



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2014 – 11:14 AM EDT

PDB ID : 4JKM
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

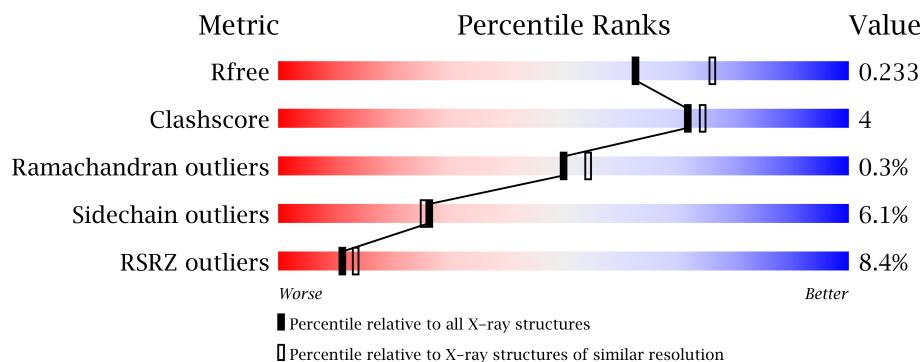
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	602	
1	B	602	
2	C	400	
2	D	400	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14718 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

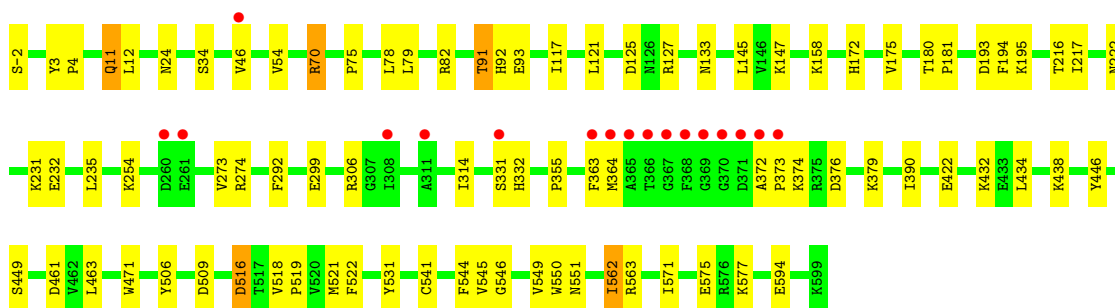
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	265	Total O 265 265	0	0
3	B	174	Total O 174 174	0	0
3	D	49	Total O 49 49	0	0
3	C	24	Total O 24 24	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

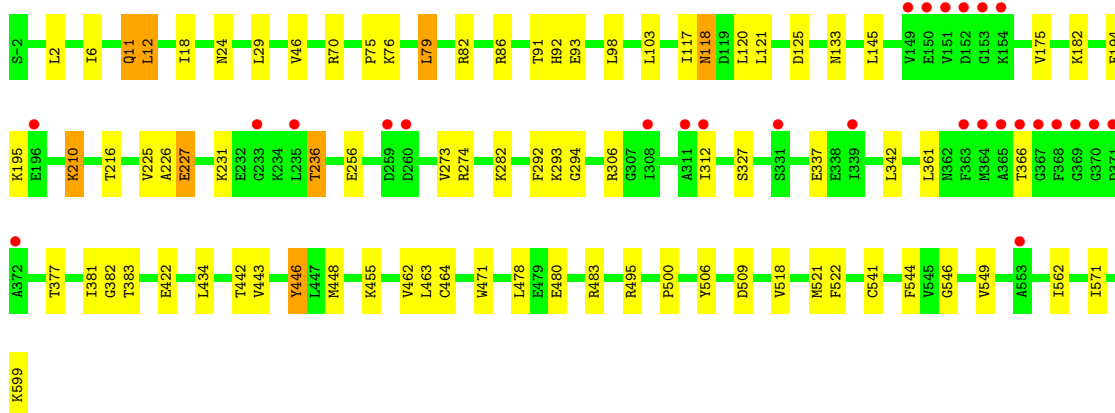
• Molecule 1: Beta-glucuronidase

Chain A: 



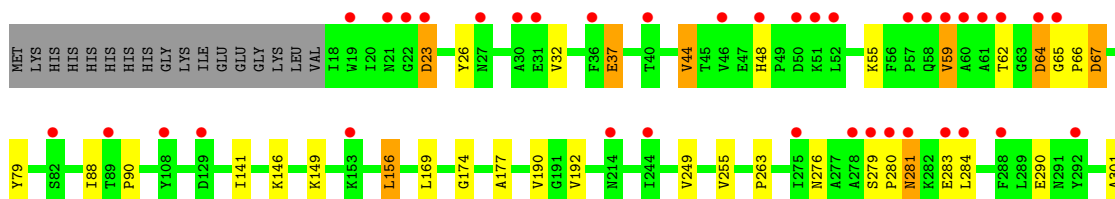
• Molecule 1: Beta-glucuronidase

Chain B: 



