



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:34 PM EDT

PDB ID : 4JKM / pdb_00004jkm
Title : Crystal Structure of Clostridium perfringens beta-glucuronidase
Authors : Wallace, B.D.; Redinbo, M.R.
Deposited on : 2013-03-09
Resolution : 2.26 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

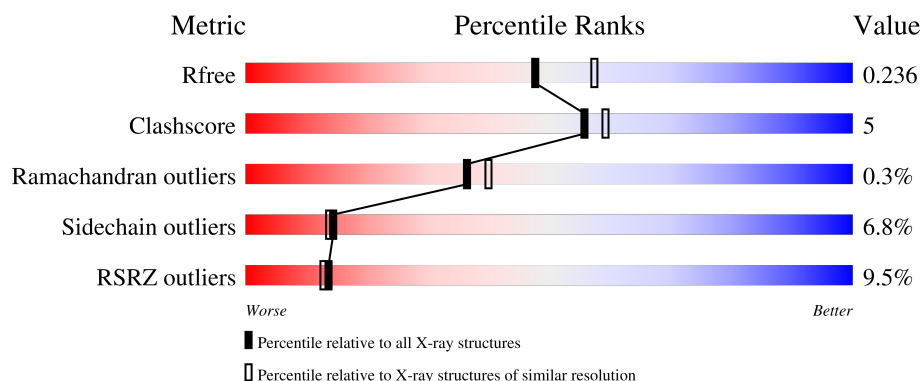
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	602	2% 85% 14% .
1	B	602	5% 85% 14% .
2	C	400	16% 48% 13% . 37%
2	D	400	16% 78% 10% . 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14718 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	1	0
			4863	3107	811	926	19			
1	B	602	Total	C	N	O	S	0	1	0
			4851	3098	808	926	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8XP19
A	-1	ASN	-	expression tag	UNP Q8XP19
A	0	ALA	-	expression tag	UNP Q8XP19
B	-2	SER	-	expression tag	UNP Q8XP19
B	-1	ASN	-	expression tag	UNP Q8XP19
B	0	ALA	-	expression tag	UNP Q8XP19

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	362	Total	C	N	O	S	0	0	0
			2653	1693	433	521	6			
2	C	252	Total	C	N	O	S	0	0	0
			1839	1168	302	363	6			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP P0AEX9
D	2	LYS	-	expression tag	UNP P0AEX9
D	3	HIS	-	expression tag	UNP P0AEX9
D	4	HIS	-	expression tag	UNP P0AEX9
D	5	HIS	-	expression tag	UNP P0AEX9
D	6	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	7	HIS	-	expression tag	UNP P0AEX9
D	8	HIS	-	expression tag	UNP P0AEX9
D	9	GLY	-	expression tag	UNP P0AEX9
D	25	ALA	GLY	SEE REMARK 999	UNP P0AEX9
D	376	ASN	-	expression tag	UNP P0AEX9
D	377	SER	-	expression tag	UNP P0AEX9
D	378	SER	-	expression tag	UNP P0AEX9
D	379	SER	-	expression tag	UNP P0AEX9
D	380	ASN	-	expression tag	UNP P0AEX9
D	381	ASN	-	expression tag	UNP P0AEX9
D	382	ASN	-	expression tag	UNP P0AEX9
D	383	ASN	-	expression tag	UNP P0AEX9
D	384	ASN	-	expression tag	UNP P0AEX9
D	385	ASN	-	expression tag	UNP P0AEX9
D	386	ASN	-	expression tag	UNP P0AEX9
D	387	ASN	-	expression tag	UNP P0AEX9
D	388	ASN	-	expression tag	UNP P0AEX9
D	389	ASN	-	expression tag	UNP P0AEX9
D	390	ARG	-	expression tag	UNP P0AEX9
D	391	ASP	-	expression tag	UNP P0AEX9
D	392	LEU	-	expression tag	UNP P0AEX9
D	393	GLY	-	expression tag	UNP P0AEX9
D	394	THR	-	expression tag	UNP P0AEX9
D	395	GLU	-	expression tag	UNP P0AEX9
D	396	ASN	-	expression tag	UNP P0AEX9
D	397	LEU	-	expression tag	UNP P0AEX9
D	398	TYR	-	expression tag	UNP P0AEX9
D	399	PHE	-	expression tag	UNP P0AEX9
D	400	GLN	-	expression tag	UNP P0AEX9
C	1	MET	-	expression tag	UNP P0AEX9
C	2	LYS	-	expression tag	UNP P0AEX9
C	3	HIS	-	expression tag	UNP P0AEX9
C	4	HIS	-	expression tag	UNP P0AEX9
C	5	HIS	-	expression tag	UNP P0AEX9
C	6	HIS	-	expression tag	UNP P0AEX9
C	7	HIS	-	expression tag	UNP P0AEX9
C	8	HIS	-	expression tag	UNP P0AEX9
C	9	GLY	-	expression tag	UNP P0AEX9
C	25	ALA	GLY	SEE REMARK 999	UNP P0AEX9
C	376	ASN	-	expression tag	UNP P0AEX9
C	377	SER	-	expression tag	UNP P0AEX9
C	378	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	379	SER	-	expression tag	UNP P0AEX9
C	380	ASN	-	expression tag	UNP P0AEX9
C	381	ASN	-	expression tag	UNP P0AEX9
C	382	ASN	-	expression tag	UNP P0AEX9
C	383	ASN	-	expression tag	UNP P0AEX9
C	384	ASN	-	expression tag	UNP P0AEX9
C	385	ASN	-	expression tag	UNP P0AEX9
C	386	ASN	-	expression tag	UNP P0AEX9
C	387	ASN	-	expression tag	UNP P0AEX9
C	388	ASN	-	expression tag	UNP P0AEX9
C	389	ASN	-	expression tag	UNP P0AEX9
C	390	ARG	-	expression tag	UNP P0AEX9
C	391	ASP	-	expression tag	UNP P0AEX9
C	392	LEU	-	expression tag	UNP P0AEX9
C	393	GLY	-	expression tag	UNP P0AEX9
C	394	THR	-	expression tag	UNP P0AEX9
C	395	GLU	-	expression tag	UNP P0AEX9
C	396	ASN	-	expression tag	UNP P0AEX9
C	397	LEU	-	expression tag	UNP P0AEX9
C	398	TYR	-	expression tag	UNP P0AEX9
C	399	PHE	-	expression tag	UNP P0AEX9
C	400	GLN	-	expression tag	UNP P0AEX9

