



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 1V3J / pdb_00001v3j
Title : Crystal structure of F283L 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

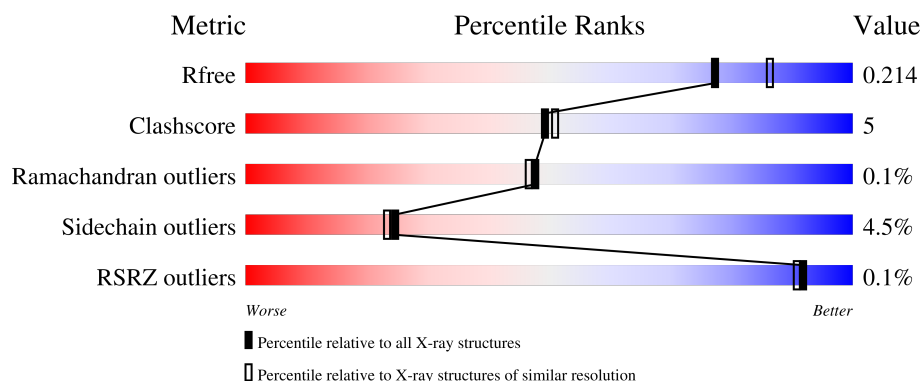
1 Overall quality at a glance

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	75% 21% . .
1	B	686	74% 22% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11226 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
			5309	3351	906	1036	16			
1	B	686	Total	C	N	O	S	0	0	0
			5309	3351	906	1036	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LEU	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	LEU	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		

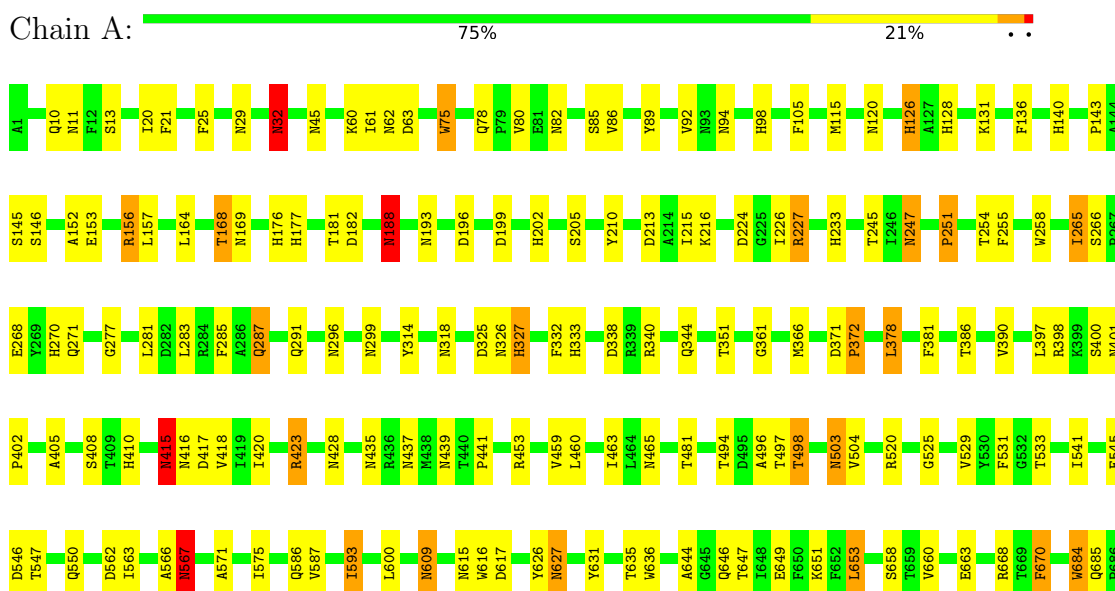
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	297	Total	O	0	0
			297	297		
3	B	307	Total	O	0	0
			307	307		

