



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:20 AM UTC

PDB ID : 8ZCX / pdb_00008zcx
Title : Crystal Structure of a novel Aldehyde Dehydrogenase from *Klebsiella pneumoniae*
Authors : Zhang, J.; Han, Y.; Liu, W.; Zhang, W.
Deposited on : 2024-04-30
Resolution : 2.44 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

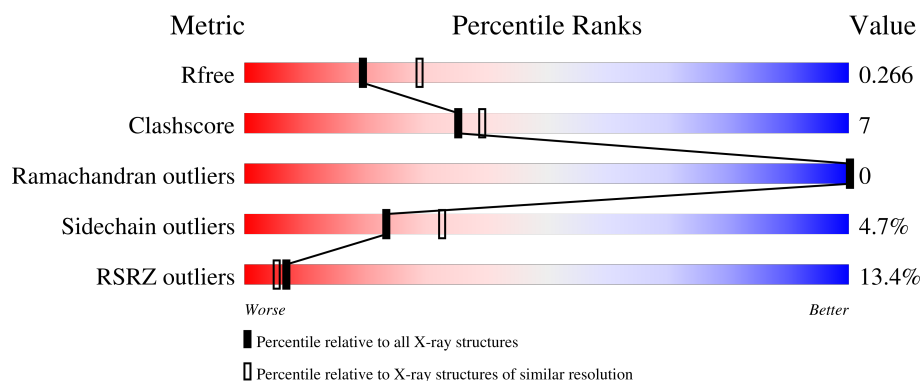
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	489	22% 69% 21% • 8%
1	B	489	10% 81% 13% 5%
1	C	489	10% 78% 16% • 5%
1	D	489	8% 83% 10% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14061 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 Aldehyde dehydrogenase.

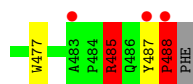
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3384	2147	605	629	3			
1	B	466	Total	C	N	O	S	0	0	0
			3505	2222	632	646	5			
1	C	465	Total	C	N	O	S	0	0	0
			3496	2211	628	654	3			
1	D	460	Total	C	N	O	S	0	0	0
			3484	2201	634	646	3			

There are 4 discrepancies between the modelled and reference sequences:

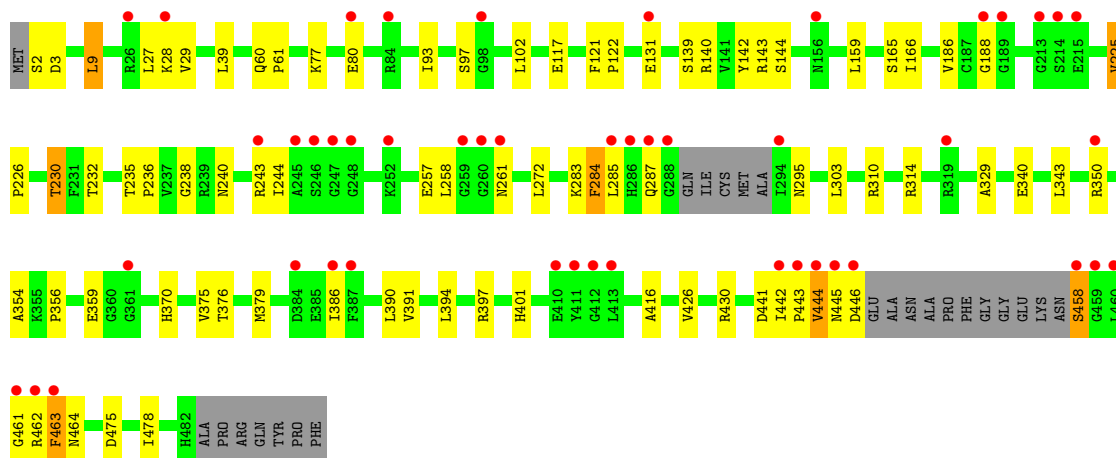
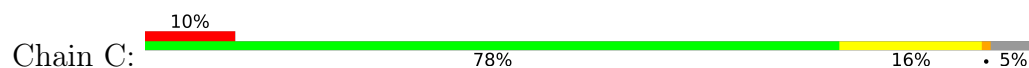
Chain	Residue	Modelled	Actual	Comment	Reference
A	277	SER	ASN	conflict	UNP A0A069Q1D5
B	277	SER	ASN	conflict	UNP A0A069Q1D5
C	277	SER	ASN	conflict	UNP A0A069Q1D5
D	277	SER	ASN	conflict	UNP A0A069Q1D5

- Molecule 2 is water.

