



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:51 PM UTC

PDB ID : 2V5D / pdb_00002v5d
Title : Structure of a Family 84 Glycoside Hydrolase and a Family 32 Carbohydrate-Binding Module in Tandem from *Clostridium perfringens*.
Authors : Ficko-Blean, E.; Gregg, K.J.; Adams, J.J.; Hehemann, J.H.; Smith, S.J.; Czjzek, M.; Boraston, A.B.
Deposited on : 2008-10-02
Resolution : 3.30 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

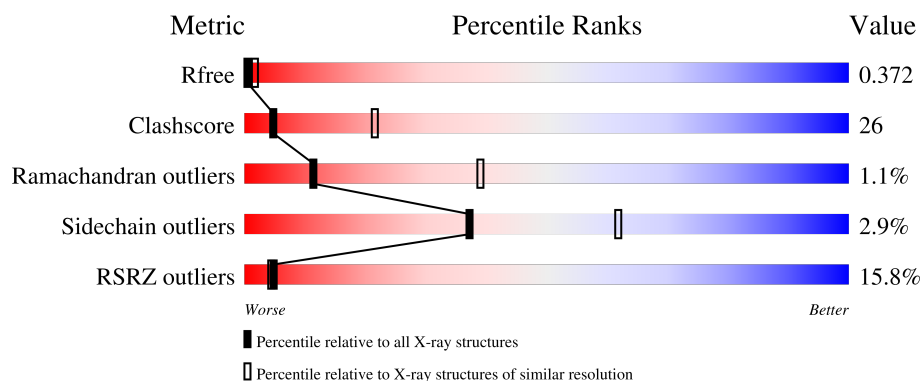
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	737	15% 78% 15% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5706 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 O-GLCNACASE NAGJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	722	Total	C	N	O	S	0	0	0
			5676	3560	939	1159	18			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		

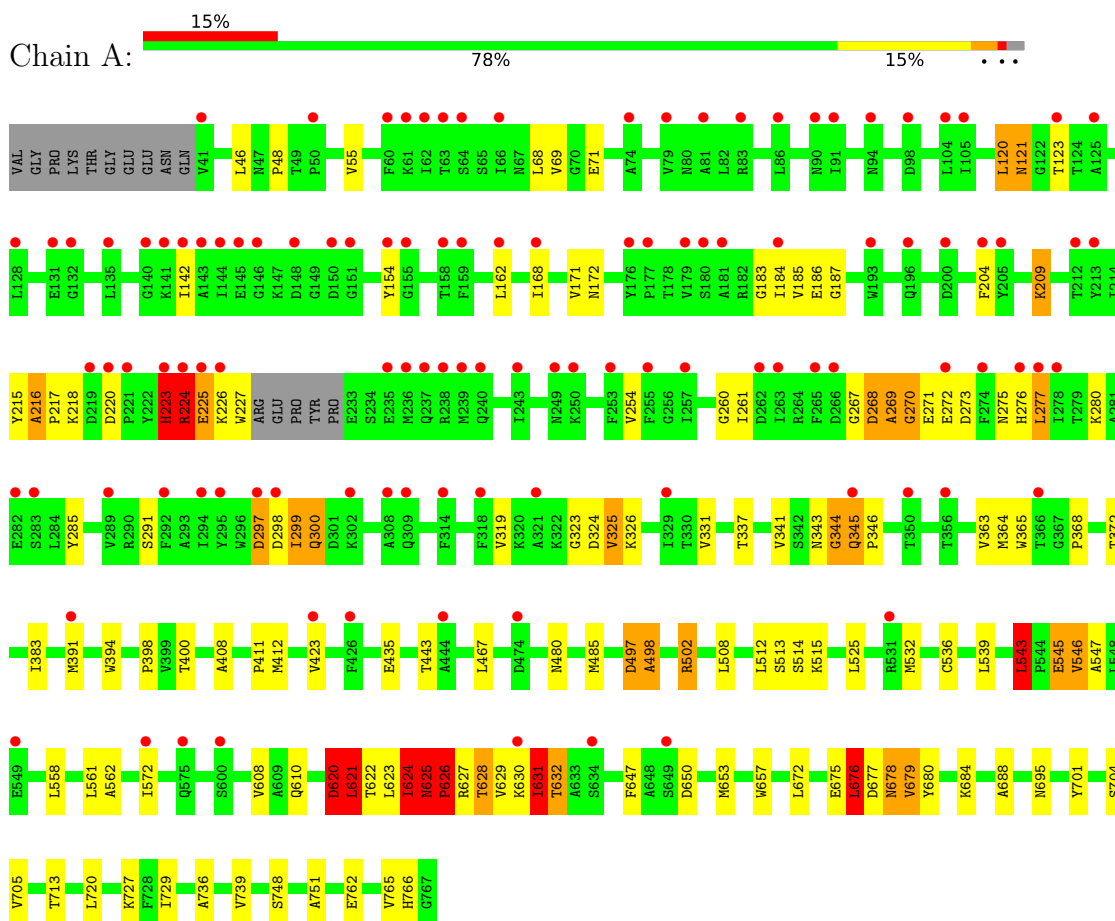
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		

3 Residue-property plots [i](#)

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: O-GLCNACASE NAGJ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.85Å 69.55Å 136.78Å 90.00° 95.78° 90.00°	Depositor
Resolution (Å)	141.42 – 3.30 136.09 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (141.42-3.30) 92.7 (136.09-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.322 , 0.370 0.324 , 0.372	Depositor DCC
R_{free} test set	594 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 11.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5706	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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	0.58	6/5792 (0.1%)	1.00	37/7861 (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	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	ALA	CA-CB	-9.58	1.44	1.52
1	A	498	ALA	C-O	-8.10	1.19	1.23
1	A	498	ALA	CA-C	-7.40	1.48	1.53
1	A	224	ARG	CA-C	6.76	1.61	1.52