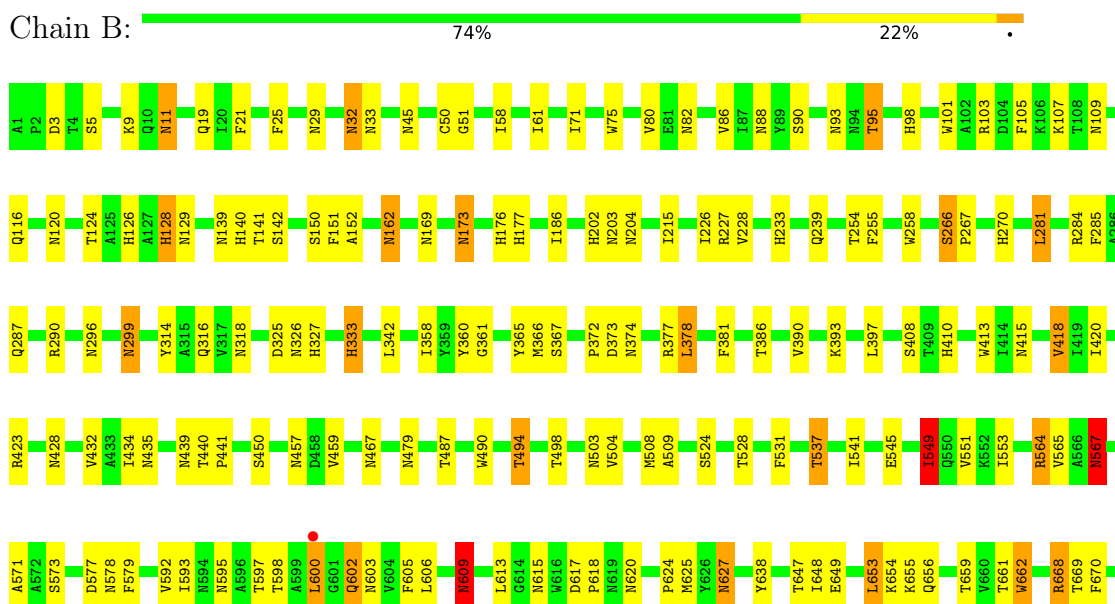
3 Residue-property plots

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



T679		
V680		
M681		
W684		
Q685		
P686		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.93Å 73.66Å 78.20Å 85.11° 104.96° 100.97°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.2 (10.00-2.00) 85.6 (10.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.170 , 0.242 0.152 , 0.214	Depositor DCC
R_{free} test set	4750 reflections (6.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11226	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 5.07% 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	1.12	15/5442 (0.3%)	1.73	106/7424 (1.4%)
1	B	1.10	22/5442 (0.4%)	1.76	110/7424 (1.5%)
All	All	1.11	37/10884 (0.3%)	1.75	216/14848 (1.5%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	549	ILE	CA-CB	7.89	1.65	1.54
1	B	140	HIS	CD2-NE2	-7.54	1.29	1.37
1	A	177	HIS	CD2-NE2	-7.21	1.29	1.37
1	B	128	HIS	CD2-NE2	-7.17	1.29	1.37
1	B	98	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	333	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	140	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	202	HIS	CD2-NE2	-6.83	1.30	1.37
1	B	126	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	233	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	128	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	333	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	177	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	327	HIS	CD2-NE2	-6.60	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.58	1.30	1.37
1	B	410	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	176	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	233	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	270	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	176	HIS	CD2-NE2	-6.16	1.31	1.37
1	B	258	TRP	CG-CD2	-5.92	1.33	1.43
1	B	378	LEU	CB-CG	-5.91	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	HIS	CG-ND1	-5.85	1.31	1.38
1	A	351	THR	CA-CB	5.83	1.63	1.53
1	B	202	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	270	HIS	CD2-NE2	-5.37	1.31	1.37
1	B	128	HIS	CG-ND1	-5.31	1.32	1.38
1	B	333	HIS	CG-ND1	-5.29	1.32	1.38
1	A	251	PRO	CA-CB	-5.25	1.46	1.53
1	B	314	TYR	CA-CB	-5.25	1.46	1.53
1	B	233	HIS	CG-ND1	-5.24	1.32	1.38
1	A	176	HIS	CG-ND1	-5.17	1.32	1.38
1	B	98	HIS	CG-ND1	-5.10	1.32	1.38
1	A	410	HIS	CD2-NE2	-5.10	1.32	1.37
1	B	126	HIS	CG-ND1	-5.04	1.32	1.38

