



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 AM UTC

PDB ID : 4CGT / pdb_00004cgt
Title : DELETION MUTANT DELTA(145-150), F151D OF CYCLODEXTRIN
GLYCOSYLTRANSFERASE
Authors : Parsiegla, G.; Schulz, G.E.
Deposited on : 1998-06-06
Resolution : 2.60 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

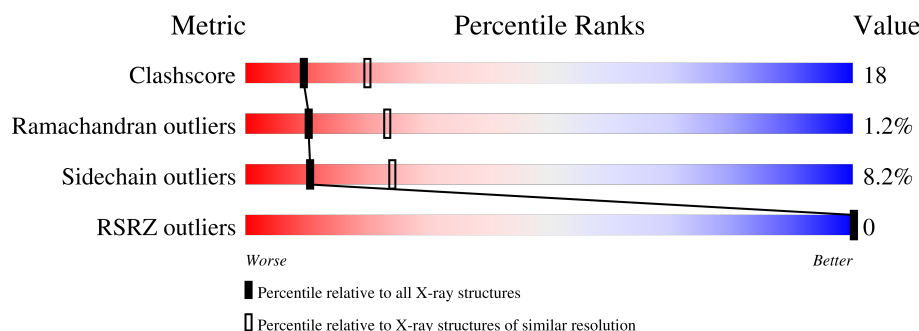
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	678	60% 34% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5381 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 GLYCOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	678	Total	C	N	O	S	0	0	0
			5219	3293	885	1029	12			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP P30920
A	?	-	GLU	deletion	UNP P30920
A	?	-	THR	deletion	UNP P30920
A	?	-	ASP	deletion	UNP P30920
A	?	-	THR	deletion	UNP P30920
A	?	-	SER	deletion	UNP P30920
A	151	ASP	PHE	engineered mutation	UNP P30920

- 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		

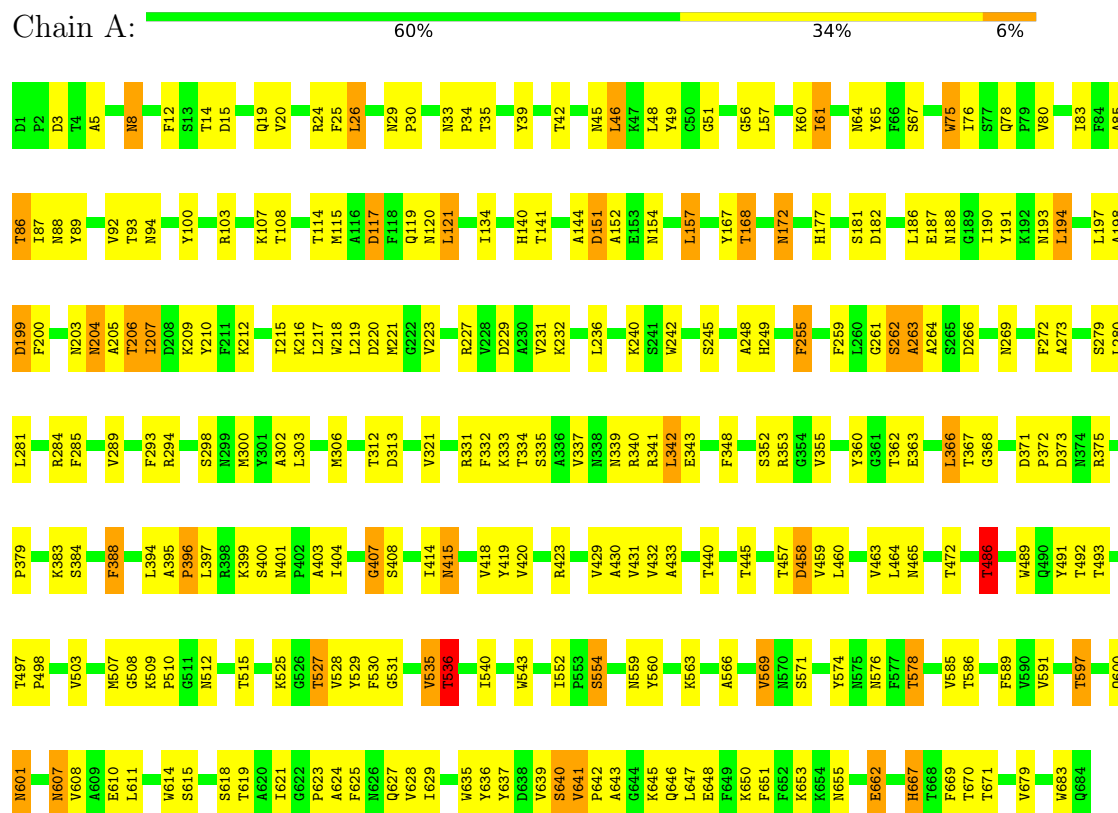
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		

