



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:27 PM UTC

PDB ID : 8HCY / pdb_00008hcy
Title : Legionella glycosyltransferase
Authors : Chen, T.T.; Ouyang, S.Y.
Deposited on : 2022-11-03
Resolution : 2.64 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

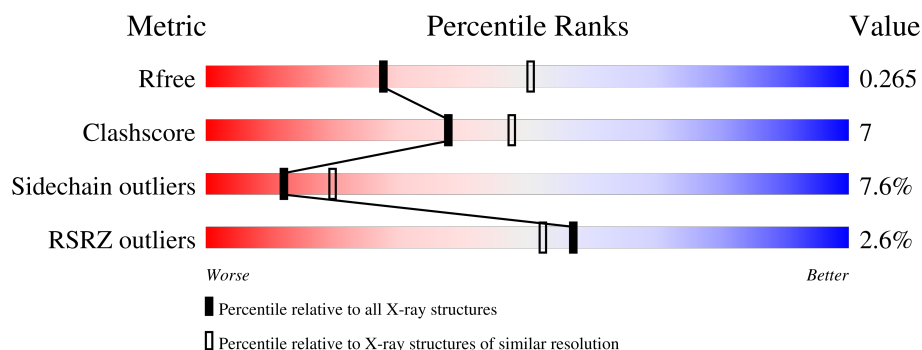
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	865	3% 45% 12% • 42%
1	B	865	47% 10% • 42%
1	C	865	2% 44% 12% • 42%
1	D	865	• 46% 10% • 42%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16216 atoms, of which 0 are hydrogens and 0 are deuteriums.

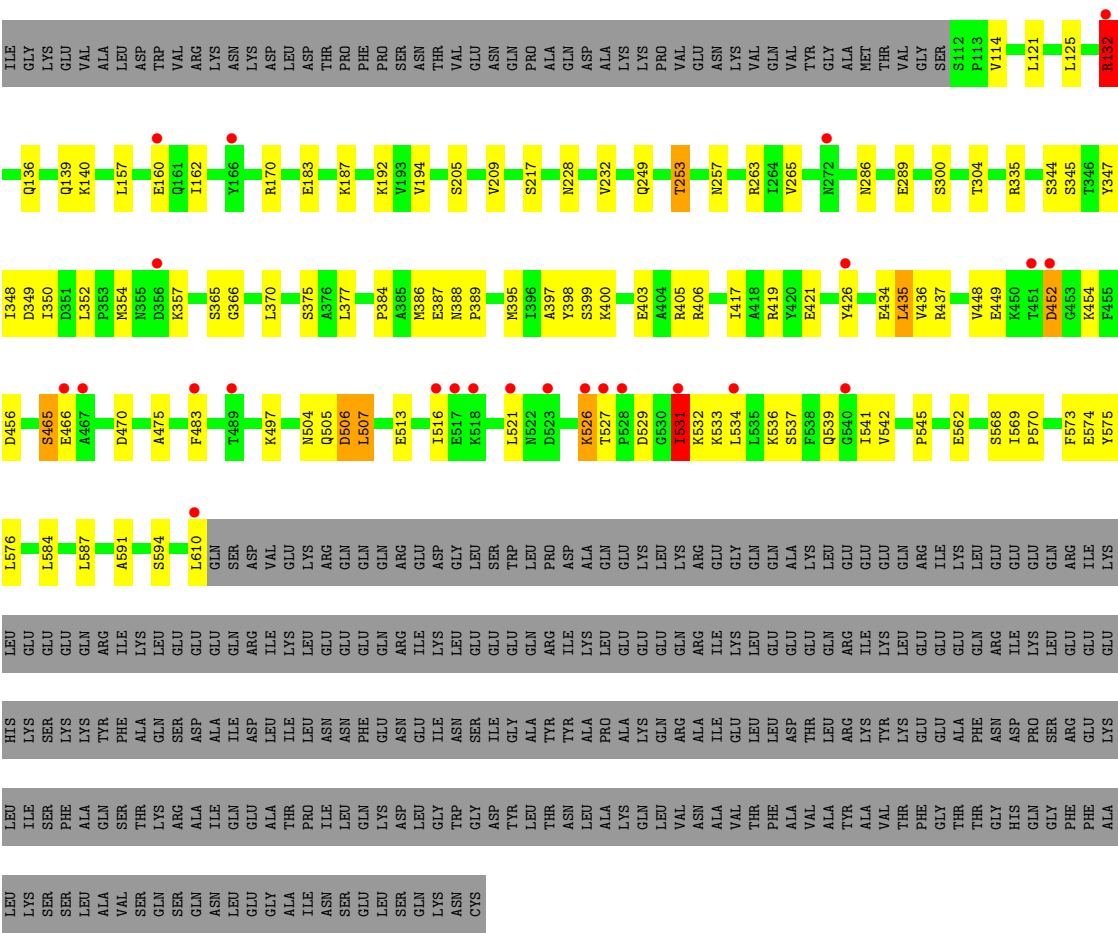
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dot/Icm secretion system substrate.

