



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:22 PM UTC

PDB ID : 1CGT / pdb_00001cgt
Title : STRUCTURE OF CYCLODEXTRIN GLYCOSYLTRANSFERASE RE-
FINED AT 2.0 ANGSTROMS RESOLUTION
Authors : Klein, C.; Schulz, G.E.
Deposited on : 1992-06-10
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

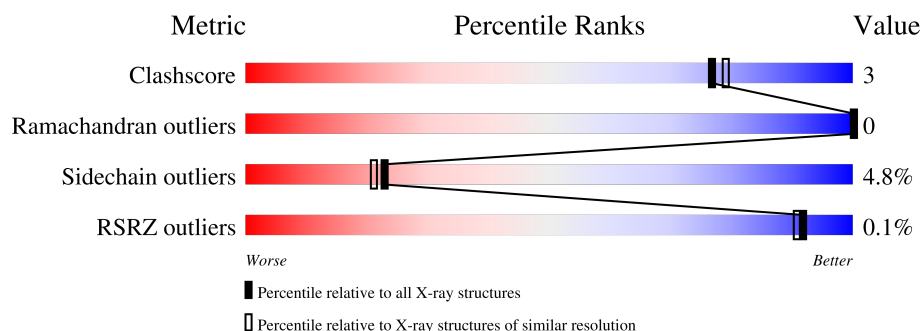
1 Overall quality at a glance

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))
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	684	 84% 12% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5857 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 GLYCOSYL-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	684	Total	C	N	O	S	0	0	0
			5267	3323	891	1040	13			

- 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		

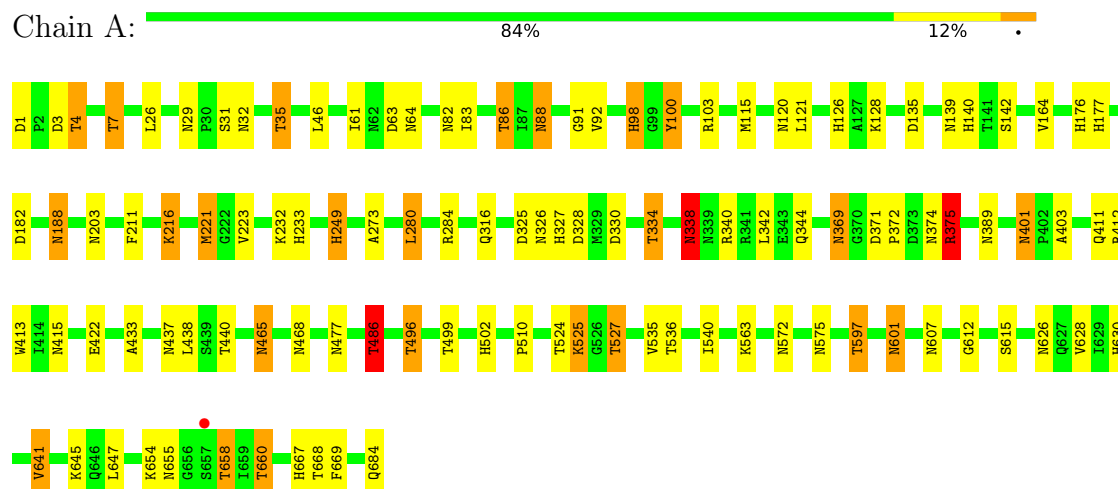
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	588	Total	O	0	0
			588	588		

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 GLYCOSYL-TRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.80Å 104.70Å 114.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.00 7.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.00) 90.0 (7.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.166 , (Not available) 0.158 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 87.2	EDS
L-test for twinning ¹	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5857	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.00	15/5398 (0.3%)	1.65	81/7366 (1.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	667	HIS	CD2-NE2	-7.75	1.29	1.37
1	A	126	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	486	THR	CA-CB	6.74	1.65	1.53
1	A	140	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	502	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	327	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	177	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	223	VAL	CA-CB	5.86	1.60	1.54
1	A	249	HIS	CD2-NE2	-5.48	1.31	1.37
1	A	499	THR	CA-CB	5.25	1.62	1.53
1	A	176	HIS	CG-ND1	-5.12	1.32	1.38
1	A	660	THR	CA-CB	5.11	1.61	1.53
1	A	630	HIS	CD2-NE2	-5.09	1.32	1.37
1	A	126	HIS	CG-ND1	-5.04	1.32	1.38