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 GLYCOSYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.50Å 104.60Å 113.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 10.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (10.00-2.60) 87.1 (10.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.60Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.272 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5381	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	0.75	1/5349 (0.0%)	1.16	40/7300 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	THR	CA-CB	5.14	1.62	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	GLY	N-CA-C	-10.74	101.79	111.67
1	A	100	TYR	N-CA-C	7.83	122.47	113.15
1	A	627	GLN	N-CA-C	7.59	123.27	114.62
1	A	407	GLY	N-CA-C	7.50	120.56	111.93
1	A	611	LEU	N-CA-C	-7.10	104.49	113.72
1	A	205	ALA	N-CA-C	6.74	119.46	111.71
1	A	388	PHE	N-CA-C	-6.54	104.23	111.36
1	A	117	ASP	N-CA-C	-6.49	103.83	111.03
1	A	281	LEU	N-CA-C	-6.33	99.32	109.96
1	A	191	TYR	N-CA-C	6.27	120.94	113.16
1	A	352	SER	N-CA-C	6.18	119.56	110.59
1	A	263	ALA	N-CA-C	-6.13	105.76	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	TRP	N-CA-C	6.03	119.86	111.90
1	A	404	ILE	N-CA-C	-5.95	105.05	110.82
1	A	418	VAL	N-CA-C	5.95	117.57	108.71
1	A	536	THR	N-CA-C	5.93	117.98	109.14
1	A	648	GLU	N-CA-C	-5.91	99.76	109.40
1	A	332	PHE	N-CA-C	-5.90	104.92	111.36
1	A	671	THR	N-CA-C	5.76	118.50	110.20
1	A	394	LEU	N-CA-C	5.72	118.73	111.69
1	A	203	ASN	N-CA-C	-5.72	105.56	112.54
1	A	667	HIS	N-CA-C	-5.69	102.87	110.55
1	A	662	GLU	N-CA-C	-5.68	102.48	110.50
1	A	5	ALA	N-CA-C	5.66	118.28	110.35
1	A	640	SER	N-CA-C	-5.64	101.29	110.20
1	A	607	ASN	N-CA-C	5.48	122.48	110.80
1	A	574	TYR	N-CA-C	-5.46	99.84	108.73
1	A	384	SER	N-CA-C	5.42	120.00	112.90
1	A	362	THR	N-CA-C	-5.39	105.06	111.69
1	A	400	SER	N-CA-C	5.35	118.27	111.69
1	A	29	ASN	CA-C-N	5.33	125.02	119.64
1	A	29	ASN	C-N-CA	5.33	125.02	119.64
1	A	578	THR	N-CA-C	5.17	117.16	109.25
1	A	61	ILE	N-CA-C	-5.13	105.70	110.53
1	A	65	TYR	N-CA-C	-5.13	105.58	111.07
1	A	259	PHE	N-CA-C	5.13	117.67	110.23
1	A	207	ILE	N-CA-C	-5.07	105.77	110.53
1	A	3	ASP	CA-C-N	5.06	127.02	120.44
1	A	3	ASP	C-N-CA	5.06	127.02	120.44
1	A	51	GLY	N-CA-C	5.05	121.71	114.64

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	TYR	Sidechain
1	A	49	TYR	Sidechain
1	A	491	TYR	Sidechain

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	5219	0	4965	181	0
2	A	2	0	0	0	0
3	A	160	0	0	9	0
All	All	5381	0	4965	181	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 18.