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ASN	OD1-CG-ND2	-11.31	111.29	122.60
1	A	627	ASN	OD1-CG-ND2	-10.90	111.70	122.60
1	B	32	ASN	OD1-CG-ND2	-10.29	112.31	122.60
1	B	95	THR	N-CA-CB	-9.45	95.24	111.69
1	B	415	ASN	CA-CB-CG	8.84	121.44	112.60
1	A	45	ASN	OD1-CG-ND2	-8.09	114.51	122.60
1	A	415	ASN	CA-CB-CG	8.01	120.61	112.60
1	B	204	ASN	OD1-CG-ND2	-7.94	114.66	122.60
1	B	299	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	B	327	HIS	CB-CG-CD2	-7.87	120.97	131.20
1	B	299	ASN	CB-CG-ND2	7.84	128.16	116.40
1	B	325	ASP	CA-CB-CG	7.77	120.37	112.60
1	B	609	ASN	OD1-CG-ND2	-7.75	114.86	122.60
1	A	627	ASN	CB-CG-ND2	7.71	127.97	116.40
1	B	173	ASN	CA-CB-CG	-7.69	104.91	112.60
1	A	327	HIS	CB-CG-CD2	-7.64	121.27	131.20
1	B	11	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	B	151	PHE	CA-C-O	-7.61	112.25	120.92
1	B	567	ASN	OD1-CG-ND2	-7.51	115.09	122.60
1	A	177	HIS	CB-CG-CD2	-7.45	121.52	131.20
1	B	326	ASN	CA-CB-CG	7.39	119.99	112.60
1	A	586	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	B	162	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	A	325	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	496	ALA	N-CA-C	-7.11	98.97	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	685	GLN	OE1-CD-NE2	-7.11	115.50	122.60
1	A	213	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	541	ILE	N-CA-C	-7.08	96.68	107.73
1	A	32	ASN	CA-CB-CG	7.06	119.66	112.60
1	B	609	ASN	CB-CG-ND2	7.05	126.97	116.40
1	B	327	HIS	CB-CG-ND1	7.03	133.24	122.70
1	A	299	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	A	202	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	B	103	ARG	N-CA-C	-6.84	105.56	114.04
1	B	45	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	A	435	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	B	177	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	A	63	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	109	ASN	CA-C-N	6.72	126.67	119.28
1	B	109	ASN	C-N-CA	6.72	126.67	119.28
1	A	503	ASN	CB-CG-ND2	6.71	126.46	116.40
1	B	579	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	62	ASN	N-CA-C	6.68	118.21	111.07
1	B	61	ILE	N-CA-C	-6.64	104.38	110.82
1	A	437	ASN	CA-CB-CG	-6.64	105.96	112.60
1	B	86	VAL	N-CA-C	-6.59	98.38	107.99
1	A	503	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	B	680	VAL	N-CA-C	-6.55	98.31	107.80
1	A	415	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	B	685	GLN	CG-CD-NE2	6.54	126.20	116.40
1	A	617	ASP	CA-C-N	6.49	126.72	119.32
1	A	617	ASP	C-N-CA	6.49	126.72	119.32
1	A	126	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	B	415	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	B	577	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	602	GLN	N-CA-C	-6.48	99.08	109.96
1	B	203	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	567	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	B	615	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	B	32	ASN	CB-CG-ND2	6.38	125.97	116.40
1	B	567	ASN	CB-CG-ND2	6.38	125.97	116.40
1	A	327	HIS	CB-CG-ND1	6.36	132.24	122.70
1	B	479	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	A	410	HIS	CA-CB-CG	6.29	120.09	113.80
1	B	51	GLY	CA-C-N	6.28	125.95	119.92
1	B	51	GLY	C-N-CA	6.28	125.95	119.92
1	B	617	ASP	CA-CB-CG	6.28	118.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ASN	CA-C-O	6.20	128.91	121.65