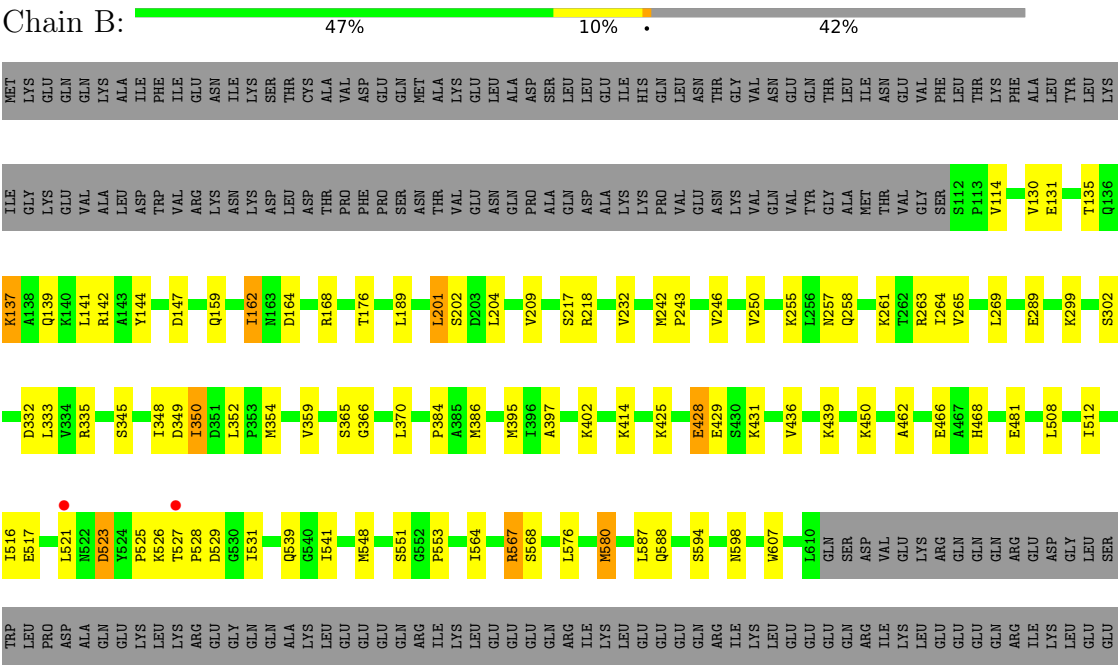
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			
1	A	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			
1	B	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			
1	D	499	Total	C	N	O	S	0	0	0
			3956	2500	676	767	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	91	Total	O	0	0
			91	91		
2	A	83	Total	O	0	0
			83	83		
2	B	99	Total	O	0	0
			99	99		
2	D	119	Total	O	0	0
			119	119		



● Molecule 1: Dot/Icm secretion system substrate



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.36Å 112.61Å 125.80Å 90.00° 108.14° 90.00°	Depositor
Resolution (Å)	29.31 – 2.64 29.31 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.31-2.64) 95.7 (29.31-2.64)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.240 , 0.256 (Not available) , 0.265	Depositor DCC
R_{free} test set	2001 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16216	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6758e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.38	1/4027 (0.0%)	0.68	8/5441 (0.1%)
1	B	0.44	0/4027	0.75	6/5441 (0.1%)
1	C	0.43	0/4027	0.80	12/5441 (0.2%)
1	D	0.41	0/4027	0.75	7/5441 (0.1%)
All	All	0.41	1/16108 (0.0%)	0.75	33/21764 (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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	ILE	CB-CG1	5.40	1.64	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	GLU	CB-CA-C	10.18	130.22	110.67
1	A	526	LYS	CG-CD-CE	-9.04	90.52	111.30
1	A	526	LYS	N-CA-CB	-9.03	97.38	110.56
1	B	189	LEU	CB-CG-CD2	-8.76	84.43	110.70
1	C	120	ARG	CB-CG-CD	-8.59	91.55	111.30
1	D	201	LEU	CB-CA-C	8.45	126.17	110.70
1	B	201	LEU	CB-CA-C	8.22	125.65	110.11
1	C	120	ARG	CG-CD-NE	-8.06	94.26	112.00
1	A	132	ARG	CB-CA-C	7.94	122.28	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	531	ILE	CB-CG1-CD1	7.94	130.47	113.80
1	C	120	ARG	NE-CZ-NH2	-7.80	112.18	119.20
1	C	201	LEU	CB-CA-C	7.38	124.50	109.67
1	D	501	GLN	CA-CB-CG	-7.18	99.74	114.10
1	C	569	ILE	CG1-CB-CG2	-7.14	89.29	110.70
1	D	449	GLU	CB-CA-C	6.33	120.82	109.29
1	D	450	LYS	N-CA-C	-6.33	104.00	111.03
1	D	450	LYS	CB-CA-C	6.30	120.71	110.95
1	C	201	LEU	N-CA-C	-6.21	104.76	112.90
1	B	137	LYS	N-CA-C	-5.92	105.70	113.17
1	C	520	HIS	N-CA-CB	-5.76	103.03	112.25
1	B	189	LEU	CD1-CG-CD2	-5.62	98.44	110.80
1	C	120	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	A	526	LYS	CB-CG-CD	-5.57	98.49	111.30