1	A	631	ILE	CA-CB	-6.09	1.48	1.54
1	A	621	LEU	N-CA	-6.00	1.38	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	CA-C-N	17.47	153.15	121.70
1	A	268	ASP	C-N-CA	17.47	153.15	121.70
1	A	344	GLY	CA-C-N	15.14	142.46	120.51
1	A	344	GLY	C-N-CA	15.14	142.46	120.51
1	A	268	ASP	N-CA-C	15.10	127.74	111.28
1	A	277	LEU	CA-C-N	13.37	137.84	120.60
1	A	277	LEU	C-N-CA	13.37	137.84	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	GLN	CA-C-N	13.15	134.00	119.92
1	A	345	GLN	C-N-CA	13.15	134.00	119.92
1	A	268	ASP	O-C-N	-10.79	110.69	122.12
1	A	269	ALA	N-CA-C	10.24	139.68	111.00
1	A	223	HIS	O-C-N	8.98	134.54	122.59
1	A	543	LEU	N-CA-C	8.91	121.14	109.83
1	A	121	ASN	N-CA-C	8.73	123.44	111.39
1	A	209	LYS	N-CA-C	7.95	122.01	111.28
1	A	269	ALA	CA-C-O	-7.50	108.06	120.80
1	A	620	ASP	CA-C-N	7.21	133.84	122.74
1	A	620	ASP	C-N-CA	7.21	133.84	122.74
1	A	626	PRO	CA-N-CD	-7.15	101.98	112.00
1	A	325	VAL	N-CA-C	6.84	118.90	109.80
1	A	120	LEU	N-CA-C	6.71	118.39	111.14
1	A	270	GLY	N-CA-C	-6.71	93.84	113.30
1	A	223	HIS	CA-C-N	6.45	133.86	121.54
1	A	223	HIS	C-N-CA	6.45	133.86	121.54
1	A	267	GLY	N-CA-C	6.17	120.80	112.17
1	A	299	ILE	N-CA-C	6.05	121.93	109.34
1	A	275	ASN	N-CA-C	-5.99	104.75	111.28
1	A	323	GLY	N-CA-C	-5.85	108.12	115.08
1	A	270	GLY	CA-C-N	-5.62	112.74	120.28
1	A	270	GLY	C-N-CA	-5.62	112.74	120.28
1	A	676	LEU	O-C-N	-5.52	116.80	123.03
1	A	624	ILE	CA-C-N	5.34	131.32	121.70
1	A	624	ILE	C-N-CA	5.34	131.32	121.70
1	A	625	ASN	C-N-CD	-5.18	103.76	125.00
1	A	497	ASP	CB-CA-C	-5.16	101.63	109.89
1	A	297	ASP	CA-C-N	-5.00	115.95	123.00
1	A	297	ASP	C-N-CA	-5.00	115.95	123.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	GLY	Peptide
1	A	620	ASP	Peptide,Mainchain
1	A	624	ILE	Peptide
1	A	676	LEU	Mainchain

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	5676	0	5404	284	0
2	A	3	0	0	0	0
3	A	27	0	0	0	0
All	All	5706	0	5404	284	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 26.

