



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 12:13 PM JST

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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

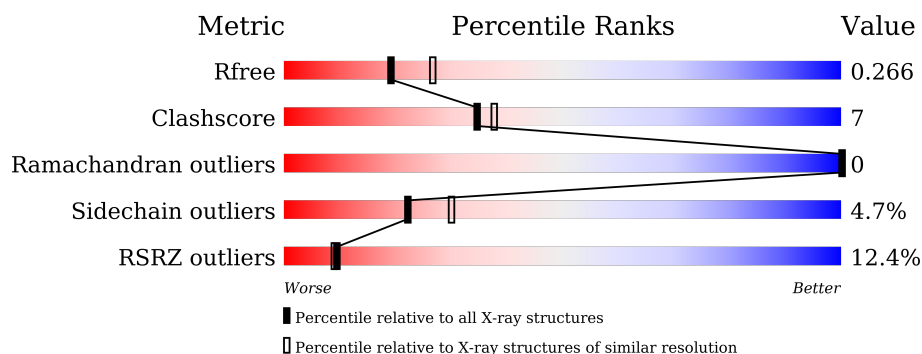
1 Overall quality at a glance

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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (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	<div> <div>20%</div> <div>69%</div> <div>21%</div> <div>• 8%</div> </div>
1	B	489	<div> <div>9%</div> <div>81%</div> <div>13%</div> <div>5%</div> </div>
1	C	489	<div> <div>9%</div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div>
1	D	489	<div> <div>8%</div> <div>83%</div> <div>10%</div> <div>• 6%</div> </div>

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

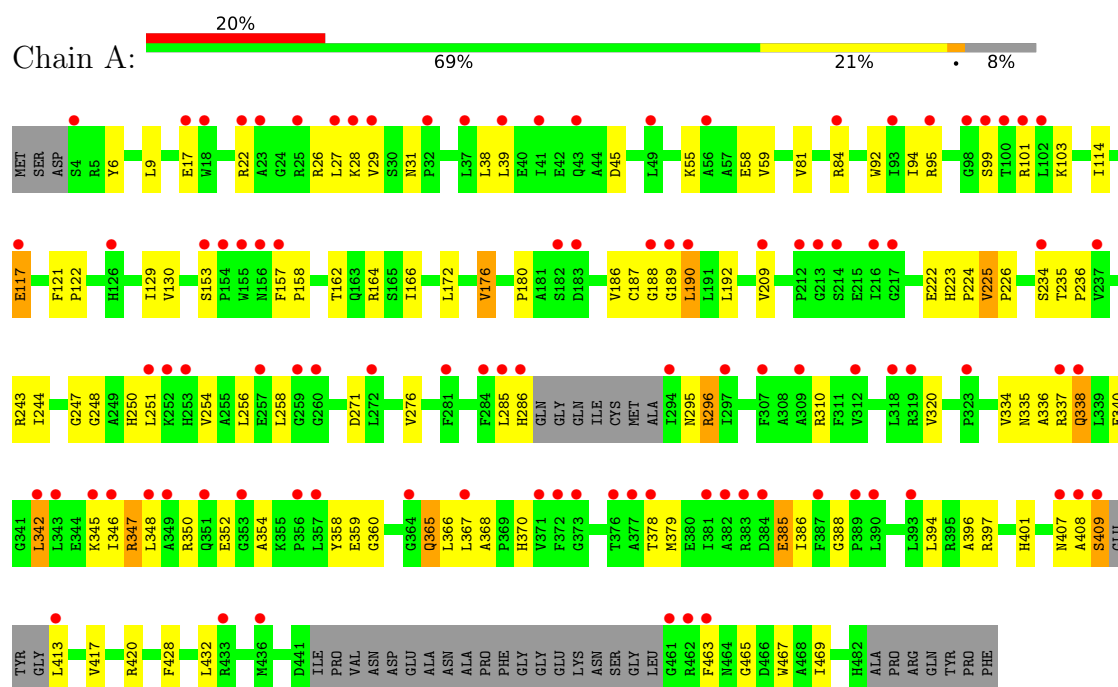
- Molecule 2 is water.

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		


3 Residue-property plots [i](#)

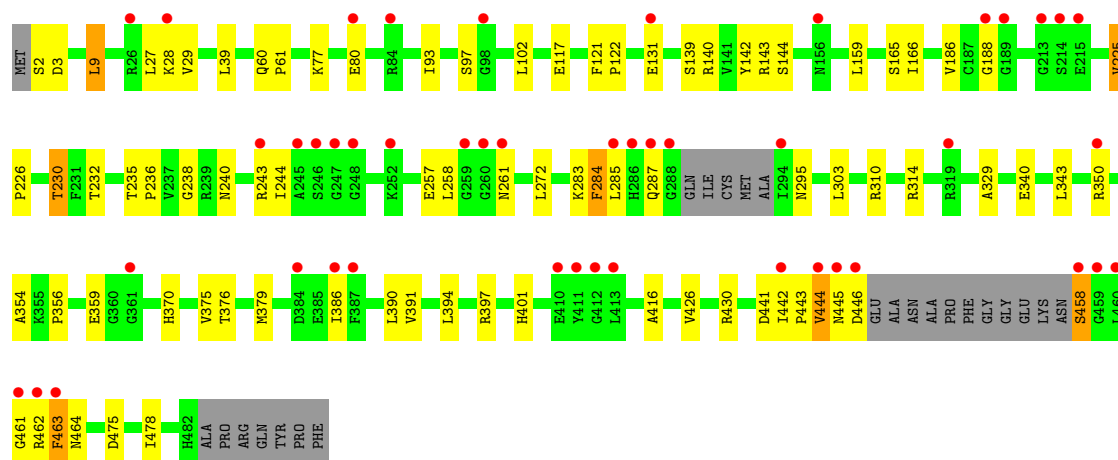
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aldehyde dehydrogenase