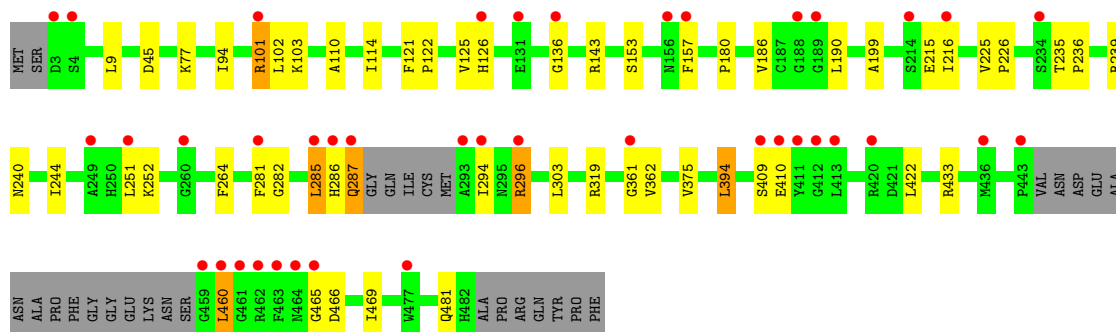
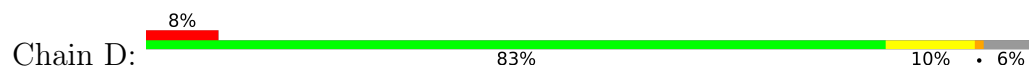
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	44	Total	O	0	0
			44	44		
2	C	53	Total	O	0	0
			53	53		
2	D	83	Total	O	0	0
			83	83		



• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.67Å 146.74Å 149.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.44 50.00 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.44) 97.9 (50.00-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.222 , 0.252 0.234 , 0.266	Depositor DCC
R_{free} test set	4316 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14061	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.74	0/3454	0.87	3/4695 (0.1%)
1	B	0.81	2/3579 (0.1%)	0.85	1/4866 (0.0%)
1	C	0.83	0/3568	0.90	2/4850 (0.0%)
1	D	0.85	0/3555	0.84	1/4828 (0.0%)
All	All	0.81	2/14156 (0.0%)	0.87	7/19239 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	ARG	C-N	-7.11	1.24	1.33
1	B	295	ASN	C-N	5.43	1.41	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	463	PHE	CA-CB-CG	6.82	120.61	113.80
1	A	190	LEU	N-CA-C	-6.11	104.62	111.28
1	C	284	PHE	CA-C-O	-5.99	113.89	120.36
1	A	26	ARG	CA-CB-CG	-5.50	103.10	114.10
1	A	378	THR	CA-CB-OG1	-5.45	101.42	109.60
1	B	488	PRO	N-CA-CB	-5.04	97.46	103.00
1	D	285	LEU	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3384	0	3336	80	0
1	B	3505	0	3465	39	0
1	C	3496	0	3444	51	0
1	D	3484	0	3458	39	0
2	A	12	0	0	0	0
2	B	44	0	0	2	0
2	C	53	0	0	0	0
2	D	83	0	0	2	0
All	All	14061	0	13703	203	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 (203) 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:D:296:ARG:NH2	1:D:409:SER:HB3	1.65	1.12
1:A:354:ALA:HB2	1:A:379:MET:HE1	1.50	0.93
1:A:342:LEU:HD11	1:A:388:GLY:HA3	1.53	0.90
1:D:296:ARG:HH22	1:D:409:SER:HB3	1.28	0.90
1:A:338:GLN:NE2	1:A:338:GLN:HA	1.87	0.88
1:D:410:GLU:HA	1:D:433:ARG:HH21	1.40	0.87
1:D:410:GLU:HA	1:D:433:ARG:NH2	1.91	0.86
1:B:261:ASN:OD1	1:B:296:ARG:HG3	1.75	0.86
1:D:94:ILE:HD11	1:D:101:ARG:HG2	1.57	0.86
1:A:166:ILE:HD12	1:A:176:VAL:HG21	1.58	0.83
1:C:77:LYS:O	1:C:80:GLU:HB2	1.80	0.82
1:A:338:GLN:HA	1:A:338:GLN:HE21	1.45	0.80
1:C:376:THR:HG22	1:C:379:MET:HG3	1.67	0.76
1:A:365:GLN:HA	1:A:365:GLN:OE1	1.85	0.75
1:C:416:ALA:HB2	1:C:443:PRO:HG3	1.67	0.75
1:D:94:ILE:HD11	1:D:101:ARG:CG	2.18	0.73
1:D:361:GLY:C	2:D:507:HOH:O	2.32	0.72
1:C:295:ASN:HD21	1:C:386:ILE:HB	1.56	0.71