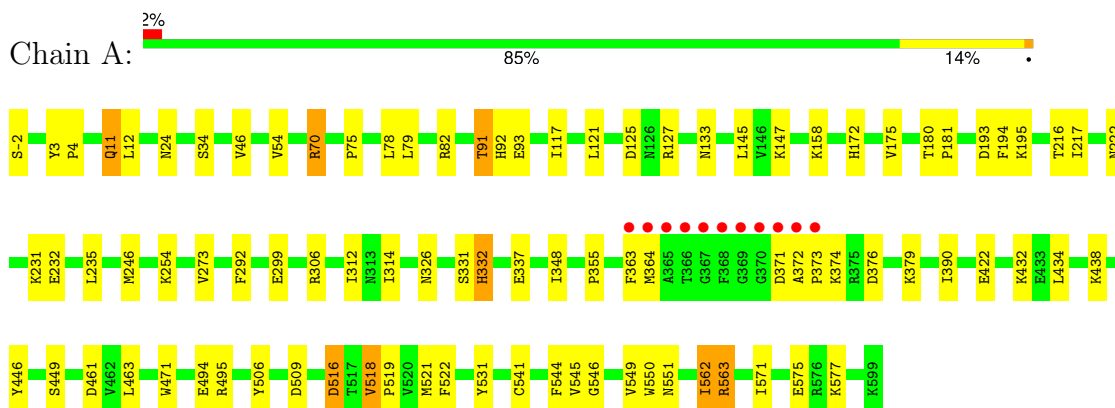
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	265	Total O 265 265	0	0
3	B	174	Total O 174 174	0	0
3	D	49	Total O 49 49	0	0
3	C	24	Total O 24 24	0	0