1	B	139	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	120	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	318	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	233	HIS	CA-CB-CG	-6.17	107.63	113.80
1	A	258	TRP	N-CA-C	-6.16	97.05	108.02
1	A	98	HIS	CB-CG-CD2	-6.16	123.20	131.20
1	A	277	GLY	N-CA-C	-6.12	106.65	115.27
1	B	620	ASN	CA-CB-CG	-6.11	106.49	112.60
1	A	416	ASN	N-CA-C	6.10	119.56	111.75
1	B	457	ASN	CB-CA-C	-6.07	99.27	109.65
1	A	398	ARG	CG-CD-NE	-6.02	98.75	112.00
1	A	333	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	B	435	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	B	541	ILE	N-CA-C	-5.93	98.47	107.73
1	B	287	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	631	TYR	N-CA-C	-5.90	100.09	109.23
1	B	595	ASN	CA-CB-CG	5.89	118.49	112.60
1	B	531	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	439	ASN	CB-CA-C	-5.87	100.86	110.08
1	A	525	GLY	O-C-N	5.87	127.69	123.35
1	A	145	SER	N-CA-C	-5.86	98.73	108.34
1	A	398	ARG	NE-CZ-NH2	-5.86	113.92	119.20
1	A	546	ASP	N-CA-C	5.86	118.61	111.82
1	B	627	ASN	CB-CG-ND2	5.84	125.16	116.40
1	A	333	HIS	CA-CB-CG	-5.83	107.97	113.80
1	B	281	LEU	N-CA-C	-5.82	101.79	110.23
1	A	216	LYS	CB-CG-CD	-5.82	97.92	111.30
1	A	10	GLN	OE1-CD-NE2	-5.81	116.79	122.60
1	B	318	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	B	662	TRP	CG-CD2-CE3	5.80	139.71	133.90
1	B	494	THR	CA-CB-OG1	-5.78	100.93	109.60
1	B	393	LYS	CG-CD-CE	-5.76	98.06	111.30
1	B	169	ASN	CA-CB-CG	-5.75	106.85	112.60
1	B	617	ASP	CA-C-N	5.74	125.59	119.28
1	B	617	ASP	C-N-CA	5.74	125.59	119.28
1	A	550	GLN	CA-CB-CG	-5.73	102.63	114.10
1	B	627	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	B	450	SER	N-CA-C	-5.72	105.89	112.92
1	B	393	LYS	CA-CB-CG	-5.71	102.67	114.10
1	B	545	GLU	CA-CB-CG	5.71	125.53	114.10
1	B	95	THR	CB-CA-C	5.71	122.64	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ASN	CB-CG-ND2	5.70	124.95	116.40
1	A	82	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	B	410	HIS	N-CA-CB	-5.67	102.22	110.84
1	A	401	ASN	CA-C-N	5.67	126.05	119.47
1	A	401	ASN	C-N-CA	5.67	126.05	119.47
1	A	182	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	338	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	285	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	270	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	B	51	GLY	N-CA-C	5.63	121.18	114.48
1	A	86	VAL	N-CA-C	-5.63	99.12	107.51
1	A	314	TYR	N-CA-C	-5.62	99.57	108.73
1	A	299	ASN	CA-CB-CG	5.61	118.21	112.60
1	B	457	ASN	N-CA-CB	5.60	118.20	109.97
1	B	3	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	531	PHE	N-CA-C	-5.59	98.10	107.99
1	A	245	THR	CA-CB-OG1	-5.57	101.24	109.60
1	A	78	GLN	CA-C-N	5.57	126.05	120.04
1	A	78	GLN	C-N-CA	5.57	126.05	120.04
1	B	296	ASN	CB-CG-ND2	5.56	124.74	116.40
1	B	142	SER	N-CA-CB	-5.56	104.29	111.35
1	A	497	THR	N-CA-CB	-5.56	102.36	110.53
1	B	21	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	586	GLN	CG-CD-NE2	5.54	124.72	116.40
1	A	20	ILE	N-CA-C	5.53	116.27	108.36
1	A	287	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	B	21	PHE	N-CA-C	-5.51	100.13	108.67
1	A	136	PHE	N-CA-C	-5.50	98.58	108.48
1	B	290	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	332	PHE	N-CA-C	-5.49	105.30	111.28
1	B	239	GLN	CA-CB-CG	-5.49	103.13	114.10
1	A	281	LEU	N-CA-C	-5.47	101.76	109.96
1	B	467	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	566	ALA	O-C-N	-5.46	116.85	123.29
1	B	169	ASN	CA-C-O	5.44	128.89	122.14