1:A:350:ARG:NH1	1:A:359:GLU:OE1	2.24	0.71
1:A:38:LEU:HD11	1:A:95:ARG:HD2	1.71	0.70
1:A:296:ARG:HH22	1:A:409:SER:HB3	1.58	0.68
1:A:189:GLY:HA2	1:A:192:LEU:HB2	1.76	0.68
1:B:296:ARG:HD3	1:B:382:ALA:O	1.94	0.67
1:A:408:ALA:O	1:A:409:SER:C	2.38	0.66
1:B:134:VAL:HG11	1:B:485:ARG:HH11	1.60	0.66
1:C:235:THR:HA	1:C:258:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HG3	1:A:394:LEU:HD13	1.78	0.65
1:A:117:GLU:OE1	1:A:463:PHE:CE2	2.50	0.65
1:B:186:VAL:HA	1:B:190:LEU:HB2	1.78	0.64
1:C:143:ARG:NH1	1:C:475:ASP:OD2	2.30	0.64
1:C:442:ILE:HG13	1:C:444:VAL:HB	1.79	0.64
1:B:463:PHE:O	1:B:467:TRP:HB3	1.97	0.64
1:A:346:ILE:O	1:A:350:ARG:HG2	1.98	0.64
1:A:6:TYR:HB3	1:A:9:LEU:HD21	1.79	0.63
1:B:269:ASP:O	1:B:420:ARG:HG3	1.98	0.63
1:A:338:GLN:HE21	1:A:338:GLN:CA	2.07	0.63
1:B:485:ARG:HD3	1:C:441:ASP:OD2	1.98	0.63
1:A:348:LEU:HD21	1:A:352:GLU:OE2	1.99	0.61
1:B:290:ILE:HG22	1:B:292:MET:H	1.65	0.61
1:B:268:GLY:O	1:B:303:LEU:HD11	2.01	0.60
1:D:153:SER:HB2	1:D:180:PRO:HA	1.83	0.60
1:A:254:VAL:HG12	1:A:256:LEU:HG	1.84	0.60
1:A:186:VAL:C	1:A:188:GLY:H	2.10	0.59
1:A:295:ASN:ND2	1:A:386:ILE:H	2.00	0.59
1:C:29:VAL:HB	1:C:39:LEU:HD23	1.83	0.59
1:A:463:PHE:O	1:A:467:TRP:HB3	2.02	0.59
1:D:240:ASN:O	1:D:244:ILE:HG12	2.03	0.59
1:A:342:LEU:O	1:A:346:ILE:HG13	2.03	0.58
1:A:22:ARG:HB3	1:A:45:ASP:OD2	2.03	0.58
1:C:272:LEU:HD13	1:C:303:LEU:HD13	1.85	0.58
1:D:296:ARG:HH21	1:D:409:SER:HB3	1.61	0.58
1:C:354:ALA:HB2	1:C:379:MET:HE1	1.86	0.58
1:A:117:GLU:OE1	1:A:463:PHE:CD2	2.57	0.57
1:A:251:LEU:H	1:A:251:LEU:HD23	1.69	0.56
1:B:283:LYS:HD2	1:B:294:ILE:O	2.05	0.56
1:A:38:LEU:CD1	1:A:95:ARG:HD2	2.35	0.56
1:A:243:ARG:O	1:A:247:GLY:N	2.34	0.56
1:C:235:THR:N	1:C:236:PRO:HD2	2.21	0.56
1:C:240:ASN:O	1:C:244:ILE:HG12	2.06	0.55
1:A:235:THR:HB	1:A:236:PRO:HD3	1.87	0.55
1:B:134:VAL:CG1	1:B:485:ARG:HH11	2.18	0.55
1:B:487:TYR:O	1:B:488:PRO:C	2.49	0.55
1:C:350:ARG:NH1	1:C:356:PRO:HG2	2.22	0.55
1:A:465:GLY:O	1:A:469:ILE:HG13	2.06	0.54
1:D:103:LYS:HE3	1:D:157:PHE:CZ	2.42	0.54
1:B:6:TYR:HD1	1:B:194:ARG:HH21	1.54	0.54
1:A:285:LEU:O	1:A:286:HIS:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:HH12	1:C:356:PRO:HG2	1.73	0.54
1:D:319:ARG:HH11	1:D:319:ARG:HG2	1.73	0.54
1:D:362:VAL:N	2:D:507:HOH:O	2.40	0.54
1:D:110:ALA:O	1:D:114:ILE:HG12	2.08	0.54
1:A:31:ASN:HB2	1:A:38:LEU:HD21	1.89	0.54
1:B:117:GLU:OE1	1:B:459:GLY:HA3	2.08	0.53
1:A:346:ILE:HD13	1:A:370:HIS:CD2	2.43	0.53