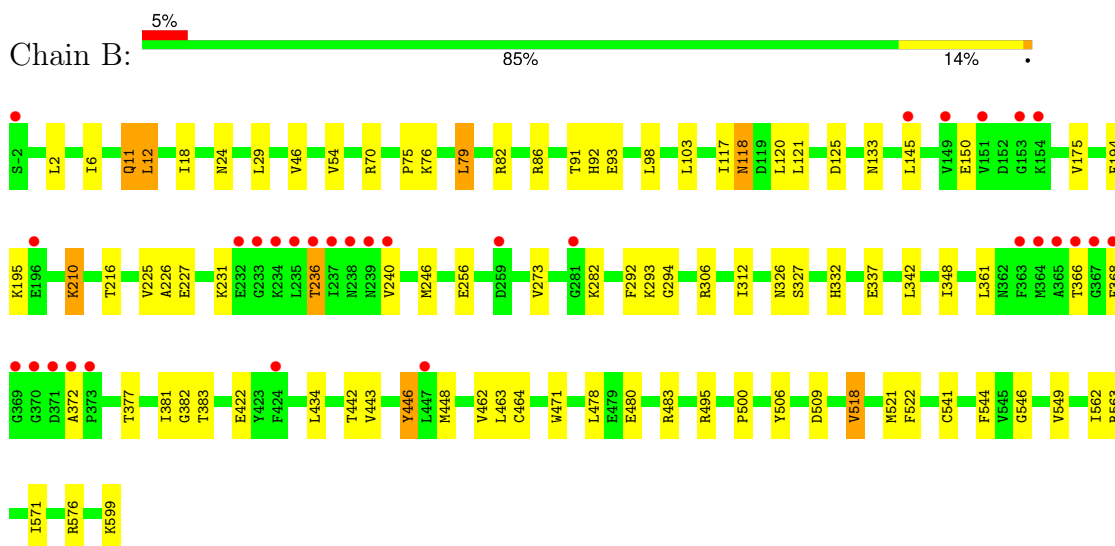
3 Residue-property plots

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.

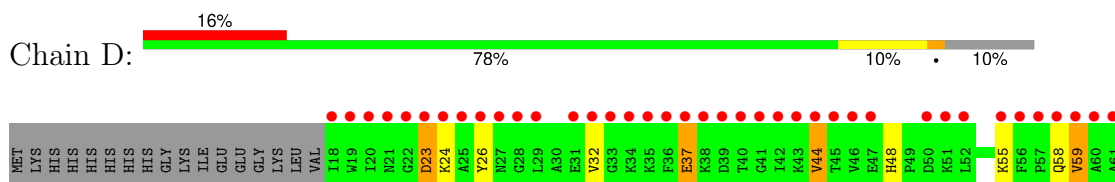
• Molecule 1: Beta-glucuronidase

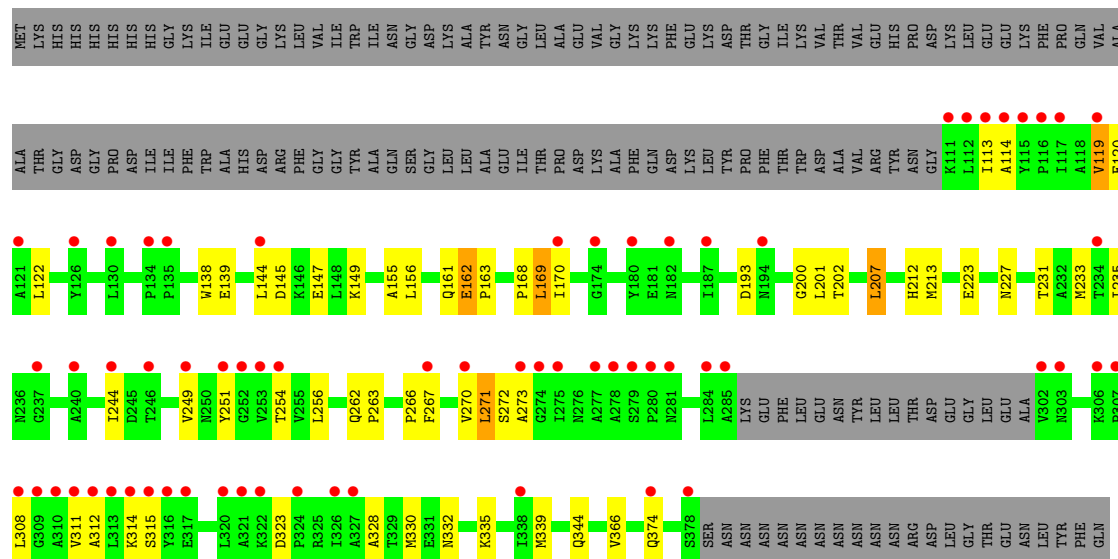


• Molecule 1: Beta-glucuronidase



• Molecule 2: Maltose-binding periplasmic protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.51Å 292.61Å 239.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.79 – 2.26 47.79 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.79-2.26) 99.6 (47.79-2.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.207 , 0.234 0.208 , 0.236	Depositor DCC
R_{free} test set	5862 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14718	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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

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	0.33	2/4977 (0.0%)	0.72	3/6740 (0.0%)
1	B	0.29	0/4965	0.74	5/6728 (0.1%)
2	C	0.32	0/1879	0.84	5/2569 (0.2%)
2	D	0.33	0/2717	0.79	3/3718 (0.1%)
All	All	0.32	2/14538 (0.0%)	0.75	16/19755 (0.1%)

