



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:50 am GMT

PDB ID : 2V5D
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

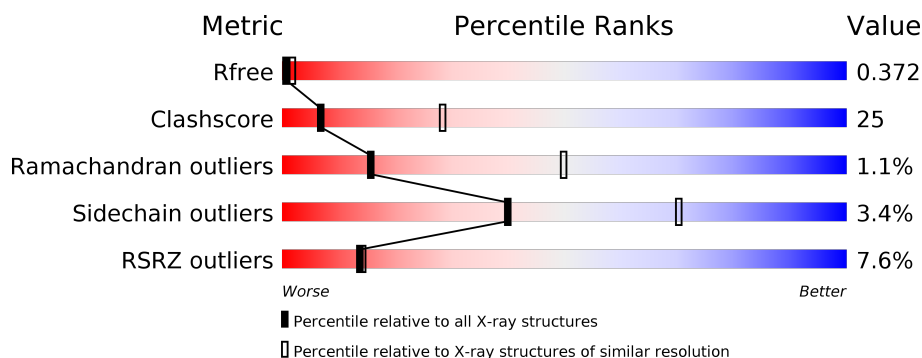
1 Overall quality at a glance

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}	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>7%</div> <div>79%</div> <div>16%</div> <div>...</div> </div>

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 (three-letter code: CA) (formula: Ca).

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

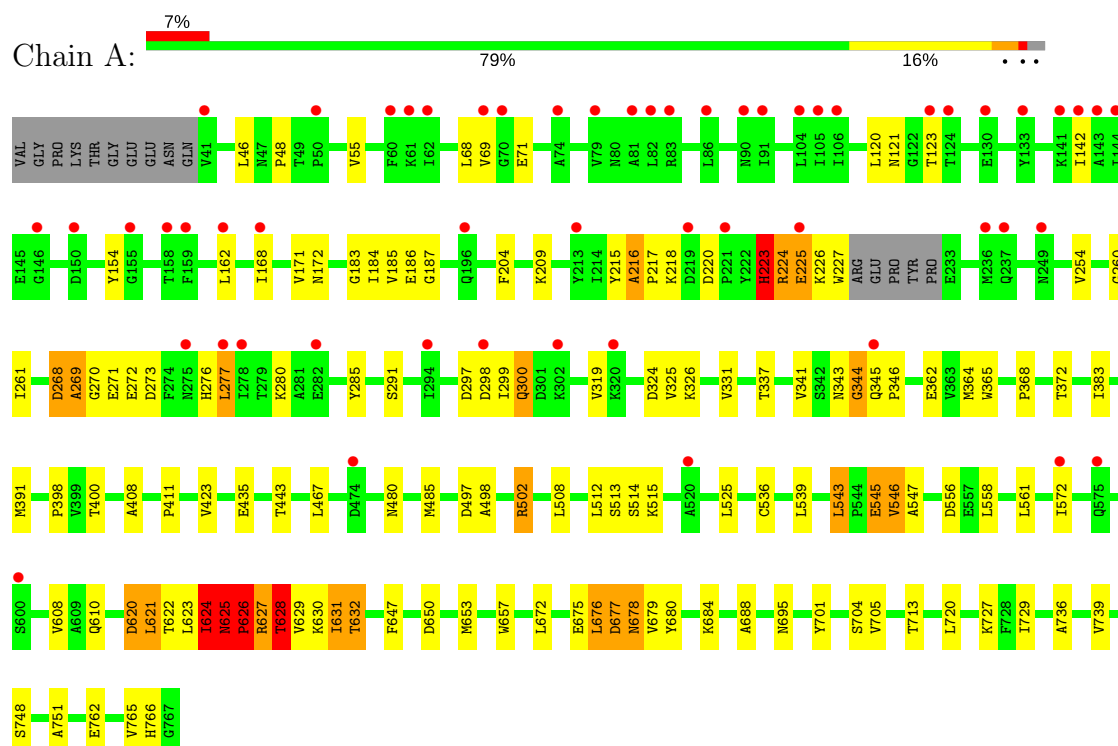
- Molecule 3 is water.

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 and DNA 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 48.64 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (141.42-3.30) 92.8 (48.64-3.30)	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 (4.78%)	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)	0.27 , 14.5	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	0.43	0/5792	0.64	14/7861 (0.2%)

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	C-N-CA	12.58	153.15	121.70
1	A	269	ALA	N-CA-C	10.62	139.68	111.00
1	A	344	GLY	C-N-CA	8.30	142.46	121.70
1	A	270	GLY	N-CA-C	-7.70	93.84	113.10
1	A	625	ASN	C-N-CD	-7.65	103.76	120.60
1	A	268	ASP	O-C-N	-7.51	110.69	122.70
1	A	223	HIS	O-C-N	7.40	134.54	122.70
1	A	269	ALA	CA-C-N	7.13	130.46	116.20
1	A	626	PRO	CA-N-CD	-6.80	101.98	111.50
1	A	277	LEU	C-N-CA	6.46	137.84	121.70
1	A	268	ASP	N-CA-C	6.20	127.74	111.00
1	A	268	ASP	CA-C-N	6.14	130.70	117.20
1	A	269	ALA	CA-C-O	-5.74	108.06	120.10
1	A	628	THR	N-CA-C	5.18	125.00	111.00

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	Mainchain,Peptide
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	275	0
2	A	3	0	0	0	0
3	A	27	0	0	0	0
All	All	5706	0	5404	275	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 25.