All (284) 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:345:GLN:CD	1:A:346:PRO:HD2	1.31	1.48
1:A:224:ARG:NH1	1:A:225:GLU:HA	1.18	1.48
1:A:224:ARG:HH11	1:A:225:GLU:CA	1.29	1.44
1:A:621:LEU:CA	1:A:622:THR:HG22	1.49	1.42
1:A:626:PRO:C	1:A:628:THR:HB	1.44	1.39
1:A:224:ARG:HD2	1:A:225:GLU:N	1.37	1.35
1:A:631:ILE:HD12	1:A:632:THR:N	1.35	1.35
1:A:621:LEU:C	1:A:621:LEU:HD23	1.50	1.28
1:A:269:ALA:HA	1:A:272:GLU:N	1.49	1.27
1:A:621:LEU:HA	1:A:622:THR:CG2	1.68	1.23
1:A:269:ALA:CB	1:A:272:GLU:HG2	1.68	1.22
1:A:217:PRO:HG2	1:A:218:LYS:HE2	1.21	1.21
1:A:345:GLN:CD	1:A:346:PRO:CD	2.13	1.20
1:A:217:PRO:CG	1:A:218:LYS:HE2	1.73	1.19
1:A:627:ARG:N	1:A:628:THR:HB	1.58	1.18
1:A:345:GLN:CG	1:A:346:PRO:HD2	1.70	1.18
1:A:224:ARG:CD	1:A:225:GLU:N	2.05	1.18
1:A:260:GLY:C	1:A:299:ILE:HD13	1.71	1.16
1:A:269:ALA:N	1:A:272:GLU:H	1.42	1.14
1:A:626:PRO:CB	1:A:627:ARG:HB3	1.78	1.13
1:A:626:PRO:HB3	1:A:627:ARG:CB	1.79	1.11
1:A:621:LEU:N	1:A:622:THR:HG22	1.64	1.11
1:A:186:GLU:O	1:A:216:ALA:O	1.68	1.10
1:A:217:PRO:CB	1:A:218:LYS:HD3	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PRO:HB3	1:A:218:LYS:HD3	1.19	1.10
1:A:217:PRO:CB	1:A:218:LYS:CD	2.30	1.10
1:A:217:PRO:CB	1:A:218:LYS:CE	2.30	1.10
1:A:269:ALA:CB	1:A:272:GLU:CG	2.30	1.09
1:A:269:ALA:CA	1:A:272:GLU:H	1.66	1.09
1:A:217:PRO:CG	1:A:218:LYS:CE	2.30	1.08
1:A:300:GLN:HE21	1:A:300:GLN:N	1.49	1.08
1:A:624:ILE:N	1:A:625:ASN:HB3	1.68	1.08
1:A:621:LEU:HG	1:A:623:LEU:H	1.09	1.07
1:A:299:ILE:HD12	1:A:299:ILE:O	1.55	1.06
1:A:621:LEU:HA	1:A:622:THR:HG22	1.23	1.06
1:A:217:PRO:CB	1:A:218:LYS:HE2	1.84	1.05
1:A:217:PRO:HB2	1:A:218:LYS:CD	1.87	1.04
1:A:269:ALA:HB1	1:A:272:GLU:HG2	1.36	1.04
1:A:624:ILE:CA	1:A:625:ASN:HB3	1.84	1.04
1:A:260:GLY:O	1:A:299:ILE:CD1	2.05	1.04
1:A:224:ARG:HD3	1:A:224:ARG:C	1.83	1.03
1:A:621:LEU:CA	1:A:622:THR:CG2	2.31	1.03
1:A:621:LEU:HD23	1:A:621:LEU:O	1.57	1.03
1:A:626:PRO:HB3	1:A:627:ARG:HB3	1.34	1.03
1:A:621:LEU:C	1:A:621:LEU:CD2	2.30	1.03
1:A:621:LEU:HG	1:A:623:LEU:N	1.71	1.03
1:A:269:ALA:CA	1:A:272:GLU:HG2	1.88	1.02
1:A:626:PRO:C	1:A:628:THR:CB	2.32	1.02
1:A:224:ARG:CD	1:A:224:ARG:C	2.30	1.02
1:A:629:VAL:HG12	1:A:675:GLU:O	1.59	1.02
1:A:224:ARG:O	1:A:225:GLU:O	1.80	0.99
1:A:626:PRO:HB3	1:A:627:ARG:HA	1.45	0.99
1:A:629:VAL:CG1	1:A:675:GLU:O	2.09	0.99
1:A:626:PRO:HB3	1:A:627:ARG:CA	1.93	0.98
1:A:217:PRO:HG2	1:A:218:LYS:CE	1.91	0.98
1:A:300:GLN:HA	1:A:300:GLN:NE2	1.77	0.97
1:A:217:PRO:CG	1:A:218:LYS:NZ	2.30	0.95
1:A:623:LEU:HD13	1:A:766:HIS:CE1	2.01	0.95
1:A:260:GLY:O	1:A:299:ILE:HD11	1.66	0.93
1:A:217:PRO:HB3	1:A:218:LYS:CD	1.97	0.93