1:B:22:ARG:HD3	2:B:501:HOH:O	2.08	0.53
1:D:94:ILE:CD1	1:D:101:ARG:CG	2.86	0.53
1:A:29:VAL:HB	1:A:39:LEU:HD23	1.90	0.53
1:C:310:ARG:O	1:C:314:ARG:HG2	2.09	0.53
1:A:320:VAL:HG12	1:A:366:LEU:HD13	1.91	0.52
1:B:460:LEU:HA	2:B:502:HOH:O	2.08	0.52
1:D:215:GLU:HG2	1:D:216:ILE:HG23	1.91	0.52
1:D:409:SER:O	1:D:410:GLU:HG3	2.08	0.52
1:A:345:LYS:NZ	1:A:385:GLU:O	2.43	0.52
1:A:347:ARG:O	1:A:350:ARG:HB2	2.10	0.51
1:C:238:GLY:HA3	1:C:258:LEU:HD21	1.91	0.51
1:A:397:ARG:HG2	1:A:401:HIS:ND1	2.25	0.51
1:B:189:GLY:HA2	1:B:192:LEU:HB2	1.92	0.51
1:B:223:HIS:O	1:B:252:LYS:HE2	2.10	0.51
1:A:346:ILE:HG22	1:A:350:ARG:HE	1.76	0.51
1:C:225:VAL:HG22	1:C:226:PRO:HD3	1.93	0.51
1:A:222:GLU:HG3	1:A:244:ILE:HG22	1.92	0.50
1:B:91:ASP:OD2	1:B:95:ARG:CZ	2.59	0.50
1:C:232:THR:HG22	1:C:257:GLU:HB2	1.93	0.50
1:D:282:GLY:HA3	1:D:294:ILE:HD12	1.92	0.50
1:C:283:LYS:HD3	1:C:391:VAL:HB	1.94	0.50
1:B:477:TRP:CZ3	1:C:461:GLY:HA2	2.47	0.50
1:B:235:THR:N	1:B:236:PRO:HD2	2.27	0.50
1:A:296:ARG:NH2	1:A:409:SER:HB3	2.26	0.50
1:A:103:LYS:HE3	1:A:157:PHE:CZ	2.47	0.49
1:A:271:ASP:HB2	1:A:420:ARG:HD2	1.95	0.49
1:A:248:GLY:O	1:D:239:ARG:NH2	2.46	0.49
1:D:94:ILE:CD1	1:D:101:ARG:HG3	2.42	0.49
1:A:360:GLY:HA3	1:A:368:ALA:HB3	1.94	0.49
1:A:81:VAL:HA	1:A:84:ARG:HB3	1.93	0.49
1:B:238:GLY:HA3	1:B:258:LEU:HD21	1.95	0.49
1:C:295:ASN:ND2	1:C:386:ILE:HB	2.25	0.49
1:C:117:GLU:OE2	1:C:458:SER:HA	2.14	0.48
1:C:225:VAL:N	1:C:226:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:O	1:A:413:LEU:HD21	2.14	0.48
1:A:337:ARG:HA	1:A:340:GLU:HG3	1.94	0.48
1:C:370:HIS:HB2	1:C:390:LEU:HD23	1.96	0.48
1:B:225:VAL:N	1:B:226:PRO:HD2	2.29	0.48
1:B:264:PHE:HB2	1:B:294:ILE:HG23	1.96	0.48
1:C:186:VAL:C	1:C:188:GLY:H	2.20	0.48
1:A:234:SER:HB3	1:A:236:PRO:HD2	1.96	0.48
1:A:235:THR:HA	1:A:258:LEU:HD13	1.95	0.47
1:D:143:ARG:HH11	1:D:469:ILE:HG22	1.79	0.47
1:C:93:ILE:O	1:C:97:SER:OG	2.32	0.47
1:C:426:VAL:O	1:C:430:ARG:HG2	2.13	0.47
1:D:186:VAL:HA	1:D:190:LEU:HB2	1.96	0.47
1:A:162:THR:O	1:A:166:ILE:HG12	2.14	0.47
1:A:114:ILE:HG23	1:A:463:PHE:CZ	2.50	0.47
1:D:481:GLN:HA	1:D:481:GLN:OE1	2.14	0.47
1:A:225:VAL:N	1:A:226:PRO:HD2	2.30	0.46
1:B:261:ASN:OD1	1:B:296:ARG:CG	2.58	0.46
1:A:130:VAL:HG11	1:D:460:LEU:O	2.16	0.46
1:A:55:LYS:HD3	1:A:58:GLU:OE2	2.16	0.46
1:B:180:PRO:HB3	1:B:188:GLY:O	2.16	0.46
1:B:460:LEU:HD13	1:C:131:GLU:O	2.16	0.45
1:C:165:SER:OG	1:C:230:THR:HG21	2.16	0.45