1	A	177	HIS	CB-CG-ND1	5.42	130.84	122.70
1	A	29	ASN	CA-C-N	5.41	125.23	119.28
1	A	29	ASN	C-N-CA	5.41	125.23	119.28
1	B	258	TRP	CE2-CD2-CE3	5.41	124.20	118.80
1	B	228	VAL	CA-C-O	5.39	126.96	120.65
1	B	204	ASN	CB-CG-ND2	5.39	124.48	116.40
1	A	75	TRP	CG-CD2-CE3	5.38	139.28	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ILE	CA-C-O	5.38	125.98	120.39
1	B	88	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	266	SER	CA-C-N	5.36	124.70	118.85
1	A	266	SER	C-N-CA	5.36	124.70	118.85
1	A	156	ARG	N-CA-C	5.36	118.00	110.23
1	B	679	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	567	ASN	CA-CB-CG	5.33	117.94	112.60
1	B	186	ILE	N-CA-C	-5.31	105.54	110.53
1	A	615	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	188	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	B	490	TRP	CE2-CD2-CG	-5.27	100.88	107.20
1	A	670	PHE	CA-CB-CG	-5.26	108.53	113.80
1	A	567	ASN	CB-CG-ND2	5.26	124.29	116.40
1	A	405	ALA	O-C-N	-5.25	116.16	122.15
1	A	616	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	B	266	SER	CA-C-N	5.25	124.42	118.97
1	B	266	SER	C-N-CA	5.25	124.42	118.97
1	B	373	ASP	N-CA-C	5.24	119.30	113.01
1	B	5	SER	CA-C-O	-5.23	116.01	121.55
1	A	423	ARG	N-CA-C	-5.22	100.67	109.07
1	B	120	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	B	29	ASN	CA-C-N	5.21	124.72	119.19
1	B	29	ASN	C-N-CA	5.21	124.72	119.19
1	A	62	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	B	98	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	B	258	TRP	N-CA-C	-5.21	98.75	108.02
1	A	420	ILE	N-CA-C	-5.20	100.16	107.75
1	A	684	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	326	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	646	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	545	GLU	CA-CB-CG	5.18	124.46	114.10
1	A	415	ASN	CB-CG-ND2	5.18	124.17	116.40
1	A	75	TRP	CE2-CD2-CG	-5.17	100.99	107.20
1	B	413	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	B	684	TRP	CG-CD2-CE3	5.17	139.06	133.90
1	B	413	TRP	CB-CG-CD1	-5.16	119.16	126.90
1	A	428	ASN	CA-CB-CG	-5.16	107.44	112.60
1	A	247	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	164	LEU	N-CA-C	-5.15	106.68	113.12
1	A	498	THR	N-CA-C	-5.15	102.55	110.32
1	B	9	LYS	CB-CG-CD	-5.14	99.48	111.30
1	A	285	PHE	CA-CB-CG	5.14	118.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	ILE	CB-CG1-CD1	-5.13	103.03	113.80
1	B	358	ILE	CB-CG1-CD1	-5.13	103.03	113.80
1	B	128	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	176	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	428	ASN	N-CA-C	-5.12	101.35	109.96
1	A	205	SER	N-CA-C	5.12	117.60	111.71
1	A	233	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	A	61	ILE	N-CA-C	-5.12	105.86	110.82
1	A	439	ASN	CA-CB-CG	5.11	117.71	112.60
1	B	662	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	B	374	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	566	ALA	N-CA-C	-5.07	100.91	109.07
1	B	139	ASN	CB-CG-ND2	5.06	123.99	116.40
1	B	152	ALA	CB-CA-C	-5.06	110.72	116.54
1	B	296	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	129	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	439	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	B	684	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	A	196	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	284	ARG	N-CA-CB	-5.01	102.74	110.01
1	A	131	LYS	O-C-N	-5.01	117.30	122.96
1	A	152	ALA	CB-CA-C	-5.01	110.78	116.54
1	A	168	THR	N-CA-C	-5.00	102.29	110.20