• Molecule 2: Maltose-binding periplasmic protein

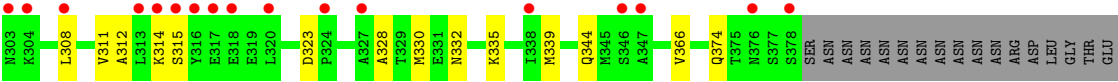
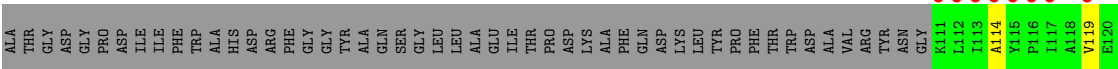
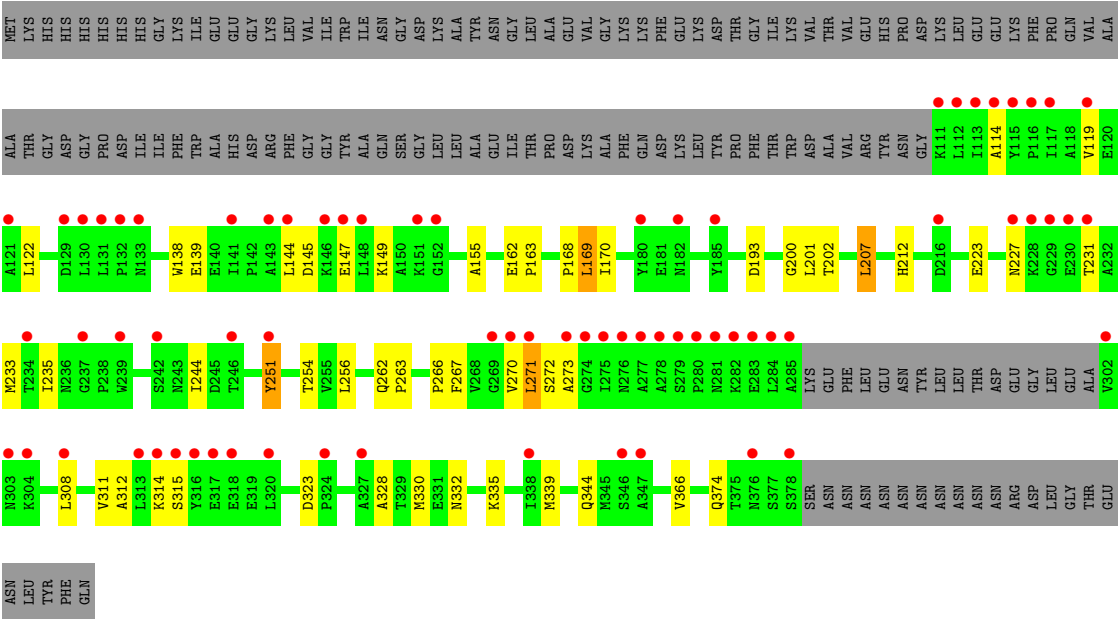
Chain D: 





• Molecule 2: Maltose-binding periplasmic protein

Chain C:



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 (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.207 , 0.234 0.205 , 0.233	Depositor DCC
R_{free} test set	5865 reflections (5.01%)	DCC
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 , 32.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 117089 reflections	Xtriage
F_o, F_c correlation	0.94	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.