1:A:99:SER:OG	1:A:103:LYS:HD3	2.16	0.45
1:A:186:VAL:C	1:A:188:GLY:N	2.74	0.45
1:D:235:THR:N	1:D:236:PRO:HD2	2.32	0.45
1:A:55:LYS:O	1:A:59:VAL:HG22	2.17	0.45
1:C:261:ASN:OD1	1:C:295:ASN:HB3	2.17	0.45
1:B:128:ARG:HG3	1:B:141:VAL:HB	1.98	0.45
1:B:485:ARG:HE	1:B:485:ARG:HB3	1.59	0.45
1:A:158:PRO:HB2	1:A:187:CYS:O	2.17	0.44
1:C:186:VAL:C	1:C:188:GLY:N	2.76	0.44
1:A:38:LEU:HD13	1:A:95:ARG:HH21	1.82	0.44
1:A:407:ASN:HD21	1:A:432:LEU:HA	1.82	0.44
1:B:29:VAL:HB	1:B:39:LEU:HD23	1.99	0.44
1:C:121:PHE:N	1:C:122:PRO:CD	2.80	0.44
1:A:9:LEU:HD12	1:A:92:TRP:CZ2	2.53	0.44
1:A:22:ARG:HB3	1:A:45:ASP:CG	2.42	0.44
1:C:140:ARG:HD2	1:C:142:TYR:OH	2.18	0.44
1:C:397:ARG:HG2	1:C:401:HIS:ND1	2.33	0.44
1:D:45:ASP:HA	1:D:215:GLU:OE2	2.17	0.44
1:C:2:SER:OG	1:C:3:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ILE:HD13	1:D:101:ARG:HG3	1.99	0.44
1:A:153:SER:HB3	1:A:180:PRO:HA	2.00	0.43
1:C:261:ASN:CG	1:C:295:ASN:HB3	2.43	0.43
1:D:303:LEU:HD23	1:D:303:LEU:HA	1.92	0.43
1:A:27:LEU:HD12	1:A:28:LYS:N	2.33	0.43
1:C:284:PHE:O	1:C:285:LEU:HB2	2.16	0.43
1:C:350:ARG:NH1	1:C:359:GLU:OE2	2.51	0.43
1:D:264:PHE:HB2	1:D:294:ILE:HG23	2.00	0.43
1:D:281:PHE:CD1	1:D:285:LEU:HD12	2.54	0.43
1:A:358:TYR:CD2	1:A:358:TYR:C	2.97	0.43
1:B:268:GLY:HA2	1:B:303:LEU:HD13	2.01	0.43
1:A:31:ASN:N	1:A:38:LEU:HD23	2.34	0.42
1:B:360:GLY:HA3	1:B:368:ALA:HB3	2.01	0.42
1:C:102:LEU:HD22	1:C:285:LEU:HD23	2.01	0.42
1:A:276:VAL:HG11	1:A:310:ARG:HB3	2.00	0.42
1:A:335:ASN:CG	1:A:336:ALA:N	2.76	0.42
1:D:296:ARG:HH22	1:D:409:SER:CB	2.15	0.42
1:B:323:PRO:HG3	1:B:332:PRO:CD	2.50	0.42
1:B:323:PRO:HG3	1:B:332:PRO:HD3	2.02	0.42
1:D:287:GLN:HE21	1:D:287:GLN:HB2	1.63	0.42
1:A:121:PHE:N	1:A:122:PRO:CD	2.82	0.42
1:B:134:VAL:CG1	1:B:485:ARG:NH1	2.82	0.42
1:A:335:ASN:CG	1:A:336:ALA:H	2.27	0.42
1:A:396:ALA:HA	1:A:401:HIS:ND1	2.35	0.42
1:A:417:VAL:HG21	1:A:428:PHE:CD2	2.55	0.42
1:C:350:ARG:NH1	1:C:356:PRO:CG	2.83	0.42
1:C:375:VAL:CG2	1:C:394:LEU:HG	2.50	0.42
1:D:121:PHE:CZ	1:D:465:GLY:HA2	2.55	0.42
1:B:114:ILE:HG23	1:B:463:PHE:CZ	2.55	0.41
1:C:9:LEU:HD13	1:C:9:LEU:HA	1.91	0.41
1:A:271:ASP:OD1	1:A:271:ASP:C	2.63	0.41
1:A:428:PHE:CE2	1:A:432:LEU:HD21	2.55	0.41
1:B:99:SER:HB2	1:B:103:LYS:HE3	2.02	0.41
1:D:121:PHE:N	1:D:122:PRO:CD	2.83	0.41
1:A:350:ARG:CZ	1:A:359:GLU:OE1	2.68	0.41
1:B:14:LEU:O	1:B:17:GLU:HG2	2.20	0.41
1:C:77:LYS:C	1:C:80:GLU:HB2	2.43	0.41