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	5309	0	5051	55	0
1	B	5309	0	5051	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	297	0	0	3	0
3	B	307	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11226	0	10102	112	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 5.

All (112) 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:340:ARG:HH12	1:A:465:ASN:HD22	1.35	0.73
1:B:564:ARG:HD2	1:B:573:SER:O	1.95	0.66
1:B:124:THR:O	1:B:128:HIS:HD2	1.83	0.61
1:A:651:LYS:HE2	1:A:663:GLU:O	2.00	0.61
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.83	0.61
1:A:361:GLY:HA3	1:A:366:MET:SD	2.42	0.59
1:B:80:VAL:HB	1:B:105:PHE:HA	1.86	0.57
1:B:361:GLY:HA3	1:B:366:MET:SD	2.45	0.56
1:A:11:ASN:ND2	3:A:1166:HOH:O	2.38	0.56
1:A:609:ASN:ND2	1:A:649:GLU:H	2.05	0.55
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.88	0.55
1:B:333:HIS:HD2	3:B:758:HOH:O	1.89	0.55
1:B:397:LEU:HD11	1:B:459:VAL:HG11	1.87	0.55
1:B:316:GLN:HG2	3:B:1262:HOH:O	2.07	0.55
1:B:600:LEU:HG	1:B:656:GLN:NE2	2.21	0.55
1:A:126:HIS:HE1	1:A:224:ASP:OD2	1.90	0.55
1:A:397:LEU:HD11	1:A:459:VAL:HG11	1.87	0.55
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.43	0.54
1:A:115:MET:HE3	1:A:115:MET:HA	1.88	0.54
1:B:11:ASN:ND2	3:B:1259:HOH:O	2.40	0.54
1:A:567:ASN:ND2	1:A:571:ALA:H	2.05	0.54
1:B:605:PHE:HB2	1:B:653:LEU:HG	1.90	0.54
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.43	0.53
1:B:434:ILE:HG12	1:B:487:THR:HG23	1.90	0.53
1:B:528:THR:HG23	1:B:537:THR:HG23	1.90	0.53
1:B:653:LEU:HD12	1:B:655:LYS:HG3	1.91	0.52
1:B:316:GLN:HE22	1:B:578:ASN:HD22	1.56	0.52
1:B:605:PHE:CE1	1:B:655:LYS:HB2	2.44	0.52
1:A:415:ASN:ND2	1:A:417:ASP:H	2.07	0.52
1:A:247:ASN:HA	1:A:251:PRO:HB3	1.92	0.52
1:B:226:ILE:HB	1:B:254:THR:HG23	1.92	0.51
1:A:25:PHE:HB3	3:A:1175:HOH:O	2.09	0.51
1:A:80:VAL:HB	1:A:105:PHE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PRO:HB2	1:A:481:THR:CG2	2.42	0.50
1:B:75:TRP:CZ2	1:B:227:ARG:HG3	2.47	0.50
1:A:653:LEU:HD12	1:A:660:VAL:HG13	1.94	0.49
1:A:520:ARG:HD3	1:A:547:THR:HG22	1.94	0.49
1:A:193:ASN:OD1	1:A:199:ASP:HB2	2.12	0.49
1:B:408:SER:O	1:B:423:ARG:HA	2.13	0.49
1:B:598:THR:HG22	1:B:654:LYS:HD2	1.95	0.48
1:A:92:VAL:HG13	1:A:94:ASN:HD21	1.79	0.48
1:B:649:GLU:HA	1:B:668:ARG:O	2.14	0.48
1:B:93:ASN:HB2	3:B:977:HOH:O	2.14	0.48
1:A:567:ASN:HD21	1:A:571:ALA:H	1.61	0.47
1:A:21:PHE:HE2	1:A:327:HIS:HB3	1.80	0.47
1:B:25:PHE:HB3	3:B:717:HOH:O	2.14	0.47
1:A:153:GLU:O	1:A:156:ARG:HG3	2.15	0.47
1:A:146:SER:HA	1:A:168:THR:OG1	2.14	0.47
1:A:587:VAL:HG13	1:A:644:ALA:HB2	1.97	0.47
1:A:415:ASN:HD22	1:A:418:VAL:H	1.63	0.46
1:A:668:ARG:NH1	1:A:685:GLN:HG3	2.30	0.46
1:B:50:CYS:HB3	1:B:377:ARG:HH11	1.79	0.46
1:B:342:LEU:HD23	1:B:365:TYR:CD1	2.50	0.46