All (181) 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:108:THR:HG23	1:A:115:MET:HE2	1.60	0.84
1:A:285:PHE:CE1	1:A:289:VAL:HG21	2.16	0.81
1:A:650:LYS:HE2	1:A:662:GLU:O	1.81	0.79
1:A:263:ALA:O	1:A:284:ARG:HD2	1.82	0.79
1:A:600:GLN:HA	1:A:655:ASN:HB3	1.64	0.78
1:A:154:ASN:HD21	1:A:168:THR:HB	1.50	0.77
1:A:273:ALA:HB2	1:A:280:LEU:HD23	1.70	0.73
1:A:597:THR:HG22	1:A:600:GLN:HB2	1.72	0.70
1:A:157:LEU:HD11	1:A:210:TYR:CZ	2.27	0.69
1:A:219:LEU:HA	1:A:223:VAL:HG22	1.73	0.69
1:A:403:ALA:O	1:A:407:GLY:HA3	1.94	0.68
1:A:334:THR:HG22	1:A:335:SER:H	1.58	0.68
1:A:530:PHE:HD1	1:A:535:VAL:HG21	1.59	0.67
1:A:429:VAL:HG12	1:A:430:ALA:N	2.10	0.67
1:A:334:THR:HG22	1:A:335:SER:N	2.12	0.65
1:A:300:MET:HE3	1:A:419:TYR:HB2	1.79	0.65
1:A:264:ALA:O	1:A:284:ARG:HD3	1.97	0.65
1:A:429:VAL:HG12	1:A:430:ALA:H	1.62	0.65
1:A:395:ALA:HB3	1:A:396:PRO:HD3	1.77	0.64
1:A:585:VAL:HG13	1:A:643:ALA:HB2	1.80	0.62
1:A:182:ASP:H	1:A:188:ASN:HD21	1.47	0.61
1:A:78:GLN:HG2	1:A:80:VAL:HG22	1.83	0.60
1:A:34:PRO:HB2	1:A:39:TYR:HB2	1.82	0.60
1:A:220:ASP:OD1	1:A:249:HIS:HE1	1.84	0.60
1:A:144:ALA:O	1:A:151:ASP:HB2	2.01	0.60
1:A:182:ASP:N	1:A:188:ASN:HD21	2.01	0.59
1:A:157:LEU:HD22	1:A:200:PHE:CE1	2.38	0.59
1:A:331:ARG:HG2	1:A:368:GLY:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:HG21	1:A:639:VAL:HG22	1.83	0.59
1:A:172:ASN:ND2	1:A:172:ASN:H	1.99	0.59
1:A:530:PHE:CD1	1:A:535:VAL:HG21	2.37	0.58
1:A:266:ASP:HB3	1:A:269:ASN:HB3	1.86	0.58
1:A:641:VAL:HG22	1:A:642:PRO:HD2	1.85	0.57
1:A:115:MET:SD	1:A:221:MET:HE1	2.45	0.57
1:A:662:GLU:HG2	1:A:683:TRP:CE3	2.40	0.57
1:A:510:PRO:HB3	1:A:554:SER:HA	1.87	0.57
1:A:512:ASN:HB2	1:A:552:ILE:HD12	1.88	0.56
1:A:89:TYR:O	1:A:92:VAL:HG12	2.05	0.56
1:A:589:PHE:O	1:A:636:TYR:HA	2.06	0.56
1:A:624:ALA:HA	1:A:637:TYR:CD1	2.40	0.55
1:A:621:ILE:HG21	1:A:639:VAL:CG2	2.35	0.55
1:A:509:LYS:H	1:A:512:ASN:ND2	2.05	0.55
1:A:300:MET:HE3	1:A:419:TYR:CB	2.38	0.54
1:A:529:TYR:HB2	1:A:563:LYS:HB3	1.89	0.54
1:A:232:LYS:O	1:A:232:LYS:HG2	2.06	0.54
1:A:154:ASN:HD21	1:A:168:THR:H	1.56	0.54
1:A:559:ASN:HD21	1:A:576:ASN:HA	1.73	0.54
1:A:498:PRO:HB2	1:A:571:SER:HB3	1.90	0.54
1:A:186:LEU:O	1:A:190:ILE:HG13	2.07	0.53
1:A:217:LEU:C	1:A:217:LEU:HD23	2.34	0.53
1:A:57:LEU:O	1:A:61:ILE:HG13	2.07	0.53
1:A:140:HIS:CD2	1:A:197:LEU:HD13	2.44	0.53
1:A:383:LYS:HA	1:A:388:PHE:CD2	2.44	0.53
1:A:187:GLU:CD	1:A:625:PHE:HB3	2.34	0.53
1:A:154:ASN:ND2	1:A:168:THR:HB	2.20	0.52
1:A:646:GLN:HA	1:A:670:THR:HA	1.89	0.52
1:A:46:LEU:HD23	1:A:373:ASP:HA	1.91	0.52
1:A:507:MET:HA	1:A:578:THR:O	2.10	0.52
1:A:255:PHE:CD1	1:A:255:PHE:N	2.78	0.52
1:A:86:THR:CG2	1:A:93:THR:HG23	2.40	0.51
1:A:460:LEU:HD13	1:A:464:LEU:HD12	1.92	0.51