1:D:225:VAL:N	1:D:226:PRO:HD2	2.36	0.41
1:A:417:VAL:HG21	1:A:428:PHE:HD2	1.85	0.41
1:A:129:ILE:HD11	1:C:140:ARG:HG2	2.02	0.41
1:B:261:ASN:CG	1:B:295:ASN:HB2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:TYR:CD2	1:C:478:ILE:HD12	2.56	0.41
1:C:272:LEU:HD12	1:C:272:LEU:HA	1.91	0.41
1:A:186:VAL:HA	1:A:190:LEU:HB2	2.02	0.41
1:C:60:GLN:N	1:C:61:PRO:CD	2.84	0.41
1:C:462:ARG:O	1:C:464:ASN:ND2	2.54	0.40
1:D:77:LYS:HE3	1:D:199:ALA:O	2.21	0.40
1:D:136:GLY:O	1:D:481:GLN:OE1	2.38	0.40
1:D:375:VAL:O	1:D:394:LEU:HD13	2.22	0.40
1:A:94:ILE:HD11	1:A:101:ARG:HA	2.02	0.40
1:A:223:HIS:CG	1:A:224:PRO:HD2	2.56	0.40
1:C:285:LEU:HD21	1:C:329:ALA:HA	2.04	0.40
1:D:282:GLY:HA3	1:D:294:ILE:CD1	2.51	0.40
1:C:375:VAL:HG23	1:C:394:LEU:HG	2.03	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	442/489 (90%)	430 (97%)	12 (3%)	0	100	100
1	B	460/489 (94%)	445 (97%)	15 (3%)	0	100	100
1	C	459/489 (94%)	443 (96%)	16 (4%)	0	100	100
1	D	454/489 (93%)	442 (97%)	12 (3%)	0	100	100
All	All	1815/1956 (93%)	1760 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	339/377 (90%)	322 (95%)	17 (5%)	22	30
1	B	350/377 (93%)	334 (95%)	16 (5%)	24	33
1	C	352/377 (93%)	334 (95%)	18 (5%)	21	29
1	D	351/377 (93%)	337 (96%)	14 (4%)	28	39
All	All	1392/1508 (92%)	1327 (95%)	65 (5%)	23	33

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	117	GLU
1	A	164	ARG
1	A	172	LEU
1	A	176	VAL
1	A	209	VAL
1	A	225	VAL
1	A	250	HIS
1	A	296	ARG
1	A	334	VAL
1	A	338	GLN
1	A	342	LEU
1	A	347	ARG
1	A	365	GLN
1	A	367	LEU
1	A	385	GLU
1	A	409	SER
1	B	3	ASP
1	B	8	ASP
1	B	9	LEU
1	B	38	LEU
1	B	125	VAL
1	B	128	ARG
1	B	130	VAL

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Mol	Chain	Res	Type
1	B	153	SER
1	B	239	ARG
1	B	310	ARG
1	B	347	ARG
1	B	378	THR
1	B	391	VAL
1	B	427	ARG
1	B	485	ARG
1	B	488	PRO
1	C	9	LEU
1	C	27	LEU
1	C	28	LYS
1	C	139	SER
1	C	144	SER
1	C	159	LEU
1	C	166	ILE
1	C	225	VAL
1	C	230	THR
1	C	243	ARG
1	C	287	GLN
1	C	340	GLU
1	C	343	LEU
1	C	444	VAL
1	C	445	ASN
1	C	446	ASP
1	C	458	SER
1	C	463	PHE
1	D	9	LEU
1	D	101	ARG
1	D	102	LEU
1	D	125	VAL
1	D	126	HIS
1	D	251	LEU
1	D	252	LYS
1	D	286	HIS
1	D	287	GLN
1	D	296	ARG
1	D	394	LEU
1	D	422	LEU
1	D	460	LEU
1	D	466	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	A	407	ASN
1	B	43	GLN
1	C	261	ASN
1	C	295	ASN
1	C	338	GLN
1	C	365	GLN
1	C	438	HIS
1	C	445	ASN
1	D	43	GLN
1	D	240	ASN
1	D	253	HIS
1	D	287	GLN
1	D	351	GLN