1	C	137	LYS	N-CA-C	-5.47	105.40	113.61
1	A	531	ILE	CA-CB-CG1	5.41	119.59	110.40
1	D	137	LYS	N-CA-C	-5.38	105.36	112.94
1	A	399	SER	N-CA-C	5.37	117.80	110.55
1	B	523	ASP	N-CA-C	-5.30	106.59	113.16
1	C	176	THR	N-CA-C	-5.25	107.42	113.88
1	C	279	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	526	LYS	CB-CA-C	5.12	119.21	110.56
1	D	486	THR	OG1-CB-CG2	5.06	119.42	109.30
1	B	258	GLN	CB-CA-C	5.02	116.20	109.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	258	GLN	Peptide
1	D	120	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	3964	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3956	0	3964	44	0
1	C	3956	0	3964	73	0
1	D	3956	0	3964	48	0
2	A	83	0	0	2	0
2	B	99	0	0	3	0
2	C	91	0	0	2	0
2	D	119	0	0	3	0
All	All	16216	0	15856	223	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 7.

All (223) 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:C:166:TYR:HD2	1:C:167:ASN:N	1.39	1.20
1:C:166:TYR:HE2	1:C:167:ASN:CG	1.57	1.10
1:C:166:TYR:CD2	1:C:167:ASN:N	2.29	1.00
1:C:166:TYR:CE2	1:C:167:ASN:CG	2.41	0.97
1:C:166:TYR:HE2	1:C:167:ASN:OD1	1.49	0.95
1:A:527:THR:HG22	1:A:529:ASP:H	1.37	0.89
1:C:298:LEU:HD22	1:C:306:ALA:HA	1.56	0.86
1:C:166:TYR:CD2	1:C:166:TYR:C	2.56	0.83
1:C:166:TYR:CE2	1:C:170:ARG:NH1	2.45	0.82
1:D:373:MET:HE2	1:D:592:CYS:HB3	1.63	0.81
1:C:166:TYR:CE2	1:C:167:ASN:OD1	2.36	0.76
1:D:359:VAL:H	1:D:598:ASN:HD21	1.34	0.76
1:C:166:TYR:CE2	1:C:167:ASN:ND2	2.54	0.75
1:D:489:THR:HG23	1:D:491:GLU:H	1.52	0.75
1:C:166:TYR:HD2	1:C:166:TYR:C	1.95	0.74
1:A:136:GLN:O	1:A:139:GLN:NE2	2.23	0.72
1:C:373:MET:HE1	1:C:587:LEU:HB3	1.71	0.72
1:D:273:GLU:O	1:D:277:ILE:HG13	1.90	0.71
1:D:481:GLU:HA	1:D:493:ILE:HD11	1.72	0.71
1:C:166:TYR:HD2	1:C:167:ASN:H	1.37	0.70
1:C:419:ARG:NH1	2:C:902:HOH:O	2.24	0.70
1:B:255:LYS:NZ	2:B:902:HOH:O	2.25	0.69
1:C:166:TYR:CD2	1:C:170:ARG:NH1	2.60	0.69
1:A:506:ASP:OD1	1:A:506:ASP:N	2.26	0.69
1:C:527:THR:HG22	1:C:529:ASP:H	1.55	0.69
1:C:523:ASP:N	1:C:523:ASP:OD2	2.20	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:TYR:HB3	1:D:405:ARG:HD2	1.76	0.67
1:A:398:TYR:HB3	1:A:405:ARG:HD2	1.77	0.67
1:D:373:MET:HE1	1:D:587:LEU:HB3	1.76	0.66
1:B:242:MET:HE1	1:B:264:ILE:HD13	1.76	0.66
1:A:529:ASP:OD1	1:A:533:LYS:NZ	2.24	0.65
1:C:166:TYR:HE2	1:C:167:ASN:ND2	1.90	0.65
1:C:516:ILE:HA	1:C:521:LEU:HD12	1.78	0.64
1:C:250:VAL:HG11	1:C:264:ILE:HD11	1.78	0.64
1:C:548:MET:HE2	1:C:553:PRO:HD2	1.79	0.63