1:A:621:LEU:HD23	1:A:622:THR:N	1.82	0.93
1:A:631:ILE:CD1	1:A:632:THR:N	2.29	0.92
1:A:269:ALA:O	1:A:272:GLU:HG2	1.68	0.92
1:A:269:ALA:HB1	1:A:272:GLU:CG	1.96	0.92
1:A:514:SER:O	1:A:515:LYS:HB2	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:SER:HB3	1:A:713:THR:O	1.69	0.92
1:A:300:GLN:NE2	1:A:300:GLN:CA	2.30	0.91
1:A:626:PRO:HA	1:A:628:THR:O	1.71	0.90
1:A:217:PRO:HG3	1:A:218:LYS:NZ	1.86	0.90
1:A:626:PRO:HB2	1:A:627:ARG:HB3	1.52	0.89
1:A:217:PRO:HB2	1:A:218:LYS:HE2	1.48	0.89
1:A:260:GLY:CA	1:A:299:ILE:HD13	2.03	0.89
1:A:626:PRO:CA	1:A:628:THR:HB	2.02	0.89
1:A:217:PRO:HB2	1:A:218:LYS:CE	1.99	0.89
1:A:260:GLY:C	1:A:299:ILE:CD1	2.46	0.89
1:A:300:GLN:HE21	1:A:300:GLN:H	1.20	0.89
1:A:626:PRO:CB	1:A:627:ARG:CA	2.48	0.89
1:A:621:LEU:HA	1:A:622:THR:HG23	1.56	0.88
1:A:345:GLN:OE1	1:A:346:PRO:CD	2.22	0.86
1:A:224:ARG:HD2	1:A:225:GLU:H	1.03	0.86
1:A:269:ALA:N	1:A:272:GLU:N	2.24	0.85
1:A:626:PRO:CB	1:A:627:ARG:HA	2.00	0.85
1:A:620:ASP:C	1:A:622:THR:HG22	2.01	0.84
1:A:513:SER:O	1:A:624:ILE:HG23	1.77	0.84
1:A:631:ILE:HD12	1:A:631:ILE:C	1.95	0.84
1:A:624:ILE:H	1:A:625:ASN:HB3	1.43	0.83
1:A:620:ASP:OD1	1:A:622:THR:HG21	1.79	0.82
1:A:627:ARG:N	1:A:628:THR:CB	2.40	0.82
1:A:269:ALA:HB1	1:A:272:GLU:CD	2.04	0.82
1:A:678:ASN:HD22	1:A:679:VAL:N	1.78	0.82
1:A:217:PRO:HB2	1:A:218:LYS:CG	2.10	0.81
1:A:269:ALA:CA	1:A:272:GLU:N	2.29	0.81
1:A:653:MET:HE1	1:A:688:ALA:HB1	1.62	0.81
1:A:624:ILE:N	1:A:625:ASN:CB	2.41	0.81
1:A:217:PRO:CB	1:A:218:LYS:HA	2.09	0.81
1:A:631:ILE:HD12	1:A:632:THR:H	0.99	0.81
1:A:620:ASP:OD1	1:A:622:THR:CG2	2.30	0.80
1:A:657:TRP:CZ3	1:A:672:LEU:HD21	2.17	0.80
1:A:678:ASN:ND2	1:A:679:VAL:N	2.30	0.80
1:A:626:PRO:HA	1:A:628:THR:HB	1.64	0.80
1:A:626:PRO:CB	1:A:627:ARG:CB	2.46	0.79
1:A:627:ARG:CA	1:A:628:THR:HB	2.12	0.78
1:A:299:ILE:O	1:A:299:ILE:CD1	2.30	0.78
1:A:300:GLN:HE21	1:A:300:GLN:CA	1.90	0.78
1:A:620:ASP:C	1:A:622:THR:CG2	2.57	0.77
1:A:625:ASN:O	1:A:626:PRO:HB2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:ILE:HA	1:A:625:ASN:HB3	1.66	0.77
1:A:345:GLN:OE1	1:A:346:PRO:HD3	1.85	0.77
1:A:621:LEU:C	1:A:622:THR:HG22	2.09	0.77
1:A:631:ILE:CD1	1:A:632:THR:H	1.92	0.77
1:A:225:GLU:HG2	1:A:226:LYS:HG3	1.65	0.77
1:A:704:SER:CB	1:A:713:THR:O	2.32	0.77
1:A:269:ALA:CB	1:A:272:GLU:CD	2.58	0.76
1:A:269:ALA:HB2	1:A:272:GLU:CG	2.14	0.76
1:A:629:VAL:HG13	1:A:675:GLU:O	1.86	0.76
1:A:300:GLN:N	1:A:300:GLN:NE2	2.30	0.75
1:A:345:GLN:HG3	1:A:346:PRO:HD2	1.67	0.75
1:A:630:LYS:O	1:A:630:LYS:HG3	1.85	0.75
1:A:224:ARG:NH1	1:A:225:GLU:CA	2.07	0.74
1:A:625:ASN:O	1:A:625:ASN:CG	2.30	0.74