All (275) 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: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:345:GLN:CD	1:A:346:PRO:HD2	1.31	1.44
1:A:621:LEU:CA	1:A:622:THR:HG22	1.49	1.42
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:626:PRO:C	1:A:628:THR:HB	1.44	1.34
1:A:269:ALA:HA	1:A:272:GLU:N	1.49	1.27
1:A:621:LEU:HD23	1:A:621:LEU:C	1.50	1.23
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:CD	1:A:225:GLU:N	2.05	1.18
1:A:345:GLN:CD	1:A:346:PRO:CD	2.13	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:260:GLY:C	1:A:299:ILE:HD13	1.71	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
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:N	1:A:300:GLN:HE21	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:621:LEU:CA	1:A:622:THR:CG2	2.31	1.03
1:A:626:PRO:HB3	1:A:627:ARG:HB3	1.34	1.03
1:A:621:LEU:O	1:A:621:LEU:HD23	1.57	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: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:224:ARG:HD3	1:A:224:ARG:C	1.83	0.99
1:A:621:LEU:CD2	1:A:621:LEU:C	2.30	0.98
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:626:PRO:C	1:A:628:THR:CB	2.32	0.97
1:A:224:ARG:CD	1:A:224:ARG:C	2.30	0.97
1:A:300:GLN:HA	1:A:300:GLN:NE2	1.77	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:704:SER:HB3	1:A:713:THR:O	1.69	0.92
1:A:300:GLN:CA	1:A:300:GLN:NE2	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:300:GLN:H	1:A:300:GLN:HE21	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:260:GLY:C	1:A:299:ILE:CD1	2.46	0.84
1:A:513:SER:O	1:A:624:ILE:HG23	1.77	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: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: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:620:ASP:C	1:A:622:THR:HG22	2.01	0.80
1:A:626:PRO:HA	1:A:628:THR:HB	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ILE:C	1:A:631:ILE:HD12	1.95	0.79
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:CA	1:A:300:GLN:HE21	1.90	0.78
1:A:269:ALA:HB1	1:A:272:GLU:CD	2.04	0.77
1:A:345:GLN:OE1	1:A:346:PRO:HD2	1.83	0.77
1:A:625:ASN:O	1:A:626:PRO:HB2	1.83	0.77
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: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: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:630:LYS:O	1:A:630:LYS:HG3	1.85	0.75
1:A:345:GLN:HG3	1:A:346:PRO:HD2	1.67	0.75
1:A:224:ARG:NH1	1:A:225:GLU:CA	2.07	0.74
1:A:187:GLY:HA2	1:A:217:PRO:HD2	1.69	0.73
1:A:623:LEU:HG	1:A:625:ASN:HA	1.70	0.73
1:A:620:ASP:C	1:A:622:THR:CG2	2.57	0.73
1:A:260:GLY:O	1:A:299:ILE:HD13	1.78	0.72
1:A:621:LEU:C	1:A:622:THR:HG22	2.09	0.72
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:269:ALA:CB	1:A:272:GLU:CD	2.58	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:625:ASN:O	1:A:626:PRO:CB	2.37	0.69
1:A:625:ASN:CG	1:A:625:ASN:O	2.30	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:625:ASN:C	1:A:625:ASN:OD1	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:225:GLU:HG2	1:A:226:LYS:N	2.08	0.67
1:A:345:GLN:NE2	1:A:346:PRO:HD2	2.08	0.67
1:A:224:ARG:HD3	1:A:225:GLU:N	1.99	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
1:A:224:ARG:HH11	1:A:225:GLU:N	1.92	0.65
1:A:623:LEU:C	1:A:624:ILE:HG13	2.16	0.65
1:A:269:ALA:C	1:A:272:GLU:HG2	2.17	0.65
1:A:142:ILE:HD13	1:A:168:ILE:HD13	1.77	0.65
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:224:ARG:O	1:A:225:GLU:C	2.37	0.62
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: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: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:68:LEU:HD22	1:A:71:GLU:HG3	1.82	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:N	1:A:298:ASP:OD2	2.30	0.60
1:A:678:ASN:HD22	1:A:678:ASN:C	2.04	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: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:215:TYR:O	1:A:216:ALA:HB3	2.04	0.58
1:A:545:GLU:O	1:A:546:VAL:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:623:LEU:O	1:A:624:ILE:C	2.44	0.56
1:A:545:GLU:HG2	1:A:546:VAL:N	2.19	0.56
1:A:630:LYS:CG	1:A:630:LYS:O	2.54	0.56
1:A:120:LEU:CD1	1:A:123:THR:O	2.54	0.55
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:629:VAL:CG1	1:A:675:GLU:C	2.76	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: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: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:512:LEU:HD11	1:A:572:ILE:HD13	1.92	0.52
1:A:653:MET:HE1	1:A:688:ALA:HB1	1.92	0.52
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:701:TYR:CE2	1:A:729:ILE:HD13	2.47	0.50
1:A:121:ASN:O	1:A:121:ASN:OD1	2.30	0.50
1:A:269:ALA:HB2	1:A:272:GLU:CD	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:625:ASN:OD1	1:A:625:ASN:O	2.29	0.49
1:A:325:VAL:CG1	1:A:326:LYS:N	2.75	0.49
1:A:217:PRO:CB	1:A:218:LYS:CA	2.84	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: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:CG1	1:A:299:ILE:O	2.63	0.46
1:A:183:GLY:C	1:A:184:ILE:HD12	2.36	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:621:LEU:CD2	1:A:622:THR:N	2.66	0.45
1:A:629:VAL:HG13	1:A:675:GLU:C	2.36	0.45
1:A:621:LEU:HD12	1:A:623:LEU:HB3	1.98	0.45
1:A:273:ASP:O	1:A:276:HIS:C	2.54	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: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: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:701:TYR:CD2	1:A:729:ILE:HD13	2.55	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
1:A:285:TYR:HE1	1:A:324:ASP:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:185:VAL:HG13	2.20	0.42
1:A:271:GLU:O	1:A:272:GLU:C	2.57	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:653:MET:CE	1:A:688:ALA:HB1	2.49	0.41
1:A:285:TYR:CE1	1:A:324:ASP:HB3	2.55	0.41
1:A:276:HIS:CG	1:A:276:HIS:O	2.71	0.41
1:A:622:THR:O	1:A:622:THR:HG23	2.19	0.41
1:A:625:ASN:H	1:A:626:PRO:HD2	1.86	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%)	16 50