1:B:348:ILE:HG22	1:B:349:ASP:O	1.99	0.63
1:C:241:TYR:OH	1:C:247:LYS:NZ	2.31	0.63
1:D:250:VAL:HG11	1:D:264:ILE:HD11	1.80	0.62
1:C:507:LEU:HD12	1:D:495:VAL:HG13	1.82	0.62
1:A:348:ILE:HG22	1:A:349:ASP:O	2.00	0.62
1:C:183:GLU:O	1:C:187:LYS:HG2	1.99	0.62
1:A:183:GLU:O	1:A:187:LYS:HE2	2.00	0.62
1:B:567:ARG:HD3	1:B:567:ARG:H	1.64	0.62
1:C:427:ILE:HG12	1:C:435:LEU:HD22	1.82	0.61
1:A:370:LEU:HB2	1:A:397:ALA:HB3	1.83	0.61
1:D:359:VAL:H	1:D:598:ASN:ND2	2.00	0.60
1:B:250:VAL:HG11	1:B:264:ILE:HD11	1.84	0.60
1:C:301:VAL:HG22	1:C:339:VAL:HG11	1.82	0.60
1:B:232:VAL:HG22	1:B:265:VAL:HB	1.84	0.59
1:A:516:ILE:HD11	1:A:534:LEU:HD22	1.83	0.59
1:D:273:GLU:HA	1:D:276:GLN:HB2	1.85	0.58
1:B:462:ALA:O	1:B:466:GLU:HG2	2.04	0.58
1:D:152:ARG:NH2	1:D:200:GLU:OE2	2.33	0.58
1:A:531:ILE:HD12	1:A:532:LYS:N	2.19	0.57
1:C:129:VAL:HG12	1:C:202:SER:HB3	1.86	0.57
1:C:298:LEU:CD2	1:C:306:ALA:HA	2.31	0.57
1:A:232:VAL:HG22	1:A:265:VAL:HB	1.86	0.57
1:C:139:GLN:CD	1:C:139:GLN:H	2.14	0.56
1:D:359:VAL:HG22	1:D:598:ASN:ND2	2.20	0.56
1:A:465:SER:HA	1:A:539:GLN:HE21	1.71	0.55
1:A:569:ILE:HG13	1:A:570:PRO:HD2	1.87	0.55
1:A:249:GLN:O	1:A:253:THR:HG23	2.07	0.55
1:A:344:SER:HB2	1:A:400:LYS:HG3	1.88	0.55
1:C:232:VAL:HG22	1:C:265:VAL:HB	1.88	0.54
1:A:532:LYS:HD2	1:A:536:LYS:HG2	1.90	0.54
1:D:359:VAL:HG22	1:D:598:ASN:HD21	1.71	0.54
1:B:564:ILE:O	1:B:567:ARG:HD2	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:GLU:HA	1:B:439:LYS:HD3	1.90	0.54
1:C:298:LEU:HD21	1:C:309:LEU:HB2	1.90	0.54
1:A:348:ILE:HG23	1:A:352:LEU:HD12	1.90	0.54
1:A:465:SER:HA	1:A:539:GLN:NE2	2.22	0.54
1:B:567:ARG:HG2	1:B:568:SER:O	2.08	0.54
1:C:242:MET:HE3	1:C:247:LYS:HA	1.90	0.53
1:D:209:VAL:HG11	1:D:587:LEU:HD21	1.91	0.53
1:D:481:GLU:HA	1:D:493:ILE:CD1	2.39	0.53
1:D:198:LYS:O	1:D:202:SER:OG	2.26	0.52
1:C:242:MET:HG2	1:C:247:LYS:HG3	1.90	0.52
1:C:373:MET:HE2	1:C:592:CYS:HB3	1.91	0.52
1:C:490:GLN:O	1:C:493:ILE:HD12	2.09	0.52
1:D:419:ARG:NH1	1:D:549:GLU:O	2.42	0.52
1:D:250:VAL:HG11	1:D:264:ILE:CD1	2.41	0.51
1:D:548:MET:HG3	1:D:553:PRO:HD2	1.93	0.51
1:C:276:GLN:O	1:C:280:GLN:HG2	2.10	0.51
1:A:132:ARG:H	1:A:132:ARG:HE	1.57	0.51
1:A:139:GLN:H	1:A:139:GLN:CD	2.18	0.51
1:B:414:LYS:NZ	2:B:901:HOH:O	2.22	0.51
1:C:393:THR:HB	1:C:396:ILE:HD11	1.93	0.51
1:A:140:LYS:HB3	1:A:384:PRO:HD3	1.93	0.51
1:B:246:VAL:HG13	1:B:350:ILE:CD1	2.41	0.51
1:C:153:LEU:HD22	1:C:189:LEU:HD22	1.93	0.50