1:A:187:GLY:HA2	1:A:217:PRO:HD2	1.69	0.73
1:A:625:ASN:OD1	1:A:625:ASN:C	2.30	0.73
1:A:623:LEU:HG	1:A:625:ASN:HA	1.70	0.73
1:A:217:PRO:CG	1:A:218:LYS:HZ1	2.01	0.72
1:A:285:TYR:OH	1:A:324:ASP:HB2	1.90	0.72
1:A:621:LEU:O	1:A:621:LEU:CD2	2.31	0.71
1:A:513:SER:O	1:A:624:ILE:CG2	2.38	0.71
1:A:216:ALA:HB1	1:A:223:HIS:NE2	2.06	0.70
1:A:623:LEU:HG	1:A:625:ASN:CA	2.20	0.70
1:A:705:VAL:O	1:A:713:THR:HG22	1.92	0.70
1:A:269:ALA:C	1:A:272:GLU:HG2	2.17	0.69
1:A:625:ASN:O	1:A:626:PRO:CB	2.37	0.69
1:A:325:VAL:HG12	1:A:326:LYS:O	1.91	0.69
1:A:46:LEU:HD21	1:A:162:LEU:CD1	2.23	0.69
1:A:626:PRO:HA	1:A:628:THR:CB	2.23	0.69
1:A:285:TYR:OH	1:A:324:ASP:CB	2.41	0.69
1:A:623:LEU:CD1	1:A:766:HIS:CE1	2.76	0.69
1:A:120:LEU:HD13	1:A:123:THR:O	1.93	0.68
1:A:623:LEU:C	1:A:624:ILE:HG13	2.16	0.68
1:A:628:THR:O	1:A:628:THR:HG22	1.93	0.68
1:A:269:ALA:HB2	1:A:272:GLU:HB3	1.73	0.68
1:A:345:GLN:CG	1:A:346:PRO:CD	2.62	0.68
1:A:224:ARG:O	1:A:225:GLU:C	2.37	0.67
1:A:225:GLU:HG2	1:A:226:LYS:N	2.08	0.67
1:A:269:ALA:N	1:A:271:GLU:N	2.44	0.66
1:A:217:PRO:HG3	1:A:218:LYS:HZ1	1.58	0.66
1:A:624:ILE:H	1:A:625:ASN:CB	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:HH11	1:A:225:GLU:N	1.92	0.65
1:A:142:ILE:HD13	1:A:168:ILE:HD13	1.77	0.65
1:A:678:ASN:HD22	1:A:678:ASN:C	2.04	0.65
1:A:363:VAL:HG12	1:A:391:MET:HE1	1.80	0.64
1:A:319:VAL:HG23	1:A:325:VAL:HG12	1.79	0.63
1:A:217:PRO:HB3	1:A:218:LYS:HA	1.81	0.63
1:A:628:THR:HA	1:A:629:VAL:HB	1.80	0.63
1:A:269:ALA:HB2	1:A:272:GLU:CB	2.28	0.63
1:A:545:GLU:O	1:A:546:VAL:C	2.40	0.63
1:A:299:ILE:O	1:A:300:GLN:HB2	2.00	0.62
1:A:46:LEU:HD21	1:A:162:LEU:HD12	1.81	0.62
1:A:224:ARG:HH11	1:A:225:GLU:HA	0.53	0.62
1:A:217:PRO:HB2	1:A:218:LYS:HG2	1.82	0.61
1:A:623:LEU:O	1:A:624:ILE:C	2.44	0.61
1:A:260:GLY:O	1:A:299:ILE:HD13	1.78	0.61
1:A:677:ASP:OD1	1:A:678:ASN:N	2.33	0.61
1:A:217:PRO:HG2	1:A:218:LYS:NZ	2.08	0.61
1:A:68:LEU:HD22	1:A:71:GLU:HG3	1.82	0.61
1:A:224:ARG:HH12	1:A:225:GLU:HA	1.52	0.61
1:A:631:ILE:HD11	1:A:632:THR:O	2.01	0.61
1:A:739:VAL:HG21	1:A:765:VAL:HG11	1.81	0.61
1:A:55:VAL:HA	1:A:171:VAL:HG12	1.84	0.60
1:A:631:ILE:CD1	1:A:632:THR:O	2.49	0.60
1:A:298:ASP:OD2	1:A:298:ASP:N	2.30	0.60
1:A:217:PRO:HG3	1:A:218:LYS:HZ3	1.65	0.59
1:A:276:HIS:CD2	1:A:276:HIS:O	2.56	0.59
1:A:629:VAL:CG1	1:A:675:GLU:C	2.76	0.59
1:A:225:GLU:HG2	1:A:226:LYS:H	1.67	0.59
1:A:539:LEU:O	1:A:543:LEU:HD22	2.03	0.59
1:A:269:ALA:CA	1:A:272:GLU:CG	2.71	0.58
1:A:345:GLN:NE2	1:A:346:PRO:HD2	2.08	0.58
1:A:277:LEU:O	1:A:280:LYS:HB3	2.03	0.58
1:A:695:ASN:HD22	1:A:748:SER:HB2	1.69	0.57
1:A:260:GLY:HA3	1:A:299:ILE:HD13	1.85	0.57