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
2	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	ALA	C-N	5.95	1.41	1.33
1	A	373	PRO	N-CD	5.39	1.55	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	113	ILE	N-CA-C	-9.46	104.72	113.71
2	C	162	GLU	CA-C-N	7.06	128.66	119.84
2	C	162	GLU	C-N-CA	7.06	128.66	119.84
1	B	240	VAL	N-CA-C	7.00	119.22	109.55
1	A	372	ALA	CA-C-N	-6.27	113.52	119.85
1	A	372	ALA	C-N-CA	-6.27	113.52	119.85
1	B	372	ALA	N-CA-C	5.91	121.56	113.16
1	B	368	PHE	N-CA-C	-5.87	105.94	112.57
2	D	24	LYS	N-CA-C	-5.80	104.95	111.28
1	A	371	ASP	N-CA-C	5.67	119.22	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	323	ASP	CA-C-N	5.33	126.50	119.84
2	C	323	ASP	C-N-CA	5.33	126.50	119.84
2	D	99	TYR	CA-C-N	5.20	125.24	119.32
2	D	99	TYR	C-N-CA	5.20	125.24	119.32
1	B	518	VAL	CA-C-N	5.07	125.08	119.90
1	B	518	VAL	C-N-CA	5.07	125.08	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	59	VAL	Peptide