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ARG	NE-CZ-NH2	-11.50	108.85	119.20
1	A	641	VAL	N-CA-CB	-10.98	95.84	111.21
1	A	164	VAL	N-CA-C	-10.83	101.38	111.67
1	A	401	ASN	OD1-CG-ND2	-10.49	112.11	122.60
1	A	4	THR	N-CA-CB	-8.99	96.35	110.46
1	A	563	LYS	CB-CG-CD	-8.59	91.56	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	THR	N-CA-CB	-8.14	97.36	110.63
1	A	667	HIS	CB-CG-CD2	-8.13	120.63	131.20
1	A	338	ASN	CB-CG-ND2	-8.13	104.20	116.40
1	A	284	ARG	NE-CZ-NH1	7.63	129.13	121.50
1	A	597	THR	N-CA-CB	-7.45	99.10	110.42
1	A	415	ASN	CA-CB-CG	7.37	119.97	112.60
1	A	437	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	A	233	HIS	CA-CB-CG	-6.96	106.84	113.80
1	A	63	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	667	HIS	CB-CG-ND1	6.85	132.97	122.70
1	A	86	THR	CB-CA-C	6.68	120.79	109.50
1	A	641	VAL	CB-CA-C	6.64	123.45	111.36
1	A	327	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	A	284	ARG	CB-CG-CD	-6.53	96.28	111.30
1	A	139	ASN	OD1-CG-ND2	-6.53	116.08	122.60
1	A	120	ASN	OD1-CG-ND2	-6.47	116.12	122.60
1	A	401	ASN	CB-CG-ND2	6.47	126.11	116.40
1	A	477	ASN	CB-CG-ND2	6.47	126.11	116.40
1	A	3	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	375	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	A	601	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	A	654	LYS	CB-CG-CD	-6.28	96.86	111.30
1	A	82	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	61	ILE	N-CA-C	-6.22	104.44	110.72
1	A	177	HIS	CA-CB-CG	-6.16	107.64	113.80
1	A	496	THR	CA-CB-OG1	-6.14	100.38	109.60
1	A	597	THR	CA-CB-OG1	-6.02	100.57	109.60
1	A	375	ARG	NE-CZ-NH1	6.01	127.51	121.50
1	A	98	HIS	CB-CG-CD2	-5.94	123.47	131.20
1	A	371	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	389	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	477	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	535	VAL	N-CA-C	-5.91	99.84	108.11
1	A	135	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	369	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	232	LYS	CG-CD-CE	-5.89	97.76	111.30
1	A	29	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	120	ASN	CB-CG-ND2	5.80	125.10	116.40
1	A	338	ASN	OD1-CG-ND2	5.79	128.39	122.60
1	A	35	THR	CA-CB-OG1	-5.79	100.92	109.60
1	A	325	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	32	ASN	CA-CB-CG	5.76	118.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ASN	CB-CG-ND2	5.75	125.03	116.40
1	A	626	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	A	684	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	630	HIS	N-CA-C	-5.55	100.63	109.23
1	A	4	THR	CB-CA-C	5.50	120.27	109.72
1	A	188	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	465	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	468	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	601	ASN	CB-CG-ND2	5.38	124.47	116.40
1	A	437	ASN	CB-CG-ND2	5.35	124.42	116.40
1	A	499	THR	CB-CA-C	5.35	119.01	109.65
1	A	88	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	525	LYS	CG-CD-CE	5.28	123.43	111.30
1	A	572	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	326	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	496	THR	N-CA-CB	-5.23	103.41	110.67
1	A	607	ASN	N-CA-C	5.22	118.67	112.72
1	A	100	TYR	N-CA-C	5.21	119.51	113.20
1	A	413	TRP	CB-CG-CD1	-5.21	119.09	126.90
1	A	328	ASP	CB-CA-C	-5.20	101.93	110.72
1	A	140	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	A	249	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	524	THR	CA-CB-OG1	-5.16	101.85	109.60
1	A	327	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	389	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	575	ASN	N-CA-C	5.11	117.45	110.55
1	A	142	SER	N-CA-CB	-5.09	106.05	111.29
1	A	7	THR	N-CA-CB	-5.08	101.95	110.39
1	A	203	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	221	MET	CA-CB-CG	-5.04	104.02	114.10
1	A	211	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	316	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	A	628	VAL	CA-C-O	-5.01	114.52	120.78