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	0.26	1/4977 (0.0%)	0.45	1/6740 (0.0%)
1	B	0.23	0/4965	0.45	0/6728
2	C	0.22	0/1879	0.42	0/2569
2	D	0.23	0/2717	0.44	0/3718
All	All	0.24	1/14538 (0.0%)	0.45	1/19755 (0.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	PRO	N-CD	5.32	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ALA	C-N-CD	5.42	139.77	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	59	VAL	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4863	0	4766	41	0
1	B	4851	0	4733	44	0
2	C	1839	0	1730	27	0
2	D	2653	0	2441	19	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	1	0
All	All	14718	0	13670	123	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:66:PRO:O	2:D:67:ASP:HB2	1.94	0.66
2:D:59:VAL:HG21	2:D:302:VAL:O	1.96	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
1:A:332:HIS:O	1:A:355:PRO:HA	2.12	0.49
1:B:118:ASN:N	1:B:118:ASN:OD1	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:217:ILE:HG13	1:A:235:LEU:HD23	1.97	0.47
1:A:11[B]:GLN:HG2	1:B:11[B]:GLN:NE2	2.30	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:432:LYS:NZ	1:A:461:ASP:OD2	2.48	0.47
1:A:70:ARG:NH2	3:A:623:HOH:O	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:207:LEU:HB2	2:C:212:HIS:HB2	1.99	0.44
2:D:65:GLY:HA3	2:D:66:PRO:HD2	1.86	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
1:B:98:LEU:HD23	1:B:120:LEU:HB2	2.00	0.44
1:B:541:CYS:HB3	1:B:544:PHE:HB2	1.99	0.44
1:B:76:LYS:HA	1:B:79:LEU:HD22	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:531:TYR:OH	1:A:549:VAL:HG13	2.19	0.43
1:A:438:LYS:HE3	2:D:174:GLY:HA3	2.01	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:HG2	1:B:210:LYS:H	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
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
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:C:271:LEU:HG	2:C:271:LEU:H	1.55	0.42
2:D:146:LYS:HE3	2:D:146:LYS:HB2	1.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:117:ILE:O	1:A:121:LEU:HG	2.20	0.40
1:A:11[B]:GLN:NE2	1:B:75:PRO:HG2	2.35	0.40
1:A:78:LEU:HD21	1:B:11[B]:GLN:HE22	1.86	0.40
2:C:256:LEU:HD21	3:C:520:HOH:O	2.21	0.40
2:D:59:VAL:HG22	2:D:302:VAL:HG13	2.03	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

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	601/602 (100%)	573 (95%)	28 (5%)	0	100	100
1	B	601/602 (100%)	568 (94%)	32 (5%)	1 (0%)	56	63
2	C	248/400 (62%)	227 (92%)	20 (8%)	1 (0%)	43	46
2	D	360/400 (90%)	338 (94%)	18 (5%)	4 (1%)	21	15
All	All	1810/2004 (90%)	1706 (94%)	98 (5%)	6 (0%)	50	54

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%)	499 (94%)	30 (6%)	29	29
1	B	526/531 (99%)	494 (94%)	32 (6%)	26	25
2	C	179/325 (55%)	167 (93%)	12 (7%)	23	21
2	D	251/325 (77%)	233 (93%)	18 (7%)	21	18
All	All	1485/1712 (87%)	1393 (94%)	92 (6%)	26	24

All (92) 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

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Mol	Chain	Res	Type
1	A	273	VAL
1	A	274	ARG
1	A	331	SER
1	A	374	LYS
1	A	390	ILE
1	A	422	GLU
1	A	434	LEU
1	A	446	TYR
1	A	449	SER
1	A	463	LEU
1	A	506	TYR
1	A	516	ASP
1	A	545	VAL
1	A	562	ILE
1	A	594	GLU
1	B	11[A]	GLN
1	B	11[B]	GLN
1	B	12	LEU
1	B	24	ASN
1	B	46	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	175	VAL
1	B	182	LYS
1	B	210	LYS
1	B	225	VAL
1	B	227	GLU
1	B	231	LYS
1	B	236	THR
1	B	273	VAL
1	B	274	ARG
1	B	306	ARG
1	B	312	ILE
1	B	342	LEU
1	B	422	GLU
1	B	434	LEU
1	B	446	TYR
1	B	455	LYS