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%)	592 (97%)	21 (3%)	40 70

All (21) 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	362	GLU
1	A	365	TRP
1	A	502	ARG
1	A	543	LEU
1	A	545	GLU
1	A	556	ASP
1	A	621	LEU
1	A	624	ILE
1	A	625	ASN
1	A	626	PRO
1	A	627	ARG
1	A	631	ILE
1	A	632	THR
1	A	677	ASP
1	A	678	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	89	ASN
1	A	121	ASN
1	A	276	HIS
1	A	300	GLN
1	A	453	ASN
1	A	480	ASN
1	A	614	GLN
1	A	678	ASN
1	A	695	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [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

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%)	0.53	55 (7%) 14 14	31, 48, 76, 79	4 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	PHE	4.8
1	A	143	ALA	4.2
1	A	221	PRO	4.0
1	A	278	ILE	4.0
1	A	237	GLN	4.0
1	A	60	PHE	4.0
1	A	69	VAL	3.9
1	A	158	THR	3.9
1	A	155	GLY	3.9
1	A	91	ILE	3.6
1	A	104	LEU	3.6
1	A	144	ILE	3.4
1	A	294	ILE	3.4
1	A	90	ASN	3.2
1	A	150	ASP	3.2
1	A	62	ILE	3.1
1	A	162	LEU	3.1
1	A	225	GLU	3.0
1	A	79	VAL	3.0
1	A	277	LEU	3.0
1	A	70	GLY	3.0
1	A	61	LYS	2.9
1	A	196	GLN	2.9
1	A	302	LYS	2.9
1	A	236	MET	2.8
1	A	298	ASP	2.8
1	A	74	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	50	PRO	2.7
1	A	83	ARG	2.7
1	A	142	ILE	2.7
1	A	82	LEU	2.7
1	A	41	VAL	2.5
1	A	249	ASN	2.5
1	A	520	ALA	2.5
1	A	105	ILE	2.4
1	A	575	GLN	2.4
1	A	572	ILE	2.4
1	A	275	ASN	2.4
1	A	474	ASP	2.4
1	A	106	ILE	2.3
1	A	345	GLN	2.3
1	A	123	THR	2.3
1	A	81	ALA	2.3
1	A	86	LEU	2.2
1	A	130	GLU	2.2
1	A	124	THR	2.2
1	A	320	LYS	2.2
1	A	168	ILE	2.1
1	A	600	SER	2.1
1	A	282	GLU	2.1
1	A	141	LYS	2.1
1	A	133	TYR	2.0
1	A	213	TYR	2.0
1	A	219	ASP	2.0
1	A	146	GLY	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 carbohydrates 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(\AA^2)	Q<0.9
2	CA	A	1768	1/1	0.82	0.34	49,49,49,49	0
2	CA	A	1769	1/1	0.82	0.17	132,132,132,132	0
2	CA	A	1770	1/1	0.84	0.12	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.