1	D	431	GLN
1	D	482	HIS

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 ⓘ

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	450/489 (92%)	1.33	108 (24%) 2 1	39, 79, 120, 150	0
1	B	466/489 (95%)	0.65	51 (10%) 10 8	32, 54, 91, 162	0
1	C	465/489 (95%)	0.52	47 (10%) 12 9	32, 49, 90, 150	0
1	D	460/489 (94%)	0.32	40 (8%) 16 13	27, 45, 92, 153	0
All	All	1841/1956 (94%)	0.70	246 (13%) 7 5	27, 55, 108, 162	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	288	GLY	7.9
1	C	446	ASP	7.1
1	C	361	GLY	6.9
1	B	290	ILE	6.6
1	C	285	LEU	6.6
1	A	294	ILE	6.3
1	B	442	ILE	6.3
1	C	460	LEU	6.0
1	C	458	SER	5.9
1	C	188	GLY	5.8
1	B	487	TYR	5.7
1	C	286	HIS	5.6
1	D	411	TYR	5.6
1	C	411	TYR	5.4
1	B	292	MET	5.3
1	B	443	PRO	5.3
1	A	381	ILE	5.1
1	D	293	ALA	5.1
1	D	287	GLN	5.0
1	C	459	GLY	5.0
1	D	463	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	412	GLY	4.9
1	A	22	ARG	4.9
1	C	445	ASN	4.8
1	C	294	ILE	4.8
1	A	461	GLY	4.6
1	C	444	VAL	4.6
1	D	462	ARG	4.5
1	C	287	GLN	4.5
1	D	460	LEU	4.5
1	D	459	GLY	4.5
1	A	49	LEU	4.4
1	A	189	GLY	4.4
1	C	461	GLY	4.3
1	B	291	CYS	4.3
1	A	387	PHE	4.3
1	B	459	GLY	4.2
1	C	215	GLU	4.2
1	A	286	HIS	4.1
1	D	361	GLY	4.1
1	B	488	PRO	4.1
1	D	464	ASN	4.1
1	A	4	SER	4.1
1	A	413	LEU	4.1
1	A	348	LEU	4.0
1	D	443	PRO	4.0
1	B	461	GLY	4.0
1	C	462	ARG	4.0
1	A	323	PRO	4.0
1	D	101	ARG	4.0
1	C	246	SER	4.0
1	A	84	ARG	4.0
1	D	126	HIS	3.9
1	A	342	LEU	3.9
1	B	411	TYR	3.9
1	C	259	GLY	3.9
1	B	281	PHE	3.8
1	A	384	ASP	3.8
1	C	214	SER	3.7
1	B	361	GLY	3.7
1	A	251	LEU	3.7
1	B	293	ALA	3.6
1	A	216	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	281	PHE	3.6
1	A	382	ALA	3.6
1	A	409	SER	3.5
1	D	286	HIS	3.5
1	B	126	HIS	3.5
1	A	102	LEU	3.5
1	A	408	ALA	3.5
1	B	460	LEU	3.4
1	B	189	GLY	3.4
1	B	128	ARG	3.4
1	A	319	ARG	3.4
1	C	387	PHE	3.3
1	A	346	ILE	3.3
1	A	126	HIS	3.3
1	A	188	GLY	3.3
1	B	412	GLY	3.3
1	D	461	GLY	3.3
1	A	212	PRO	3.3
1	A	357	LEU	3.2
1	C	245	ALA	3.2
1	D	251	LEU	3.2
1	A	56	ALA	3.2
1	B	463	PHE	3.2
1	D	3	ASP	3.2
1	A	27	LEU	3.2
1	A	285	LEU	3.2
1	C	156	ASN	3.2
1	A	213	GLY	3.2
1	A	389	PRO	3.2
1	B	410	GLU	3.2
1	A	377	ALA	3.1
1	B	462	ARG	3.1
1	A	190	LEU	3.1
1	A	260	GLY	3.1
1	D	296	ARG	3.1
1	A	376	THR	3.1
1	D	216	ILE	3.1
1	D	413	LEU	3.1
1	C	410	GLU	3.0
1	A	463	PHE	3.0
1	A	312	VAL	3.0
1	B	387	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	157	PHE	2.9
1	B	409	SER	2.9
1	C	213	GLY	2.9
1	B	156	ASN	2.9