1:B:71:ILE:HD13	1:B:71:ILE:HA	1.72	0.46
1:A:340:ARG:O	1:A:344:GLN:HG3	2.15	0.46
1:B:418:VAL:HA	1:B:434:ILE:O	2.15	0.46
1:A:89:TYR:O	1:A:92:VAL:HG12	2.15	0.46
1:A:397:LEU:HA	1:A:400:SER:HG	1.81	0.46
1:A:386:THR:O	1:A:390:VAL:HG23	2.16	0.46
1:B:603:ASN:HB3	1:B:624:PRO:HB3	1.98	0.46
1:B:593:ILE:HD13	1:B:684:TRP:HE3	1.82	0.45
1:B:564:ARG:HG3	1:B:565:VAL:N	2.32	0.45
1:B:386:THR:O	1:B:390:VAL:HG23	2.17	0.45
1:B:618:PRO:HG3	1:B:662:TRP:CZ2	2.52	0.44
1:A:503:ASN:HD22	1:A:504:VAL:H	1.66	0.44
1:B:58:ILE:HG23	1:B:124:THR:HG21	2.00	0.44
1:A:460:LEU:O	1:A:463:ILE:HG12	2.18	0.44
1:B:549:ILE:HD11	1:B:551:VAL:HB	1.99	0.44
1:A:647:THR:HA	1:A:670:PHE:O	2.18	0.44
1:B:266:SER:HA	1:B:267:PRO:HD3	1.84	0.44
1:A:371:ASP:HA	1:A:372:PRO:HA	1.78	0.44
1:B:420:ILE:HA	1:B:432:VAL:O	2.18	0.44
1:A:21:PHE:CE2	1:A:327:HIS:HB3	2.54	0.43
1:B:648:ILE:O	1:B:669:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:HD21	1:B:381:PHE:CZ	2.53	0.43
1:B:592:VAL:HB	1:B:681:ASN:HA	1.99	0.43
1:B:609:ASN:ND2	1:B:649:GLU:H	2.16	0.43
1:A:296:ASN:HB2	3:A:774:HOH:O	2.17	0.43
1:B:647:THR:HA	1:B:670:PHE:O	2.18	0.43
1:A:593:ILE:O	1:A:635:THR:HA	2.19	0.43
1:A:283:LEU:O	1:A:287:GLN:HG2	2.19	0.43
1:A:227:ARG:HG2	1:A:255:PHE:CE1	2.54	0.43
1:A:408:SER:O	1:A:423:ARG:HA	2.19	0.43
1:B:567:ASN:ND2	1:B:571:ALA:H	2.17	0.43
1:A:181:THR:HA	1:A:188:ASN:HD21	1.84	0.42
1:B:503:ASN:HD22	1:B:504:VAL:H	1.67	0.42
1:B:598:THR:HB	1:B:602:GLN:HB3	2.00	0.42
1:B:603:ASN:O	1:B:654:LYS:HA	2.19	0.42
1:A:626:TYR:O	1:A:636:TRP:HA	2.19	0.42
1:B:101:TRP:HA	1:B:141:THR:O	2.20	0.42
1:A:287:GLN:O	1:A:291:GLN:HG3	2.20	0.42
1:A:378:LEU:HD21	1:A:381:PHE:CE1	2.54	0.42
1:B:227:ARG:HA	1:B:255:PHE:O	2.20	0.42
1:B:19:GLN:O	1:B:360:TYR:HB3	2.20	0.42
1:B:508:MET:HE2	1:B:508:MET:HB3	1.76	0.42
1:B:440:THR:HA	1:B:441:PRO:HD3	1.92	0.41
1:A:215:ILE:HD12	1:A:215:ILE:HA	1.91	0.41
1:A:402:PRO:HG3	1:A:520:ARG:CZ	2.51	0.41
1:B:50:CYS:HB3	1:B:377:ARG:NH1	2.35	0.41
1:B:509:ALA:HB3	1:B:553:ILE:CD1	2.51	0.41
1:A:32:ASN:C	1:A:32:ASN:HD22	2.29	0.41
1:A:340:ARG:HH12	1:A:465:ASN:ND2	2.10	0.41
1:B:656:GLN:O	1:B:659:THR:HG22	2.20	0.41
1:B:215:ILE:HD12	1:B:215:ILE:HA	1.91	0.41
1:B:624:PRO:HD2	3:B:1276:HOH:O	2.20	0.41
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.78	0.41
1:A:157:LEU:HD11	1:A:210:TYR:CE2	2.56	0.40
1:A:649:GLU:HA	1:A:668:ARG:O	2.21	0.40
1:A:226:ILE:O	1:A:254:THR:HA	2.22	0.40
1:A:593:ILE:HD11	1:A:684:TRP:HA	2.03	0.40
1:B:80:VAL:HA	1:B:107:LYS:O	2.21	0.40
1:B:281:LEU:HA	1:B:281:LEU:HD23	1.84	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%)	667 (98%)	17 (2%)	0	100	100
1	B	684/686 (100%)	661 (97%)	21 (3%)	2 (0%)	36	35
All	All	1368/1372 (100%)	1328 (97%)	38 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	SER
1	B	600	LEU