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	5267	0	5008	30	0
2	A	2	0	0	0	0
3	A	588	0	0	4	0
All	All	5857	0	5008	30	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 (30) 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:98:HIS:HD2	1:A:100:TYR:H	1.30	0.80
1:A:340:ARG:HH12	1:A:465:ASN:HD22	1.40	0.68
1:A:334:THR:HG21	3:A:1111:HOH:O	1.93	0.67
1:A:340:ARG:HH12	1:A:465:ASN:ND2	1.99	0.60
1:A:88:ASN:HD21	1:A:91:GLY:H	1.52	0.57
1:A:647:LEU:HD12	3:A:1238:HOH:O	2.04	0.56
1:A:273:ALA:HB2	1:A:280:LEU:HD22	1.87	0.56
1:A:655:ASN:OD1	1:A:658:THR:HG23	2.07	0.55
1:A:338:ASN:HD21	1:A:438:LEU:HD11	1.72	0.54
1:A:527:THR:HB	1:A:536:THR:HG22	1.90	0.54
1:A:401:ASN:HD22	1:A:403:ALA:H	1.57	0.53
1:A:64:ASN:OD1	1:A:128:LYS:NZ	2.41	0.52
1:A:330:ASP:HB3	1:A:369:ASN:HD22	1.78	0.48
1:A:525:LYS:HD2	1:A:540:ILE:HB	1.95	0.48
1:A:401:ASN:ND2	1:A:403:ALA:H	2.11	0.48
1:A:612:GLY:O	1:A:615:SER:HB3	2.13	0.47
1:A:115:MET:SD	1:A:221:MET:HE1	2.54	0.47
1:A:88:ASN:ND2	1:A:91:GLY:H	2.11	0.46
1:A:344:GLN:HG2	1:A:486:THR:CG2	2.45	0.46
1:A:1:ASP:OD2	1:A:7:THR:HG21	2.16	0.46
1:A:330:ASP:HB3	1:A:369:ASN:ND2	2.32	0.44
1:A:645:LYS:NZ	3:A:1253:HOH:O	2.51	0.44
1:A:669:PHE:HD2	3:A:1238:HOH:O	2.00	0.44
1:A:182:ASP:H	1:A:188:ASN:HD21	1.65	0.43
1:A:344:GLN:HG2	1:A:486:THR:HG21	2.01	0.43
1:A:83:ILE:HA	1:A:103:ARG:HD3	2.00	0.42
1:A:433:ALA:O	1:A:486:THR:HA	2.19	0.42
1:A:216:LYS:HG3	1:A:249:HIS:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:HH11	1:A:422:GLU:CD	2.28	0.41
1:A:374:ASN:OD1	1:A:375:ARG:HD3	2.22	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	682/684 (100%)	665 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	566/566 (100%)	539 (95%)	27 (5%)	23	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	26	LEU
1	A	31	SER
1	A	35	THR

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	86	THR
1	A	92	VAL
1	A	121	LEU
1	A	216	LYS
1	A	280	LEU
1	A	334	THR
1	A	338	ASN
1	A	342	LEU
1	A	372	PRO
1	A	375	ARG
1	A	411	GLN
1	A	440	THR
1	A	486	THR
1	A	496	THR
1	A	510	PRO
1	A	527	THR
1	A	597	THR
1	A	601	ASN
1	A	641	VAL
1	A	658	THR
1	A	660	THR
1	A	668	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	29	ASN
1	A	55	GLN
1	A	88	ASN
1	A	98	HIS
1	A	160	ASN
1	A	178	ASN
1	A	188	ASN
1	A	204	ASN
1	A	249	HIS
1	A	320	GLN
1	A	338	ASN
1	A	369	ASN
1	A	401	ASN
1	A	410	GLN

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Mol	Chain	Res	Type
1	A	465	ASN
1	A	575	ASN
1	A	631	GLN
1	A	684	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 2 ligands modelled in this entry, 2 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	684/684 (100%)	-1.13	1 (0%) 92 91	11, 20, 39, 67	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	657	SER	2.3

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	686	1/1	0.95	0.05	18,18,18,18	0
2	CA	A	685	1/1	0.99	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.