1:B:144:TYR:HB2	1:B:384:PRO:HD2	1.92	0.50
1:D:523:ASP:OD1	1:D:523:ASP:N	2.31	0.50
1:B:201:LEU:O	1:B:576:LEU:HD13	2.12	0.50
1:D:364:HIS:O	1:D:596:LYS:HE3	2.11	0.50
1:B:512:ILE:HG21	1:B:531:ILE:HG23	1.94	0.49
1:B:218:ARG:HD2	1:B:580:MET:HG3	1.94	0.49
1:D:528:PRO:O	1:D:531:ILE:HG13	2.12	0.49
1:C:493:ILE:HB	1:C:494:PRO:HD3	1.95	0.49
1:A:435:LEU:CD1	1:A:545:PRO:HB2	2.43	0.49
1:A:209:VAL:HG11	1:A:587:LEU:HD21	1.95	0.49
1:A:516:ILE:HA	1:A:521:LEU:HD12	1.95	0.49
1:B:348:ILE:HG23	1:B:352:LEU:HD12	1.93	0.49
1:D:468:HIS:CG	1:D:539:GLN:HB2	2.47	0.49
1:A:574:GLU:HB2	1:A:575:TYR:CD2	2.47	0.49
1:C:429:GLU:OE2	2:C:901:HOH:O	2.20	0.49
1:A:437:ARG:HG3	1:A:437:ARG:HH11	1.78	0.49
1:A:465:SER:HB2	1:A:539:GLN:HE22	1.78	0.49
1:C:373:MET:CE	1:C:587:LEU:HB3	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:THR:HG22	1:B:529:ASP:H	1.78	0.48
1:D:196:GLU:OE1	1:D:199:ARG:NH2	2.38	0.48
1:B:250:VAL:HG23	1:B:350:ILE:HD13	1.94	0.48
1:D:382:GLN:NE2	2:D:904:HOH:O	2.28	0.48
1:A:263:ARG:HG2	1:A:289:GLU:HB3	1.96	0.48
1:A:504:ASN:ND2	1:A:507:LEU:H	2.12	0.48
1:A:419:ARG:HG2	1:A:426:TYR:CD2	2.48	0.48
1:D:354:MET:HG2	1:D:599:PHE:CE2	2.49	0.47
1:B:567:ARG:HD3	1:B:567:ARG:N	2.24	0.47
1:B:517:GLU:CD	1:B:526:LYS:HD2	2.39	0.47
1:D:120:ARG:NH2	2:D:916:HOH:O	2.47	0.47
1:B:525:PRO:C	1:B:527:THR:H	2.22	0.47
1:C:364:HIS:O	1:C:596:LYS:HE3	2.14	0.47
1:A:526:LYS:HE3	1:A:526:LYS:HB2	1.49	0.47
1:B:425:LYS:O	1:B:429:GLU:HG3	2.14	0.47
1:D:293:ILE:O	1:D:296:ILE:HG22	2.15	0.47
1:C:293:ILE:HA	1:C:296:ILE:HD12	1.97	0.47
1:A:513:GLU:HG2	1:A:526:LYS:HG2	1.96	0.47
1:D:244:GLN:HE22	1:D:248:THR:HG23	1.78	0.47
1:D:116:LYS:HD3	1:D:116:LYS:HA	1.63	0.47
1:A:170:ARG:NH1	1:B:147:ASP:OD2	2.47	0.47
1:B:370:LEU:HB2	1:B:397:ALA:HB3	1.96	0.47
1:D:501:GLN:O	1:D:501:GLN:HG3	2.15	0.47
1:B:164:ASP:O	1:B:168:ARG:HG3	2.15	0.46
1:B:359:VAL:HG22	1:B:598:ASN:OD1	2.15	0.46
1:B:516:ILE:HA	1:B:521:LEU:HD12	1.97	0.46
1:D:201:LEU:O	1:D:576:LEU:HD13	2.14	0.46
1:A:125:LEU:HD22	1:A:194:VAL:HG13	1.98	0.46
1:B:468:HIS:CG	1:B:539:GLN:HB2	2.50	0.46
1:C:273:GLU:H	1:C:273:GLU:HG2	1.59	0.46
1:A:257:ASN:HB2	1:A:354:MET:HE1	1.97	0.46
1:B:263:ARG:HG2	1:B:289:GLU:HB3	1.97	0.46
1:A:587:LEU:HA	1:A:591:ALA:HB3	1.97	0.46
1:C:469:GLN:O	1:C:532:LYS:NZ	2.48	0.46
1:B:139:GLN:OE1	1:B:142:ARG:NH1	2.49	0.46
1:C:469:GLN:O	1:C:532:LYS:HG2	2.16	0.46
1:D:211:ILE:HB	1:D:367:PHE:CZ	2.51	0.46
1:B:159:GLN:HA	1:B:162:ILE:HG12	1.98	0.45