1:A:620:ASP:OD1	1:A:622:THR:HG23	2.04	0.57
1:A:623:LEU:HG	1:A:625:ASN:HB2	1.87	0.57
1:A:398:PRO:HB2	1:A:408:ALA:HB3	1.87	0.57
1:A:545:GLU:HG2	1:A:546:VAL:N	2.19	0.56
1:A:215:TYR:O	1:A:216:ALA:HB3	2.04	0.56
1:A:630:LYS:O	1:A:630:LYS:CG	2.54	0.56
1:A:120:LEU:CD1	1:A:123:THR:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ARG:HG2	1:A:608:VAL:HG22	1.88	0.55
1:A:269:ALA:CB	1:A:272:GLU:CB	2.85	0.55
1:A:154:TYR:HB3	1:A:209:LYS:HE3	1.89	0.55
1:A:269:ALA:HB2	1:A:272:GLU:CD	2.31	0.55
1:A:623:LEU:HG	1:A:625:ASN:CB	2.36	0.54
1:A:269:ALA:O	1:A:272:GLU:CG	2.49	0.54
1:A:630:LYS:HB3	1:A:675:GLU:HB3	1.90	0.54
1:A:68:LEU:HD23	1:A:69:VAL:N	2.22	0.54
1:A:620:ASP:HB3	1:A:621:LEU:CA	2.38	0.54
1:A:225:GLU:CG	1:A:226:LYS:H	2.22	0.53
1:A:647:PHE:HA	1:A:650:ASP:HB2	1.89	0.53
1:A:331:VAL:HG22	1:A:364:MET:HB2	1.91	0.53
1:A:368:PRO:HD2	1:A:372:THR:HG21	1.91	0.53
1:A:48:PRO:HD2	1:A:209:LYS:HD2	1.91	0.53
1:A:532:MET:HE2	1:A:562:ALA:HB2	1.91	0.53
1:A:218:LYS:O	1:A:220:ASP:N	2.38	0.52
1:A:435:GLU:HB2	1:A:546:VAL:HG22	1.90	0.52
1:A:364:MET:HE2	1:A:394:TRP:HB2	1.91	0.52
1:A:620:ASP:HB3	1:A:621:LEU:HA	1.91	0.52
1:A:142:ILE:CD1	1:A:168:ILE:HD13	2.39	0.52
1:A:225:GLU:O	1:A:227:TRP:CD1	2.62	0.52
1:A:497:ASP:O	1:A:608:VAL:HG21	2.10	0.52
1:A:319:VAL:HG23	1:A:325:VAL:CG1	2.38	0.52
1:A:412:MET:HE2	1:A:412:MET:HA	1.92	0.52
1:A:512:LEU:HD11	1:A:572:ILE:HD13	1.92	0.52
1:A:183:GLY:C	1:A:184:ILE:HD12	2.36	0.51
1:A:300:GLN:NE2	1:A:300:GLN:H	1.98	0.51
1:A:268:ASP:O	1:A:271:GLU:HB3	2.12	0.50
1:A:629:VAL:HG13	1:A:675:GLU:C	2.36	0.50
1:A:701:TYR:CE2	1:A:729:ILE:HD13	2.47	0.50
1:A:121:ASN:OD1	1:A:121:ASN:O	2.30	0.50
1:A:225:GLU:CG	1:A:226:LYS:N	2.71	0.50
1:A:545:GLU:O	1:A:547:ALA:N	2.45	0.50
1:A:273:ASP:O	1:A:276:HIS:C	2.54	0.50
1:A:273:ASP:O	1:A:276:HIS:O	2.30	0.50
1:A:625:ASN:OD1	1:A:626:PRO:O	2.29	0.50
1:A:224:ARG:NE	1:A:261:ILE:HD11	2.27	0.49
1:A:536:CYS:SG	1:A:558:LEU:HD23	2.51	0.49
1:A:269:ALA:HA	1:A:272:GLU:CA	2.39	0.49
1:A:298:ASP:OD2	1:A:298:ASP:O	2.30	0.49
1:A:325:VAL:CG1	1:A:326:LYS:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:PRO:CB	1:A:218:LYS:CA	2.84	0.49
1:A:625:ASN:O	1:A:625:ASN:OD1	2.29	0.49
1:A:217:PRO:HG2	1:A:218:LYS:HZ1	1.68	0.48
1:A:623:LEU:CG	1:A:625:ASN:HB2	2.43	0.48
1:A:319:VAL:HA	1:A:325:VAL:HB	1.95	0.48
1:A:299:ILE:HD12	1:A:299:ILE:C	2.25	0.47
1:A:325:VAL:HG12	1:A:326:LYS:N	2.28	0.47
1:A:625:ASN:N	1:A:626:PRO:HD2	2.29	0.47
1:A:142:ILE:HD11	1:A:168:ILE:HG21	1.97	0.47
1:A:629:VAL:HG11	1:A:676:LEU:O	2.15	0.47
1:A:299:ILE:O	1:A:299:ILE:CG1	2.63	0.46
1:A:363:VAL:CG1	1:A:391:MET:HE1	2.44	0.46