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	4863	0	4766	43	0
1	B	4851	0	4733	46	0
2	C	1839	0	1730	28	0
2	D	2653	0	2441	22	0
3	A	265	0	0	4	0
3	B	174	0	0	4	0
3	C	24	0	0	3	0
3	D	49	0	0	2	0
All	All	14718	0	13670	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (131) 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:B:246:MET:HE1	1:B:348:ILE:HG12	1.66	0.77
1:A:246:MET:HE1	1:A:348:ILE:HG12	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LEU:H	1:B:377:THR:HG22	1.57	0.70
2:D:280:PRO:HD2	2:D:283:GLU:HB3	1.76	0.67
2:D:59:VAL:HG21	2:D:302:VAL:O	1.96	0.66
2:D:66:PRO:O	2:D:67:ASP:HB2	1.94	0.66
1:B:216:THR:HG22	1:B:227:GLU:HG3	1.78	0.65
1:B:292:PHE:HB2	1:B:546:GLY:HA3	1.77	0.64
1:B:2:LEU:O	1:B:86:ARG:NH2	2.32	0.63
1:A:292:PHE:HB2	1:A:546:GLY:HA3	1.81	0.63
2:C:223:GLU:O	2:C:227:ASN:ND2	2.30	0.62
2:D:88:ILE:HG13	2:D:90:PRO:HD3	1.82	0.62
2:D:276:ASN:HB3	2:D:280:PRO:HG3	1.82	0.62
1:A:563:ARG:NH2	3:A:810:HOH:O	2.34	0.61
1:B:246:MET:HE3	1:B:326:ASN:HA	1.82	0.60
1:A:246:MET:HE3	1:A:326:ASN:HA	1.83	0.59
2:C:308:LEU:HA	2:C:312:ALA:HA	1.85	0.58
1:A:34:SER:O	1:A:127:ARG:NH2	2.31	0.57
1:B:462:VAL:HG22	1:B:500:PRO:HG2	1.86	0.57
1:B:442:THR:HG21	1:B:464:CYS:SG	2.45	0.56
2:D:67:ASP:OD2	2:D:280:PRO:HB2	2.05	0.56
2:C:119:VAL:H	2:C:315:SER:H	1.55	0.55
2:D:141:ILE:HD13	2:D:156:LEU:HD12	1.89	0.54
2:C:193:ASP:HB2	2:C:374:GLN:HB2	1.90	0.54
2:D:281:ASN:ND2	3:D:533:HOH:O	2.40	0.53
1:A:516:ASP:OD1	3:A:652:HOH:O	2.19	0.53
2:C:328:ALA:O	2:C:332:ASN:ND2	2.40	0.53
2:C:114:ALA:HB3	2:C:273:ALA:HB2	1.90	0.53
1:B:337:GLU:OE1	3:B:760:HOH:O	2.19	0.53
2:D:301:ALA:HA	2:D:304:LYS:HD3	1.90	0.53
2:D:263:PRO:HB3	2:D:335:LYS:HD3	1.91	0.52
2:C:201:LEU:HD23	2:C:366:VAL:HG13	1.91	0.52
1:A:93:GLU:HB3	1:A:133:ASN:HB3	1.92	0.51
1:A:11[A]:GLN:NE2	1:B:11[A]:GLN:OE1	2.44	0.51
2:D:138:TRP:NE1	3:D:523:HOH:O	2.42	0.51
2:C:207:LEU:HD13	2:C:213:MET:HE2	1.93	0.51
2:D:23:ASP:O	2:D:26:TYR:CB	2.60	0.50
1:A:575:GLU:HG2	1:A:577:LYS:HG2	1.92	0.50
1:B:93:GLU:HB3	1:B:133:ASN:HB3	1.94	0.49
1:B:480:GLU:OE2	1:B:483:ARG:NH2	2.33	0.49
2:C:235:ILE:HG23	3:C:520:HOH:O	2.12	0.49
2:D:37:GLU:CB	2:D:64:ASP:HA	2.42	0.49
2:C:263:PRO:HB3	2:C:335:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:HIS:O	1:A:355:PRO:HA	2.12	0.49
1:B:118:ASN:OD1	1:B:118:ASN:N	2.26	0.49
2:C:170:ILE:HA	2:C:200:GLY:HA3	1.94	0.49
1:B:381:ILE:HG13	1:B:383:THR:HG23	1.95	0.48
1:A:82:ARG:HH11	1:A:180:THR:HG21	1.79	0.48
1:B:562:ILE:HG12	3:B:691:HOH:O	2.13	0.48
1:A:145:LEU:HD11	1:A:147:LYS:HE3	1.96	0.48
1:A:180:THR:HG23	1:A:181:PRO:O	2.13	0.48
1:B:381:ILE:HG23	1:B:382:GLY:H	1.79	0.48
1:A:376:ASP:HB3	1:A:379:LYS:HG2	1.96	0.47
1:B:29:LEU:HD21	3:B:698:HOH:O	2.13	0.47
1:B:91:THR:HA	1:B:92:HIS:HA	1.64	0.47
2:C:254:THR:HA	2:C:328:ALA:HB1	1.97	0.47
1:A:549:VAL:HG11	1:A:571:ILE:HD11	1.96	0.47
1:A:11[B]:GLN:HG2	1:B:11[B]:GLN:NE2	2.30	0.47
1:A:217:ILE:HG13	1:A:235:LEU:HD23	1.97	0.47
1:B:361:LEU:H	1:B:377:THR:CG2	2.27	0.47
1:A:78:LEU:HD11	1:B:11[B]:GLN:HE22	1.80	0.47
1:B:471:TRP:CZ2	1:B:509:ASP:HB2	2.50	0.47
1:B:549:VAL:HG11	1:B:571:ILE:HD11	1.97	0.47
1:A:70:ARG:NH2	3:A:623:HOH:O	2.48	0.47
1:A:432:LYS:NZ	1:A:461:ASP:OD2	2.48	0.47