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Mol	Chain	Res	Type
1	B	463	LEU
1	B	478	LEU
1	B	495	ARG
1	B	506	TYR
1	B	518	VAL
2	D	23	ASP
2	D	44	VAL
2	D	48	HIS
2	D	55	LYS
2	D	62	THR
2	D	64	ASP
2	D	149	LYS
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	325	ARG
2	D	344	GLN
2	D	374	GLN
2	C	139	GLU
2	C	144	LEU
2	C	147	GLU
2	C	169	LEU
2	C	207	LEU
2	C	231	THR
2	C	251	TYR
2	C	271	LEU
2	C	311	VAL
2	C	323	ASP
2	C	330	MET
2	C	344	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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%)	0.04	17 (2%)	50	57	18, 29, 55, 162	0
1	B	602/602 (100%)	0.19	27 (4%)	32	36	24, 43, 79, 171	0
2	C	252/400 (63%)	1.37	71 (28%)	1	1	56, 82, 119, 139	0
2	D	362/400 (90%)	0.41	38 (10%)	7	8	28, 61, 104, 117	0
All	All	1818/2004 (90%)	0.35	153 (8%)	11	13	18, 44, 105, 171	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	PHE	13.9
1	B	369	GLY	13.5
1	A	367	GLY	13.0
1	A	371	ASP	12.1
1	B	367	GLY	12.0
2	C	280	PRO	11.5
1	A	366	THR	11.1
1	A	368	PHE	10.0
1	A	365	ALA	9.6
2	C	273	ALA	9.4
2	D	22	GLY	8.9
1	B	371	ASP	8.8
2	C	279	SER	8.7
2	D	46	VAL	8.2
1	A	370	GLY	8.0
1	B	365	ALA	7.7
1	A	364	MET	6.9
1	B	364	MET	6.8
2	C	111	LYS	6.8
2	C	302	VAL	6.7
2	C	112	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	370	GLY	6.4
2	D	284	LEU	6.3
2	C	275	ILE	6.3
2	D	23	ASP	6.3
2	C	281	ASN	6.1
2	C	316	TYR	5.8
1	B	372	ALA	5.8
1	A	369	GLY	5.7
1	B	151	VAL	5.6
1	A	372	ALA	5.6
2	D	57	PRO	5.4
2	C	116	PRO	5.3
2	D	27	ASN	5.3
2	C	284	LEU	5.0
2	C	132	PRO	4.9
2	D	52	LEU	4.5
2	C	317	GLU	4.4
1	B	235	LEU	4.3
2	D	62	THR	4.2
2	C	115	TYR	4.2
2	C	282	LYS	4.0
2	D	288	PHE	3.9
2	C	182	ASN	3.9
2	C	278	ALA	3.8
2	D	31	GLU	3.8
1	B	152	ASP	3.8
2	C	113	ILE	3.8
2	C	304	LYS	3.7
2	C	274	GLY	3.7
2	D	153	LYS	3.7
1	B	366	THR	3.6
2	C	130	LEU	3.5
1	A	373	PRO	3.5
1	B	154	LYS	3.5
2	D	50	ASP	3.5
2	D	60	ALA	3.5
2	C	121	ALA	3.4
2	C	283	GLU	3.4
2	D	279	SER	3.4
2	C	313	LEU	3.4
1	A	363	PHE	3.4
2	C	314	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	233	GLY	3.3
2	C	251	TYR	3.3
2	C	129	ASP	3.3
2	C	152	GLY	3.3
2	C	229	GLY	3.2
2	C	237	GLY	3.2
2	C	271	LEU	3.2
2	C	119	VAL	3.2
2	D	36	PHE	3.2
2	C	324	PRO	3.2
2	D	65	GLY	3.1
1	A	260	ASP	3.1
2	C	246	THR	3.0
2	C	338	ILE	3.0
2	C	242	SER	3.0
2	C	147	GLU	3.0
2	C	269	GLY	2.9
1	B	150	GLU	2.9
1	B	196	GLU	2.8
2	D	21	ASN	2.8
1	B	311	ALA	2.8
2	D	281	ASN	2.8
1	A	311	ALA	2.8
2	C	114	ALA	2.8
2	C	270	VAL	2.8
2	C	320	LEU	2.7
2	D	59	VAL	2.7
2	C	230	GLU	2.7
2	D	275	ILE	2.7
2	C	285	ALA	2.7
1	B	331	SER	2.6
2	C	277	ALA	2.6
2	D	58	GLN	2.6
1	B	308	ILE	2.6
2	D	280	PRO	2.6
2	C	231	THR	2.6
1	B	149	VAL	2.6
2	C	216	ASP	2.6
1	A	261	GLU	2.5
2	D	61	ALA	2.5
2	C	131	LEU	2.5
1	B	363	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	180	TYR	2.5
2	D	48	HIS	2.5
2	C	308	LEU	2.5
2	C	117	ILE	2.5
2	C	315	SER	2.5
1	B	339	ILE	2.5
2	C	141	ILE	2.5
2	C	376	ASN	2.5
1	A	308	ILE	2.4
2	D	89	THR	2.4
2	D	64	ASP	2.4
2	D	51	LYS	2.4
2	D	82	SER	2.4
2	D	214	ASN	2.3
2	C	303	ASN	2.3
2	D	108	TYR	2.3
2	D	283	GLU	2.3
2	D	40	THR	2.3
2	C	143	ALA	2.2
1	B	153	GLY	2.2
1	B	312	ILE	2.2
2	C	276	ASN	2.2
2	D	244	ILE	2.2
2	C	228	LYS	2.2
1	A	331	SER	2.2
2	C	346	SER	2.2
2	C	151	LYS	2.1
2	C	327	ALA	2.1
2	C	133	ASN	2.1
1	A	46	VAL	2.1
1	B	553	ALA	2.1
2	D	19	TRP	2.1
2	C	234	THR	2.1
2	D	278	ALA	2.1
2	C	227	ASN	2.1
2	C	148	LEU	2.1
2	C	146	LYS	2.1
2	D	292	TYR	2.1
2	C	378	SER	2.1
1	B	260	ASP	2.1
2	D	30	ALA	2.1
2	C	347	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	259	ASP	2.0
2	D	129	ASP	2.0
2	C	318	GLU	2.0
2	C	185	TYR	2.0
2	C	144	LEU	2.0
2	C	239	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.