1:C:431:LYS:HA	1:C:431:LYS:HD3	1.58	0.45
1:A:286:ASN:ND2	2:A:909:HOH:O	2.41	0.45
1:D:370:LEU:HB2	1:D:397:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.85	0.45
1:C:446:LEU:HA	1:C:449:GLU:OE1	2.17	0.45
1:A:228:ASN:ND2	2:A:913:HOH:O	2.50	0.45
1:A:335:ARG:HG2	1:A:347:TYR:CD2	2.52	0.45
1:A:386:MET:HE3	1:A:569:ILE:HG12	1.98	0.45
1:A:532:LYS:HB3	1:A:532:LYS:HE3	1.72	0.45
1:C:492:LEU:HD23	1:C:492:LEU:HA	1.84	0.45
1:C:157:LEU:HB2	1:C:162:ILE:HG13	1.97	0.45
1:C:311:LEU:HD21	1:C:420:TYR:CD2	2.52	0.45
1:A:348:ILE:HD13	1:A:395:MET:HG3	1.98	0.45
1:D:263:ARG:HG2	1:D:289:GLU:HB3	1.99	0.45
1:C:333:LEU:HD11	1:C:416:ILE:HG21	1.99	0.44
1:B:431:LYS:N	1:B:431:LYS:HD3	2.32	0.44
1:C:263:ARG:NH2	1:C:340:ILE:O	2.51	0.44
1:D:428:GLU:CD	1:D:439:LYS:HD3	2.43	0.44
1:C:166:TYR:CZ	1:C:170:ARG:NH1	2.85	0.44
1:C:244:GLN:OE1	1:C:247:LYS:HE2	2.16	0.44
1:B:209:VAL:HG11	1:B:587:LEU:HD21	2.00	0.44
1:B:243:PRO:HD3	2:B:910:HOH:O	2.18	0.44
1:B:548:MET:HE2	1:B:553:PRO:HD2	2.00	0.43
1:A:375:SER:HB2	1:A:387:GLU:HG3	2.00	0.43
1:D:184:GLU:H	1:D:184:GLU:CD	2.26	0.43
1:C:504:ASN:CG	1:C:507:LEU:HB2	2.42	0.43
1:A:497:LYS:HB3	1:A:497:LYS:HE3	1.56	0.43
1:B:257:ASN:HA	1:B:354:MET:HE1	2.00	0.43
1:D:497:LYS:HD2	1:D:497:LYS:HA	1.61	0.43
1:A:452:ASP:HB3	1:A:454:LYS:HE3	1.99	0.43
1:D:517:GLU:HG2	1:D:526:LYS:HD2	1.99	0.43
1:C:419:ARG:HD2	1:C:550:PHE:HA	2.00	0.43
1:B:332:ASP:HB3	1:B:551:SER:O	2.18	0.43
1:B:526:LYS:HE2	1:B:526:LYS:HB2	1.87	0.43
1:C:335:ARG:HG2	1:C:347:TYR:CD2	2.54	0.43
1:A:417:ILE:O	1:A:421:GLU:HG3	2.19	0.42
1:D:212:LEU:HG	1:D:559:SER:HB3	2.02	0.42
1:D:316:LEU:O	1:D:320:ARG:HG3	2.19	0.42
1:C:301:VAL:HG13	1:C:305:ASP:CB	2.50	0.42
1:A:573:PHE:HB3	1:A:576:LEU:HG	2.02	0.42
1:A:536:LYS:HA	1:A:536:LYS:HD2	1.54	0.42
1:C:436:VAL:HA	1:C:439:LYS:HE2	2.01	0.42
1:C:113:PRO:HG2	1:C:178:SER:O	2.20	0.42
1:C:321:LYS:O	1:C:323:LYS:HG2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:LYS:HE2	1:C:425:LYS:HB2	1.88	0.42
1:B:588:GLN:HG3	1:B:607:TRP:CD1	2.54	0.42
1:C:309:LEU:O	1:C:313:LYS:HG3	2.19	0.42
1:A:157:LEU:HD12	1:A:162:ILE:HD13	2.01	0.42
1:A:386:MET:HE3	1:A:386:MET:HB3	1.85	0.42
1:A:475:ALA:HB2	1:A:483:PHE:CD1	2.54	0.42
1:A:534:LEU:O	1:A:537:SER:OG	2.35	0.42
1:A:532:LYS:O	1:A:536:LYS:HG2	2.20	0.41
1:A:470:ASP:CG	1:A:505:GLN:HE22	2.28	0.41
1:C:137:LYS:HA	1:C:139:GLN:HE22	1.85	0.41
1:C:395:MET:HE2	1:C:395:MET:HB2	1.95	0.41