1:A:471:TRP:CZ2	1:A:509:ASP:HB2	2.50	0.46
1:A:91:THR:HA	1:A:92:HIS:HA	1.59	0.46
1:A:216:THR:HG23	1:A:254:LYS:HB3	1.98	0.46
2:D:23:ASP:O	2:D:26:TYR:N	2.44	0.46
2:C:145:ASP:O	2:C:149:LYS:HB2	2.15	0.46
1:A:193:ASP:OD1	1:A:194:PHE:N	2.45	0.45
1:A:550:TRP:HA	1:A:551:ASN:HA	1.75	0.45
1:A:75:PRO:HG2	1:B:11[A]:GLN:HG2	1.99	0.45
2:D:32:VAL:HG21	2:D:79:TYR:OH	2.17	0.45
2:C:138:TRP:CE2	2:C:169:LEU:HG	2.52	0.45
2:C:122:LEU:HB3	3:C:520:HOH:O	2.16	0.44
1:B:256:GLU:O	3:B:685:HOH:O	2.21	0.44
2:D:65:GLY:HA3	2:D:66:PRO:HD2	1.86	0.44
2:C:207:LEU:HB2	2:C:212:HIS:HB2	1.99	0.44
2:C:271:LEU:O	2:C:273:ALA:N	2.45	0.44
2:C:202:THR:HG23	2:C:366:VAL:HG11	1.98	0.44
1:A:363:PHE:HA	1:A:364:MET:HA	1.70	0.44
1:A:562:ILE:H	1:A:562:ILE:HD13	1.82	0.44
1:B:282:LYS:NZ	1:B:599:LYS:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HD23	1:B:120:LEU:HB2	2.00	0.44
1:B:76:LYS:HA	1:B:79:LEU:HD22	1.99	0.44
1:B:541:CYS:HB3	1:B:544:PHE:HB2	1.99	0.44
2:C:267:PHE:HB3	2:C:339:MET:HG3	2.00	0.44
2:C:244:ILE:HD11	2:C:251:TYR:CZ	2.53	0.44
2:C:271:LEU:HD12	2:C:272:SER:N	2.33	0.44
1:B:442:THR:HG22	1:B:443:VAL:N	2.33	0.43
1:A:438:LYS:HE3	2:D:174:GLY:HA3	2.01	0.43
1:A:531:TYR:OH	1:A:549:VAL:HG13	2.19	0.43
2:C:314:LYS:HA	2:C:315:SER:HA	1.53	0.43
1:B:82:ARG:HA	1:B:118:ASN:ND2	2.33	0.43
1:B:210:LYS:H	1:B:210:LYS:HG2	1.74	0.43
1:B:381:ILE:HG23	1:B:382:GLY:N	2.34	0.43
1:B:294:GLY:HA3	1:B:327:SER:O	2.19	0.43
1:B:521:MET:O	1:B:522:PHE:HB2	2.18	0.43
1:A:541:CYS:HB3	1:A:544:PHE:HB2	2.01	0.43
1:A:518:VAL:HA	1:A:519:PRO:HD3	1.89	0.42
1:B:117:ILE:O	1:B:121:LEU:HG	2.20	0.42
2:D:23:ASP:CG	2:D:278:ALA:CB	2.92	0.42
1:A:231:LYS:HG3	1:A:232:GLU:HG3	2.01	0.42
1:A:314:ILE:HD11	1:B:18:ILE:HD12	2.00	0.42
2:D:310:ALA:HB1	2:D:330:MET:HE2	2.01	0.42
1:A:216:THR:HG22	3:A:723:HOH:O	2.20	0.42
1:A:521:MET:O	1:A:522:PHE:HB2	2.20	0.42
2:C:162:GLU:HA	2:C:163:PRO:HD2	1.71	0.42
2:D:146:LYS:HB2	2:D:146:LYS:HE3	1.83	0.42
2:C:271:LEU:H	2:C:271:LEU:HG	1.55	0.42
1:A:172:HIS:CE1	1:A:306:ARG:HB3	2.55	0.41
1:B:6:ILE:HG12	1:B:12:LEU:HB2	2.02	0.41
1:B:194:PHE:O	1:B:195:LYS:HD2	2.19	0.41
2:D:190:VAL:HG12	2:D:192:VAL:H	1.84	0.41
1:B:82:ARG:HA	1:B:118:ASN:HD21	1.85	0.41
1:A:363:PHE:CE1	1:A:364:MET:HG2	2.56	0.41
1:B:446:TYR:CE1	1:B:448:MET:HB2	2.55	0.41
2:C:168:PRO:HG3	2:C:266:PRO:HB3	2.02	0.41
1:A:299:GLU:O	1:A:306:ARG:HA	2.21	0.41
1:A:3:TYR:HA	1:A:4:PRO:HD3	1.91	0.41
1:B:293:LYS:HB2	1:B:293:LYS:HE3	1.76	0.41
2:C:155:ALA:O	2:C:233:MET:N	2.53	0.41
1:B:210:LYS:HB3	1:B:210:LYS:HE2	1.86	0.41
1:A:11[B]:GLN:NE2	1:B:75:PRO:HG2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD21	1:B:11[B]:GLN:HE22	1.86	0.40
1:A:117:ILE:O	1:A:121:LEU:HG	2.20	0.40
2:D:59:VAL:HG22	2:D:302:VAL:HG13	2.03	0.40
2:C:256:LEU:HD21	3:C:520:HOH:O	2.21	0.40
1:B:226:ALA:HB1	1:B:236:THR:HG22	2.04	0.40
2:C:262:GLN:HA	2:C:263:PRO:HD3	1.91	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	601/602 (100%)	573 (95%)	28 (5%)	0	100	100
1	B	601/602 (100%)	568 (94%)	32 (5%)	1 (0%)	43	50
2	C	248/400 (62%)	227 (92%)	20 (8%)	1 (0%)	30	31
2	D	360/400 (90%)	338 (94%)	18 (5%)	4 (1%)	11	8
All	All	1810/2004 (90%)	1706 (94%)	98 (5%)	6 (0%)	36	40

