1	B	333	HIS
1	B	364	GLN
1	B	410	HIS
1	B	415	ASN
1	B	439	ASN
1	B	465	ASN
1	B	467	ASN
1	B	548	GLN
1	B	578	ASN
1	B	609	ASN
1	B	620	ASN
1	B	656	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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%)	-0.95	0 100 100	4, 11, 24, 42	0
1	B	686/686 (100%)	-0.80	1 (0%) 92 91	5, 15, 33, 49	0
All	All	1372/1372 (100%)	-0.88	1 (0%) 92 91	4, 13, 29, 49	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	3.0

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](#)

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	B	689	1/1	0.95	0.03	13,13,13,13	0
2	CA	A	687	1/1	0.97	0.03	7,7,7,7	0
2	CA	A	688	1/1	0.99	0.04	11,11,11,11	0
2	CA	B	690	1/1	0.99	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.