1:C:548:MET:HE3	1:C:548:MET:HB2	1.94	0.41
1:B:450:LYS:HD2	1:B:450:LYS:HA	1.92	0.41
1:D:386:MET:H	1:D:386:MET:HG2	1.72	0.41
1:C:367:PHE:CG	1:C:368:PRO:HD2	2.55	0.41
1:D:373:MET:CE	1:D:587:LEU:HB3	2.46	0.41
1:C:292:ASP:HB3	1:C:295:SER:HB2	2.02	0.41
1:A:403:GLU:HG2	1:A:406:ARG:HH21	1.85	0.41
1:B:242:MET:SD	1:B:246:VAL:HG12	2.60	0.41
1:A:217:SER:O	1:A:366:GLY:HA3	2.20	0.41
1:D:367:PHE:CG	1:D:368:PRO:HD2	2.55	0.41
1:C:534:LEU:O	1:C:537:SER:OG	2.39	0.41
1:A:388:ASN:HD22	1:A:389:PRO:HD2	1.85	0.41
1:D:368:PRO:HA	1:D:399:SER:HB2	2.03	0.40
1:D:386:MET:HE3	1:D:569:ILE:HD13	2.03	0.40
1:D:439:LYS:NZ	2:D:915:HOH:O	2.44	0.40
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.84	0.40
1:C:373:MET:CE	1:C:592:CYS:HB3	2.52	0.40
1:A:377:LEU:HA	1:A:386:MET:O	2.22	0.40
1:A:434:GLU:HG3	1:A:541:ILE:O	2.21	0.40
1:B:217:SER:O	1:B:366:GLY:HA3	2.21	0.40
1:C:257:ASN:HB2	1:C:354:MET:HE1	2.02	0.40
1:C:588:GLN:HG3	1:C:607:TRP:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	439/763 (58%)	410 (93%)	29 (7%)	15	25
1	B	439/763 (58%)	408 (93%)	31 (7%)	13	22
1	C	439/763 (58%)	409 (93%)	30 (7%)	14	23
1	D	439/763 (58%)	396 (90%)	43 (10%)	7	11
All	All	1756/3052 (58%)	1623 (92%)	133 (8%)	12	20

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	114	VAL
1	C	120	ARG
1	C	121	LEU
1	C	134	LYS
1	C	160	GLU
1	C	166	TYR
1	C	204	LEU
1	C	261	LYS
1	C	273	GLU
1	C	287	ASN
1	C	301	VAL
1	C	302	SER
1	C	304	THR
1	C	333	LEU
1	C	345	SER
1	C	350	ILE
1	C	356	ASP
1	C	365	SER
1	C	386	MET
1	C	403	GLU
1	C	428	GLU
1	C	431	LYS
1	C	433	GLU
1	C	452	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	507	LEU
1	C	520	HIS
1	C	523	ASP
1	C	548	MET
1	C	568	SER
1	C	569	ILE
1	A	114	VAL
1	A	132	ARG
1	A	160	GLU
1	A	192	LYS
1	A	205	SER
1	A	253	THR
1	A	300	SER
1	A	304	THR
1	A	345	SER
1	A	350	ILE
1	A	357	LYS
1	A	365	SER
1	A	435	LEU
1	A	436	VAL
1	A	448	VAL
1	A	449	GLU
1	A	452	ASP
1	A	456	ASP
1	A	465	SER
1	A	466	GLU
1	A	506	ASP
1	A	507	LEU
1	A	531	ILE
1	A	542	VAL
1	A	562	GLU
1	A	568	SER
1	A	584	LEU
1	A	594	SER
1	A	610	LEU
1	B	114	VAL
1	B	130	VAL
1	B	131	GLU
1	B	135	THR
1	B	137	LYS
1	B	141	LEU
1	B	162	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	THR
1	B	202	SER
1	B	204	LEU
1	B	261	LYS
1	B	299	LYS
1	B	302	SER
1	B	333	LEU
1	B	335	ARG
1	B	345	SER
1	B	350	ILE
1	B	365	SER
1	B	386	MET
1	B	395	MET
1	B	402	LYS
1	B	428	GLU
1	B	436	VAL
1	B	481	GLU
1	B	508	LEU
1	B	523	ASP
1	B	528	PRO
1	B	541	ILE