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	270	VAL
2	D	37	GLU
2	D	44	VAL
2	D	67	ASP
2	D	177	ALA
1	B	366	THR

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	529/531 (100%)	494 (93%)	35 (7%)	15	14
1	B	526/531 (99%)	493 (94%)	33 (6%)	16	16
2	C	179/325 (55%)	164 (92%)	15 (8%)	10	8
2	D	251/325 (77%)	231 (92%)	20 (8%)	11	9
All	All	1485/1712 (87%)	1382 (93%)	103 (7%)	14	13

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	11[A]	GLN
1	A	11[B]	GLN
1	A	12	LEU
1	A	24	ASN
1	A	46	VAL
1	A	54	VAL
1	A	70	ARG
1	A	79	LEU
1	A	91	THR
1	A	125	ASP
1	A	158	LYS
1	A	175	VAL
1	A	195	LYS
1	A	222	ASN
1	A	273	VAL
1	A	312	ILE
1	A	331	SER
1	A	332	HIS
1	A	337	GLU
1	A	374	LYS
1	A	390	ILE
1	A	422	GLU
1	A	434	LEU

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Mol	Chain	Res	Type
1	A	446	TYR
1	A	449	SER
1	A	463	LEU
1	A	494	GLU
1	A	495	ARG
1	A	506	TYR
1	A	516	ASP
1	A	518	VAL
1	A	545	VAL
1	A	562	ILE
1	A	563	ARG
1	B	11[A]	GLN
1	B	11[B]	GLN
1	B	12	LEU
1	B	24	ASN
1	B	46	VAL
1	B	54	VAL
1	B	70	ARG
1	B	79	LEU
1	B	103	LEU
1	B	118	ASN
1	B	125	ASP
1	B	145	LEU
1	B	150	GLU
1	B	175	VAL
1	B	210	LYS
1	B	225	VAL
1	B	231	LYS
1	B	236	THR
1	B	273	VAL
1	B	306	ARG
1	B	312	ILE
1	B	332	HIS
1	B	342	LEU
1	B	422	GLU
1	B	434	LEU
1	B	446	TYR
1	B	463	LEU
1	B	478	LEU
1	B	495	ARG
1	B	506	TYR
1	B	518	VAL

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Mol	Chain	Res	Type
1	B	563	ARG
1	B	576	ARG
2	D	23	ASP
2	D	44	VAL
2	D	48	HIS
2	D	55	LYS
2	D	58	GLN
2	D	62	THR
2	D	64	ASP
2	D	139	GLU
2	D	156	LEU
2	D	169	LEU
2	D	249	VAL
2	D	255	VAL
2	D	279	SER
2	D	281	ASN
2	D	284	LEU
2	D	290	GLU
2	D	297	GLU
2	D	325	ARG
2	D	344	GLN
2	D	374	GLN
2	C	119	VAL
2	C	120	GLU
2	C	139	GLU
2	C	144	LEU
2	C	147	GLU
2	C	156	LEU
2	C	161	GLN
2	C	169	LEU
2	C	207	LEU
2	C	231	THR
2	C	249	VAL
2	C	271	LEU
2	C	311	VAL
2	C	330	MET
2	C	344	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN

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Mol	Chain	Res	Type
1	B	62	HIS
1	B	238	ASN
2	D	281	ASN
2	C	262	GLN
2	C	303	ASN
2	C	364	GLN
2	C	374	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 ⓘ

There are no ligands in this entry.