1	D	420	ARG	2.9
1	D	131	GLU	2.9
1	A	373	GLY	2.9
1	A	99	SER	2.8
1	D	156	ASN	2.8
1	A	349	ALA	2.8
1	A	155	TRP	2.8
1	C	243	ARG	2.8
1	B	188	GLY	2.8
1	C	98	GLY	2.8
1	D	260	GLY	2.8
1	A	153	SER	2.8
1	A	156	ASN	2.8
1	A	93	ILE	2.8
1	C	26	ARG	2.8
1	A	252	LYS	2.7
1	A	383	ARG	2.7
1	A	284	PHE	2.7
1	C	248	GLY	2.7
1	B	99	SER	2.7
1	A	18	TRP	2.7
1	A	309	ALA	2.7
1	B	5	ARG	2.7
1	B	362	VAL	2.7
1	A	214	SER	2.6
1	D	214	SER	2.6
1	D	136	GLY	2.6
1	A	433	ARG	2.6
1	A	345	LYS	2.6
1	B	103	LYS	2.6
1	A	183	ASP	2.6
1	A	353	GLY	2.6
1	A	272	LEU	2.6
1	C	463	PHE	2.6
1	A	117	GLU	2.6
1	A	407	ASN	2.6
1	A	351	GLN	2.6
1	A	28	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	378	THR	2.5
1	B	95	ARG	2.5
1	C	412	GLY	2.5
1	B	294	ILE	2.5
1	A	237	VAL	2.5
1	A	253	HIS	2.5
1	A	41	ILE	2.5
1	A	257	GLU	2.5
1	B	94	ILE	2.5
1	A	209	VAL	2.5
1	B	84	ARG	2.5
1	D	189	GLY	2.5
1	A	43	GLN	2.5
1	A	95	ARG	2.5
1	A	32	PRO	2.4
1	C	131	GLU	2.4
1	B	441	ASP	2.4
1	C	442	ILE	2.4
1	B	413	LEU	2.4
1	A	364	GLY	2.4
1	D	285	LEU	2.4
1	A	157	PHE	2.4
1	A	307	PHE	2.4
1	A	337	ARG	2.4
1	A	23	ALA	2.4
1	B	246	SER	2.4
1	A	98	GLY	2.4
1	A	259	GLY	2.4
1	A	234	SER	2.4
1	D	436	MET	2.4
1	B	245	ALA	2.4
1	D	249	ALA	2.4
1	A	217	GLY	2.3
1	C	189	GLY	2.3
1	C	260	GLY	2.3
1	A	372	PHE	2.3
1	B	214	SER	2.3
1	B	299	VAL	2.3
1	C	261	ASN	2.3
1	C	247	GLY	2.3
1	D	465	GLY	2.3
1	A	318	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	84	ARG	2.3
1	C	413	LEU	2.3
1	A	367	LEU	2.2
1	A	390	LEU	2.2
1	D	4	SER	2.2
1	A	436	MET	2.2
1	A	154	PRO	2.2
1	A	356	PRO	2.2
1	A	371	VAL	2.2
1	A	338	GLN	2.2
1	A	37	LEU	2.2
1	A	182	SER	2.2
1	D	234	SER	2.2
1	B	212	PRO	2.2
1	A	29	VAL	2.2
1	A	39	LEU	2.2
1	A	393	LEU	2.2
1	B	427	ARG	2.2
1	B	483	ALA	2.1
1	A	343	LEU	2.1
1	D	188	GLY	2.1
1	A	297	ILE	2.1
1	C	386	ILE	2.1
1	A	25	ARG	2.1
1	A	101	ARG	2.1
1	C	80	GLU	2.1
1	C	28	LYS	2.1
1	A	100	THR	2.1
1	B	102	LEU	2.1
1	B	433	ARG	2.1
1	C	319	ARG	2.1
1	C	384	ASP	2.1
1	D	409	SER	2.1
1	D	281	PHE	2.1
1	B	155	TRP	2.1
1	A	303	LEU	2.1
1	B	131	GLU	2.1
1	D	410	GLU	2.1
1	B	157	PHE	2.1
1	A	247	GLY	2.1
1	B	247	GLY	2.1
1	C	350	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	17	GLU	2.1
1	B	340	GLU	2.1
1	A	302	SER	2.1
1	C	443	PRO	2.1
1	A	20	HIS	2.1
1	B	284	PHE	2.0
1	A	462	ARG	2.0
1	D	477	TRP	2.0
1	C	252	LYS	2.0
1	A	362	VAL	2.0
1	A	159	LEU	2.0
1	A	306	ALA	2.0
1	B	367	LEU	2.0
1	A	316	LYS	2.0
1	D	294	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.