1:A:508:GLY:HA3	3:A:750:HOH:O	2.08	0.51
1:A:86:THR:HG21	1:A:93:THR:HG23	1.92	0.51
1:A:433:ALA:O	1:A:486:THR:HA	2.10	0.51
1:A:144:ALA:O	1:A:151:ASP:CB	2.60	0.50
1:A:64:ASN:HA	3:A:770:HOH:O	2.11	0.50
1:A:527:THR:HB	1:A:536:THR:CG2	2.41	0.50
1:A:420:VAL:HA	1:A:432:VAL:O	2.11	0.50
1:A:601:ASN:O	1:A:653:LYS:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:LYS:HG3	1:A:646:GLN:N	2.27	0.50
1:A:248:ALA:HA	1:A:512:ASN:OD1	2.11	0.50
1:A:140:HIS:HD2	1:A:141:THR:O	1.94	0.50
1:A:284:ARG:HG3	3:A:700:HOH:O	2.11	0.50
1:A:415:ASN:OD1	1:A:415:ASN:C	2.55	0.50
1:A:510:PRO:HA	1:A:552:ILE:HG22	1.93	0.49
1:A:60:LYS:HE3	1:A:60:LYS:HA	1.93	0.49
1:A:255:PHE:CD2	1:A:321:VAL:HG21	2.47	0.49
1:A:242:TRP:O	1:A:245:SER:HB3	2.13	0.49
1:A:586:THR:HG22	3:A:828:HOH:O	2.11	0.49
1:A:333:LYS:HB2	1:A:342:LEU:HD23	1.95	0.49
1:A:321:VAL:HA	1:A:355:VAL:O	2.13	0.49
1:A:401:ASN:OD1	1:A:403:ALA:HB3	2.12	0.49
1:A:261:GLY:O	1:A:262:SER:HB3	2.13	0.49
1:A:503:VAL:HA	1:A:515:THR:O	2.13	0.49
1:A:543:TRP:C	1:A:543:TRP:CD1	2.91	0.49
1:A:334:THR:CG2	1:A:335:SER:H	2.24	0.49
1:A:45:ASN:ND2	1:A:48:LEU:HG	2.28	0.48
1:A:92:VAL:HG13	1:A:94:ASN:HD21	1.79	0.48
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.61	0.48
1:A:525:LYS:HE3	1:A:540:ILE:HB	1.95	0.48
1:A:527:THR:HB	1:A:536:THR:HG23	1.95	0.48
1:A:204:ASN:ND2	1:A:206:THR:H	2.12	0.48
1:A:653:LYS:HE3	1:A:683:TRP:CZ2	2.48	0.47
1:A:420:VAL:HG22	1:A:433:ALA:HA	1.96	0.47
1:A:303:LEU:HD11	1:A:348:PHE:CZ	2.49	0.47
1:A:463:VAL:HG23	1:A:464:LEU:HG	1.96	0.47
1:A:366:LEU:HA	3:A:758:HOH:O	2.14	0.47
1:A:24:ARG:NH2	1:A:48:LEU:O	2.47	0.47
1:A:624:ALA:HA	1:A:637:TYR:HD1	1.77	0.47
1:A:363:GLU:OE1	1:A:363:GLU:N	2.47	0.47
1:A:284:ARG:NH2	1:A:313:ASP:OD2	2.48	0.47
1:A:12:PHE:HA	1:A:15:ASP:OD2	2.15	0.47
1:A:662:GLU:CD	1:A:667:HIS:HE2	2.23	0.46
1:A:340:ARG:HH12	1:A:465:ASN:ND2	2.13	0.46
1:A:498:PRO:O	1:A:571:SER:HA	2.14	0.46
1:A:30:PRO:HA	1:A:33:ASN:ND2	2.30	0.46
1:A:334:THR:CG2	1:A:335:SER:N	2.78	0.46
1:A:19:GLN:HG3	1:A:75:TRP:CD2	2.51	0.45
1:A:608:VAL:HG12	1:A:645:LYS:HE3	1.98	0.45
1:A:371:ASP:HA	1:A:372:PRO:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG12	1:A:529:TYR:N	2.31	0.45
1:A:635:TRP:N	1:A:635:TRP:CD1	2.84	0.45
1:A:26:LEU:HB3	1:A:56:GLY:HA3	1.99	0.45
1:A:75:TRP:C	1:A:75:TRP:CD1	2.93	0.45
1:A:303:LEU:HD11	1:A:348:PHE:CE2	2.51	0.45
1:A:76:ILE:HD11	1:A:134:ILE:HG22	1.99	0.45
1:A:115:MET:O	1:A:119:GLN:HG3	2.17	0.45
1:A:193:ASN:OD1	1:A:199:ASP:HB2	2.17	0.45
1:A:431:VAL:HB	1:A:489:TRP:HE3	1.82	0.45
1:A:167:TYR:O	1:A:177:HIS:HE1	1.99	0.44
1:A:293:PHE:O	1:A:341:ARG:HD2	2.17	0.44
1:A:408:SER:O	1:A:423:ARG:HA	2.17	0.44
1:A:458:ASP:O	1:A:460:LEU:N	2.50	0.44
1:A:566:ALA:O	1:A:569:VAL:HG23	2.17	0.44