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	602/602 (100%)	-0.31	11 (1%) 67 68	18, 29, 55, 162	1 (0%)
1	B	602/602 (100%)	0.28	31 (5%) 33 32	24, 43, 79, 171	1 (0%)
2	C	252/400 (63%)	1.61	65 (25%) 1 1	56, 82, 119, 139	0
2	D	362/400 (90%)	0.98	65 (17%) 3 3	28, 61, 104, 117	0
All	All	1818/2004 (90%)	0.41	172 (9%) 14 13	18, 44, 105, 171	2 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	273	ALA	7.0
2	D	44	VAL	5.9
2	C	321	ALA	5.9
2	D	65	GLY	5.5
1	A	365	ALA	5.4
2	D	46	VAL	5.1
2	C	280	PRO	5.1
1	B	235	LEU	5.1
2	C	311	VAL	5.1
2	D	62	THR	5.0
2	C	302	VAL	4.9
1	A	364	MET	4.8
1	B	364	MET	4.8
2	D	379	SER	4.8
2	C	113	ILE	4.6
1	B	368	PHE	4.6
2	C	115	TYR	4.6
2	D	57	PRO	4.6
2	D	61	ALA	4.5
2	D	33	GLY	4.5
1	A	366	THR	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	40	THR	4.4
2	D	284	LEU	4.4
2	C	114	ALA	4.3
2	D	22	GLY	4.3
2	D	20	ILE	4.2
2	C	324	PRO	4.2
2	D	29	LEU	4.2
1	A	372	ALA	4.1
2	C	285	ALA	4.1
2	D	52	LEU	4.1
1	B	366	THR	4.1
1	B	365	ALA	4.1
1	A	368	PHE	4.1
2	C	316	TYR	3.9
1	B	151	VAL	3.9
2	D	27	ASN	3.9
1	B	233	GLY	3.9
1	B	369	GLY	3.9
2	D	21	ASN	3.9
2	D	36	PHE	3.8
2	C	116	PRO	3.8
2	C	315	SER	3.8
1	B	371	ASP	3.7
2	C	327	ALA	3.7
2	D	60	ALA	3.7
2	D	19	TRP	3.7
2	C	320	LEU	3.7
2	C	275	ILE	3.6
2	D	289	LEU	3.6
2	C	112	LEU	3.6
2	D	58	GLN	3.6
2	D	23	ASP	3.6
2	D	288	PHE	3.6
1	A	363	PHE	3.5
2	D	292	TYR	3.5
2	D	59	VAL	3.5
2	D	26	TYR	3.5
2	C	119	VAL	3.4
2	D	28	GLY	3.4
2	D	63	GLY	3.4
2	D	31	GLU	3.4
2	C	308	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	278	ALA	3.4
2	D	41	GLY	3.4
2	C	274	GLY	3.4
2	D	55	LYS	3.3
2	D	18	ILE	3.3
1	A	369	GLY	3.2
2	D	32	VAL	3.2
2	C	246	THR	3.2
2	C	253	VAL	3.2
1	A	367	GLY	3.2
2	D	43	LYS	3.1
1	B	238	ASN	3.1
2	D	51	LYS	3.1
2	C	279	SER	3.1
1	B	237	ILE	3.1
2	C	322	LYS	3.0
1	A	371	ASP	3.0
1	A	370	GLY	3.0
2	C	251	TYR	3.0
2	C	310	ALA	2.9
2	D	282	LYS	2.9
2	D	39	ASP	2.9
1	B	239	ASN	2.9
2	D	25	ALA	2.9
2	D	301	ALA	2.9
2	C	281	ASN	2.9
2	C	180	TYR	2.9
2	D	42	ILE	2.9
2	C	314	LYS	2.8
2	C	284	LEU	2.8
2	C	270	VAL	2.8
1	B	236	THR	2.8
2	C	338	ILE	2.8
2	D	66	PRO	2.8
1	B	373	PRO	2.8
2	C	111	LYS	2.8
2	D	249	VAL	2.7
2	C	312	ALA	2.7
2	D	50	ASP	2.7
2	C	170	ILE	2.7
2	D	38	LYS	2.6
2	D	64	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	281	GLY	2.6
2	C	117	ILE	2.6
2	C	378	SER	2.6
2	C	306	LYS	2.6
2	C	309	GLY	2.6
2	D	279	SER	2.6
2	C	130	LEU	2.6
2	D	305	ASP	2.6
2	D	45	THR	2.6
1	B	154	LYS	2.6
2	C	182	ASN	2.6
2	C	249	VAL	2.6
1	B	234	LYS	2.6
1	B	367	GLY	2.5
2	C	135	PRO	2.5
2	D	293	LEU	2.5
1	B	363	PHE	2.5
1	B	447	LEU	2.5
2	D	34	LYS	2.5
2	C	121	ALA	2.5
2	C	234	THR	2.4
2	D	82	SER	2.4
2	C	317	GLU	2.4
1	B	240	VAL	2.4
1	B	372	ALA	2.4
1	B	149	VAL	2.4
2	C	244	ILE	2.4
2	D	278	ALA	2.3
2	C	126	TYR	2.3
2	C	237	GLY	2.3
2	C	254	THR	2.3
2	C	326	ILE	2.3
1	B	232	GLU	2.3
2	D	24	LYS	2.3
1	A	373	PRO	2.3
2	D	214	ASN	2.3
2	C	194	ASN	2.3
2	D	280	PRO	2.3
2	C	174	GLY	2.3
2	D	285	ALA	2.3
2	D	47	GLU	2.3
2	D	56	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	267	PHE	2.2
1	B	259	ASP	2.2
2	D	35	LYS	2.2
1	B	196	GLU	2.2
2	C	134	PRO	2.2
1	B	370	GLY	2.2
1	B	-2	SER	2.2
2	D	89	THR	2.2
2	C	240	ALA	2.2
1	B	145	LEU	2.1
2	C	187	ILE	2.1
2	D	302	VAL	2.1
2	D	156	LEU	2.1
2	C	144	LEU	2.1
2	D	37	GLU	2.1
2	C	313	LEU	2.1
2	C	307	PRO	2.1
1	B	424	PHE	2.1
2	C	252	GLY	2.1
2	D	306	LYS	2.1
2	C	277	ALA	2.0
2	C	303	ASN	2.0
1	B	153	GLY	2.0
2	D	81	GLN	2.0
2	C	374	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.