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%)	540 (96%)	24 (4%)	26	25
1	B	564/564 (100%)	537 (95%)	27 (5%)	23	21
All	All	1128/1128 (100%)	1077 (96%)	51 (4%)	24	23

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	32	ASN
1	A	85	SER
1	A	143	PRO

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	227	ARG
1	A	265	ILE
1	A	268	GLU
1	A	271	GLN
1	A	372	PRO
1	A	378	LEU
1	A	415	ASN
1	A	453	ARG
1	A	494	THR
1	A	498	THR
1	A	529	VAL
1	A	533	THR
1	A	567	ASN
1	A	593	ILE
1	A	600	LEU
1	A	609	ASN
1	A	627	ASN
1	A	653	LEU
1	A	658	SER
1	B	32	ASN
1	B	82	ASN
1	B	95	THR
1	B	116	GLN
1	B	150	SER
1	B	162	ASN
1	B	173	ASN
1	B	299	ASN
1	B	367	SER
1	B	372	PRO
1	B	418	VAL
1	B	494	THR
1	B	498	THR
1	B	524	SER
1	B	537	THR
1	B	549	ILE
1	B	564	ARG
1	B	567	ASN
1	B	597	THR
1	B	606	LEU
1	B	609	ASN
1	B	613	LEU

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Mol	Chain	Res	Type
1	B	627	ASN
1	B	653	LEU
1	B	661	THR
1	B	668	ARG
1	B	685	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	32	ASN
1	A	94	ASN
1	A	116	GLN
1	A	126	HIS
1	A	128	HIS
1	A	129	ASN
1	A	172	GLN
1	A	188	ASN
1	A	296	ASN
1	A	316	GLN
1	A	333	HIS
1	A	415	ASN
1	A	465	ASN
1	A	503	ASN
1	A	550	GLN
1	A	567	ASN
1	A	603	ASN
1	A	609	ASN
1	A	627	ASN
1	B	11	ASN
1	B	32	ASN
1	B	33	ASN
1	B	55	GLN
1	B	129	ASN
1	B	188	ASN
1	B	203	ASN
1	B	239	GLN
1	B	263	ASN
1	B	270	HIS
1	B	316	GLN
1	B	333	HIS
1	B	467	ASN

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Mol	Chain	Res	Type
1	B	503	ASN
1	B	548	GLN
1	B	595	ASN
1	B	603	ASN
1	B	609	ASN
1	B	627	ASN
1	B	628	GLN
1	B	646	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 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 ⓘ

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	9, 17, 31, 71	0
1	B	686/686 (100%)	-0.82	1 (0%) 92 91	11, 20, 39, 60	0
All	All	1372/1372 (100%)	-0.89	1 (0%) 92 91	9, 18, 37, 71	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	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
2	CA	A	687	1/1	0.97	0.04	13,13,13,13	0
2	CA	A	688	1/1	0.97	0.03	19,19,19,19	0
2	CA	B	689	1/1	0.98	0.02	18,18,18,18	0
2	CA	B	690	1/1	0.98	0.03	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.