1	B	567	ARG
1	B	580	MET
1	B	594	SER
1	D	114	VAL
1	D	115	ASN
1	D	116	LYS
1	D	121	LEU
1	D	132	ARG
1	D	134	LYS
1	D	135	THR
1	D	137	LYS
1	D	184	GLU
1	D	190	LYS
1	D	199	ARG
1	D	202	SER
1	D	204	LEU
1	D	205	SER
1	D	226	THR
1	D	227	THR
1	D	248	THR
1	D	274	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	299	LYS
1	D	300	SER
1	D	304	THR
1	D	333	LEU
1	D	345	SER
1	D	350	ILE
1	D	354	MET
1	D	365	SER
1	D	403	GLU
1	D	414	LYS
1	D	436	VAL
1	D	449	GLU
1	D	465	SER
1	D	466	GLU
1	D	469	GLN
1	D	486	THR
1	D	489	THR
1	D	492	LEU
1	D	497	LYS
1	D	501	GLN
1	D	511	VAL
1	D	523	ASP
1	D	532	LYS
1	D	558	SER
1	D	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	159	GLN
1	C	286	ASN
1	C	469	GLN
1	C	490	GLN
1	C	519	GLN
1	A	115	ASN
1	A	272	ASN
1	A	307	GLN
1	A	388	ASN
1	A	504	ASN
1	A	505	GLN
1	A	514	ASN
1	A	515	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	539	GLN
1	B	119	ASN
1	B	281	GLN
1	B	407	GLN
1	B	589	HIS
1	D	115	ASN
1	D	136	GLN
1	D	139	GLN
1	D	244	GLN
1	D	258	GLN
1	D	287	ASN
1	D	589	HIS
1	D	598	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	499/865 (57%)	0.43	24 (4%) 35 29	22, 34, 66, 103	0
1	B	499/865 (57%)	0.24	2 (0%) 88 87	21, 32, 53, 82	0
1	C	499/865 (57%)	0.29	17 (3%) 48 42	21, 33, 58, 116	0
1	D	499/865 (57%)	0.30	9 (1%) 67 64	23, 35, 56, 82	0
All	All	1996/3460 (57%)	0.31	52 (2%) 57 52	21, 34, 57, 116	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	ILE	5.6
1	C	166	TYR	5.2
1	A	528	PRO	4.9
1	A	517	GLU	4.5
1	C	520	HIS	4.4
1	C	517	GLU	4.4
1	A	160	GLU	4.3
1	A	526	LYS	3.6
1	A	610	LEU	3.5
1	A	452	ASP	3.4
1	D	469	GLN	3.3
1	A	356	ASP	3.3
1	A	527	THR	3.3
1	C	456	ASP	3.2
1	C	569	ILE	3.2
1	C	524	TYR	3.1
1	B	527	THR	3.0
1	D	501	GLN	2.9
1	C	493	ILE	2.9
1	B	521	LEU	2.9
1	D	532	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	518	LYS	2.8
1	C	139	GLN	2.7
1	C	471	ALA	2.7
1	C	516	ILE	2.7
1	D	314	ASP	2.7
1	A	467	ALA	2.5
1	A	483	PHE	2.5
1	A	132	ARG	2.5
1	A	534	LEU	2.5
1	C	160	GLU	2.5
1	A	521	LEU	2.5
1	A	523	ASP	2.5
1	C	481	GLU	2.4
1	A	451	THR	2.4
1	C	534	LEU	2.4
1	C	489	THR	2.4
1	A	272	ASN	2.3
1	A	466	GLU	2.3
1	A	489	THR	2.3
1	C	528	PRO	2.3
1	A	166	TYR	2.3
1	D	471	ALA	2.2
1	A	426	TYR	2.2
1	A	540	GLY	2.2
1	A	516	ILE	2.2
1	D	123	ASN	2.1
1	C	426	TYR	2.1
1	C	521	LEU	2.1
1	D	523	ASP	2.0
1	D	433	GLU	2.0
1	D	566	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 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.