1:A:181:SER:HB2	1:A:188:ASN:O	2.17	0.44
1:A:512:ASN:HB3	3:A:717:HOH:O	2.16	0.44
1:A:525:LYS:HG3	1:A:543:TRP:HB3	1.99	0.44
1:A:231:VAL:HB	1:A:272:PHE:CZ	2.53	0.44
1:A:306:MET:HE3	1:A:306:MET:HB3	1.90	0.44
1:A:157:LEU:HD22	1:A:200:PHE:HE1	1.80	0.44
1:A:262:SER:OG	1:A:264:ALA:HB3	2.18	0.44
1:A:83:ILE:HA	1:A:103:ARG:HD3	2.00	0.43
1:A:528:VAL:HB	1:A:535:VAL:HB	2.00	0.43
1:A:559:ASN:ND2	1:A:576:ASN:HA	2.33	0.43
1:A:669:PHE:CE1	1:A:679:VAL:HB	2.53	0.43
1:A:294:ARG:HG3	1:A:337:VAL:HG21	2.00	0.43
1:A:340:ARG:HA	1:A:340:ARG:HD3	1.77	0.43
1:A:87:ILE:HD12	1:A:87:ILE:N	2.34	0.43
1:A:628:VAL:HG12	1:A:629:ILE:HD13	2.01	0.43
1:A:367:THR:HB	3:A:753:HOH:O	2.18	0.43
1:A:429:VAL:CG1	1:A:430:ALA:N	2.79	0.43
1:A:560:TYR:CD1	1:A:560:TYR:N	2.87	0.43
1:A:625:PHE:O	1:A:635:TRP:HA	2.19	0.43
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.53	0.43
1:A:25:PHE:CE2	1:A:60:LYS:HG3	2.54	0.42
1:A:83:ILE:HD12	1:A:152:ALA:HB1	2.00	0.42
1:A:240:LYS:HD3	1:A:640:SER:HB3	2.00	0.42
1:A:212:LYS:O	1:A:216:LYS:HD3	2.19	0.42
1:A:298:SER:HB3	1:A:302:ALA:CB	2.49	0.42
1:A:639:VAL:HG12	1:A:640:SER:O	2.19	0.42
1:A:30:PRO:HA	1:A:33:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:HG3	1:A:75:TRP:CE3	2.55	0.42
1:A:236:LEU:C	1:A:236:LEU:HD23	2.44	0.42
1:A:194:LEU:HD22	1:A:194:LEU:HA	1.89	0.42
1:A:14:THR:O	1:A:399:LYS:HE2	2.20	0.42
1:A:217:LEU:HD23	1:A:217:LEU:O	2.19	0.42
1:A:255:PHE:N	1:A:255:PHE:HD1	2.17	0.42
1:A:339:ASN:HB3	1:A:343:GLU:OE2	2.20	0.42
1:A:121:LEU:HD22	1:A:121:LEU:O	2.19	0.42
1:A:207:ILE:HD13	1:A:207:ILE:HA	1.79	0.42
1:A:368:GLY:HA3	1:A:373:ASP:O	2.20	0.42
1:A:64:ASN:HB3	1:A:67:SER:HB2	2.01	0.41
1:A:141:THR:OG1	1:A:198:ALA:HB3	2.20	0.41
1:A:383:LYS:HA	1:A:388:PHE:CE2	2.55	0.41
1:A:215:ILE:O	1:A:219:LEU:HG	2.19	0.41
1:A:591:VAL:HB	1:A:651:PHE:CE1	2.55	0.41
1:A:273:ALA:CB	1:A:280:LEU:HD23	2.47	0.41
1:A:527:THR:CB	1:A:536:THR:HG23	2.51	0.41
1:A:8:ASN:HB3	3:A:699:HOH:O	2.20	0.41
1:A:12:PHE:HB3	1:A:355:VAL:HG11	2.03	0.41
1:A:353:ARG:HA	3:A:803:HOH:O	2.20	0.41
1:A:114:THR:H	1:A:117:ASP:HB2	1.85	0.41
1:A:117:ASP:O	1:A:120:ASN:HB3	2.21	0.41
1:A:464:LEU:HB3	1:A:486:THR:HG23	2.01	0.41
1:A:492:THR:HG22	1:A:493:THR:N	2.35	0.41
1:A:509:LYS:N	1:A:512:ASN:ND2	2.69	0.41
1:A:601:ASN:ND2	1:A:623:PRO:HB2	2.37	0.40
1:A:157:LEU:HD22	1:A:200:PHE:CZ	2.56	0.40
1:A:108:THR:HG22	1:A:218:TRP:HH2	1.87	0.40
1:A:414:ILE:HD13	1:A:414:ILE:HG21	1.86	0.40
1:A:610:GLU:CD	1:A:642:PRO:HD3	2.46	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	676/678 (100%)	612 (90%)	56 (8%)	8 (1%)	10	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	151	ASP
1	A	459	VAL
1	A	262	SER
1	A	458	ASP
1	A	607	ASN
1	A	85	ALA
1	A	379	PRO