1:A:215:TYR:O	1:A:216:ALA:CB	2.63	0.46
1:A:391:MET:O	1:A:423:VAL:HG13	2.16	0.46
1:A:630:LYS:O	1:A:632:THR:HG22	2.16	0.46
1:A:345:GLN:HA	1:A:346:PRO:HD3	1.76	0.45
1:A:224:ARG:HD3	1:A:225:GLU:N	1.99	0.45
1:A:621:LEU:CD2	1:A:622:THR:N	2.66	0.45
1:A:621:LEU:HD12	1:A:623:LEU:HB3	1.98	0.45
1:A:398:PRO:O	1:A:400:THR:HG23	2.17	0.45
1:A:508:LEU:HD22	1:A:525:LEU:CD1	2.47	0.45
1:A:626:PRO:HA	1:A:628:THR:CG2	2.47	0.45
1:A:254:VAL:HG22	1:A:291:SER:CB	2.47	0.45
1:A:688:ALA:HB3	1:A:762:GLU:HB2	1.99	0.44
1:A:515:LYS:HE2	1:A:679:VAL:O	2.17	0.44
1:A:684:LYS:HB3	1:A:766:HIS:HB2	2.00	0.44
1:A:345:GLN:NE2	1:A:346:PRO:CD	2.75	0.44
1:A:271:GLU:O	1:A:272:GLU:C	2.57	0.43
1:A:269:ALA:CA	1:A:270:GLY:C	2.91	0.43
1:A:480:ASN:HD21	1:A:498:ALA:HA	1.83	0.43
1:A:676:LEU:HD12	1:A:736:ALA:O	2.19	0.43
1:A:678:ASN:ND2	1:A:679:VAL:H	2.11	0.43
1:A:621:LEU:HD11	1:A:624:ILE:HG12	2.01	0.43
1:A:626:PRO:C	1:A:628:THR:CG2	2.92	0.43
1:A:204:PHE:HE1	1:A:467:LEU:HD21	1.83	0.42
1:A:625:ASN:N	1:A:626:PRO:CD	2.80	0.42
1:A:620:ASP:C	1:A:622:THR:HG21	2.42	0.42
1:A:701:TYR:CD2	1:A:729:ILE:HD13	2.55	0.42
1:A:216:ALA:C	1:A:217:PRO:O	2.61	0.42
1:A:720:LEU:HD22	1:A:727:LYS:HG2	2.02	0.42
1:A:269:ALA:CA	1:A:272:GLU:CB	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TYR:HE1	1:A:324:ASP:HB3	1.85	0.42
1:A:561:LEU:HD22	1:A:610:GLN:HA	2.00	0.42
1:A:224:ARG:NH1	1:A:225:GLU:CB	2.77	0.42
1:A:185:VAL:HG13	1:A:185:VAL:O	2.20	0.42
1:A:383:ILE:HG22	1:A:391:MET:HG3	2.02	0.41
1:A:400:THR:HG22	1:A:485:MET:CE	2.50	0.41
1:A:678:ASN:O	1:A:680:TYR:CD2	2.73	0.41
1:A:285:TYR:CE1	1:A:324:ASP:HB3	2.55	0.41
1:A:276:HIS:O	1:A:276:HIS:CG	2.71	0.41
1:A:622:THR:HG23	1:A:622:THR:O	2.19	0.41
1:A:625:ASN:H	1:A:626:PRO:HD2	1.86	0.40
1:A:270:GLY:O	1:A:271:GLU:C	2.61	0.40
1:A:411:PRO:HB3	1:A:443:THR:HG21	2.02	0.40
1:A:337:THR:O	1:A:341:VAL:HG22	2.21	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	718/737 (97%)	668 (93%)	42 (6%)	8 (1%)	11 39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	GLU
1	A	625	ASN
1	A	626	PRO
1	A	223	HIS
1	A	628	THR
1	A	751	ALA
1	A	546	VAL

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Mol	Chain	Res	Type
1	A	216	ALA

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	613/627 (98%)	595 (97%)	18 (3%)	37 62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	223	HIS
1	A	224	ARG
1	A	297	ASP
1	A	300	GLN
1	A	343	ASN
1	A	365	TRP
1	A	502	ARG
1	A	543	LEU
1	A	545	GLU
1	A	621	LEU
1	A	624	ILE
1	A	625	ASN
1	A	626	PRO
1	A	631	ILE
1	A	632	THR
1	A	678	ASN
1	A	679	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	89	ASN
1	A	121	ASN
1	A	157	GLN
1	A	172	ASN
1	A	276	HIS
1	A	300	GLN
1	A	373	ASN
1	A	421	GLN
1	A	453	ASN
1	A	461	ASN
1	A	480	ASN
1	A	538	ASN
1	A	614	GLN
1	A	678	ASN
1	A	695	ASN
1	A	750	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 3 ligands modelled in this entry, 3 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	722/737 (97%)	1.15	114 (15%) 5 4	19, 48, 76, 79	4 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	PHE	8.7
1	A	531	ARG	6.8
1	A	278	ILE	5.4
1	A	155	GLY	5.1
1	A	294	ILE	5.0
1	A	298	ASP	4.9
1	A	236	MET	4.8
1	A	144	ILE	4.7
1	A	62	ILE	4.6
1	A	50	PRO	4.6
1	A	221	PRO	4.5
1	A	600	SER	4.4
1	A	158	THR	4.3
1	A	140	GLY	4.1
1	A	249	ASN	4.1
1	A	572	ILE	3.8
1	A	150	ASP	3.8
1	A	200	ASP	3.8
1	A	135	LEU	3.7
1	A	143	ALA	3.7
1	A	60	PHE	3.7
1	A	575	GLN	3.5
1	A	314	PHE	3.5
1	A	226	LYS	3.4
1	A	223	HIS	3.4
1	A	91	ILE	3.3
1	A	213	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	345	GLN	3.3
1	A	61	LYS	3.3
1	A	283	SER	3.2
1	A	426	PHE	3.2
1	A	131	GLU	3.2
1	A	162	LEU	3.1
1	A	180	SER	3.1
1	A	474	ASP	3.1
1	A	104	LEU	3.1
1	A	297	ASP	3.1
1	A	79	VAL	3.1
1	A	205	TYR	3.1
1	A	237	GLN	3.0
1	A	289	VAL	3.0
1	A	105	ILE	3.0
1	A	225	GLU	3.0
1	A	239	MET	3.0
1	A	154	TYR	3.0
1	A	634	SER	2.9
1	A	204	PHE	2.9
1	A	235	GLU	2.9
1	A	86	LEU	2.9
1	A	193	TRP	2.8
1	A	292	PHE	2.8
1	A	177	PRO	2.8
1	A	277	LEU	2.8
1	A	148	ASP	2.8
1	A	318	PHE	2.7
1	A	253	PHE	2.7
1	A	295	TYR	2.7
1	A	146	GLY	2.7
1	A	423	VAL	2.7
1	A	98	ASP	2.7
1	A	181	ALA	2.7
1	A	66	ILE	2.7
1	A	184	ILE	2.6
1	A	257	ILE	2.6
1	A	630	LYS	2.6
1	A	90	ASN	2.6
1	A	141	LYS	2.6
1	A	243	ILE	2.6
1	A	350	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	64	SER	2.5
1	A	63	THR	2.5
1	A	649	SER	2.5
1	A	240	GLN	2.5
1	A	83	ARG	2.5
1	A	366	THR	2.5
1	A	255	PHE	2.5
1	A	81	ALA	2.4
1	A	128	LEU	2.4
1	A	212	THR	2.4
1	A	74	ALA	2.4
1	A	274	PHE	2.4
1	A	41	VAL	2.4
1	A	224	ARG	2.3
1	A	302	LYS	2.3
1	A	238	ARG	2.3
1	A	391	MET	2.3
1	A	262	ASP	2.3
1	A	123	THR	2.3
1	A	309	GLN	2.3
1	A	329	ILE	2.2
1	A	321	ALA	2.2
1	A	219	ASP	2.2
1	A	220	ASP	2.2
1	A	125	ALA	2.2
1	A	250	LYS	2.2
1	A	94	ASN	2.2
1	A	176	TYR	2.1
1	A	142	ILE	2.1
1	A	308	ALA	2.1
1	A	266	ASP	2.1
1	A	179	VAL	2.1
1	A	549	GLU	2.1
1	A	263	ILE	2.1
1	A	151	GLY	2.1
1	A	265	PHE	2.1
1	A	282	GLU	2.1
1	A	276	HIS	2.1
1	A	356	THR	2.1
1	A	132	GLY	2.0
1	A	196	GLN	2.0
1	A	444	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLU	2.0
1	A	272	GLU	2.0
1	A	168	ILE	2.0

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	A	1769	1/1	0.63	0.11	132,132,132,132	0
2	CA	A	1770	1/1	0.92	0.12	34,34,34,34	0
2	CA	A	1768	1/1	0.98	0.22	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.