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	560/560 (100%)	514 (92%)	46 (8%)	10	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	26	LEU
1	A	35	THR
1	A	42	THR
1	A	46	LEU
1	A	75	TRP
1	A	86	THR
1	A	88	ASN
1	A	107	LYS
1	A	121	LEU
1	A	157	LEU

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Mol	Chain	Res	Type
1	A	168	THR
1	A	172	ASN
1	A	194	LEU
1	A	199	ASP
1	A	204	ASN
1	A	206	THR
1	A	209	LYS
1	A	229	ASP
1	A	255	PHE
1	A	279	SER
1	A	312	THR
1	A	342	LEU
1	A	366	LEU
1	A	375	ARG
1	A	396	PRO
1	A	397	LEU
1	A	415	ASN
1	A	440	THR
1	A	445	THR
1	A	457	THR
1	A	472	THR
1	A	486	THR
1	A	497	THR
1	A	527	THR
1	A	535	VAL
1	A	536	THR
1	A	554	SER
1	A	569	VAL
1	A	597	THR
1	A	601	ASN
1	A	615	SER
1	A	618	SER
1	A	619	THR
1	A	641	VAL
1	A	647	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	120	ASN
1	A	140	HIS

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Mol	Chain	Res	Type
1	A	154	ASN
1	A	172	ASN
1	A	176	HIS
1	A	178	ASN
1	A	188	ASN
1	A	201	ASN
1	A	204	ASN
1	A	249	HIS
1	A	318	ASN
1	A	369	ASN
1	A	389	ASN
1	A	411	GLN
1	A	465	ASN
1	A	477	ASN
1	A	512	ASN
1	A	559	ASN
1	A	575	ASN
1	A	576	ASN
1	A	601	ASN
1	A	684	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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

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	678/678 (100%)	-2.00	0 100 100	2, 10, 31, 53	0

There are no RSRZ outliers to report.

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	685	1/1	1.00	0.01	22,22,22,22	0
2	CA	A	686	1/1	1.00	0.02	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.