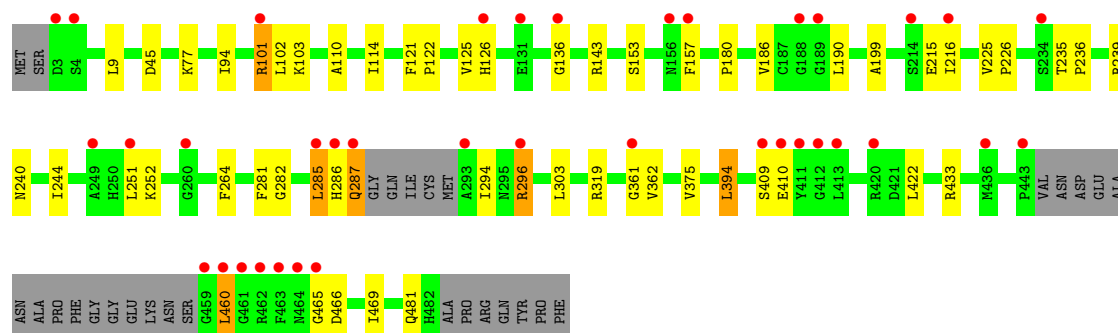
● Molecule 1: Aldehyde dehydrogenase

Chain C:  9% 78% 16% 5%



● Molecule 1: Aldehyde dehydrogenase

Chain D:  8% 83% 10% 6%



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	4396 reflections (5.21%)	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 [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	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%)	20	28
1	B	350/377 (93%)	334 (95%)	16 (5%)	23	31
1	C	352/377 (93%)	334 (95%)	18 (5%)	20	27
1	D	351/377 (93%)	337 (96%)	14 (4%)	27	36
All	All	1392/1508 (92%)	1327 (95%)	65 (5%)	22	30

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%)	1.25	100 (22%) 3 3	39, 79, 120, 150	0
1	B	466/489 (95%)	0.56	46 (9%) 14 14	32, 54, 91, 162	0
1	C	465/489 (95%)	0.43	46 (9%) 14 14	32, 49, 90, 150	0
1	D	460/489 (94%)	0.22	37 (8%) 20 19	27, 45, 92, 153	0
All	All	1841/1956 (94%)	0.61	229 (12%) 9 9	27, 55, 108, 162	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	288	GLY	7.9
1	C	446	ASP	7.2
1	C	361	GLY	6.9
1	B	290	ILE	6.6
1	C	285	LEU	6.5
1	A	294	ILE	6.3
1	B	442	ILE	6.2
1	C	460	LEU	6.0
1	C	458	SER	5.9
1	C	188	GLY	5.7
1	B	487	TYR	5.6
1	C	286	HIS	5.6
1	D	411	TYR	5.5
1	C	411	TYR	5.3
1	B	443	PRO	5.3
1	B	292	MET	5.3
1	D	293	ALA	5.0
1	A	22	ARG	5.0
1	A	381	ILE	5.0
1	D	287	GLN	5.0
1	C	459	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	412	GLY	4.9
1	C	445	ASN	4.8
1	D	463	PHE	4.8
1	C	294	ILE	4.7
1	D	462	ARG	4.7
1	A	461	GLY	4.6
1	C	444	VAL	4.5
1	C	287	GLN	4.5
1	D	460	LEU	4.4
1	D	459	GLY	4.4
1	A	189	GLY	4.3
1	A	49	LEU	4.3
1	C	461	GLY	4.3
1	C	215	GLU	4.3
1	B	291	CYS	4.2
1	B	459	GLY	4.2
1	A	387	PHE	4.1
1	C	462	ARG	4.1
1	A	286	HIS	4.1
1	D	361	GLY	4.1
1	D	464	ASN	4.1
1	B	488	PRO	4.1
1	D	101	ARG	4.1
1	A	4	SER	4.0
1	A	84	ARG	4.0
1	D	443	PRO	4.0
1	B	461	GLY	4.0
1	A	413	LEU	4.0
1	A	348	LEU	3.9
1	A	323	PRO	3.9
1	C	246	SER	3.9
1	D	126	HIS	3.9
1	A	342	LEU	3.8
1	C	259	GLY	3.8
1	A	384	ASP	3.8
1	B	411	TYR	3.8
1	C	214	SER	3.7
1	B	281	PHE	3.7
1	B	361	GLY	3.6
1	A	251	LEU	3.6
1	B	293	ALA	3.6
1	A	216	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	382	ALA	3.5
1	B	128	ARG	3.5
1	A	409	SER	3.5
1	D	286	HIS	3.5
1	A	281	PHE	3.5
1	B	126	HIS	3.5
1	A	319	ARG	3.4
1	A	408	ALA	3.4
1	A	102	LEU	3.4
1	B	189	GLY	3.4
1	B	460	LEU	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	346	ILE	3.2
1	A	212	PRO	3.2
1	C	387	PHE	3.2
1	B	410	GLU	3.2
1	D	3	ASP	3.2
1	B	462	ARG	3.2
1	C	245	ALA	3.2
1	A	357	LEU	3.1
1	C	156	ASN	3.1
1	A	56	ALA	3.1
1	D	296	ARG	3.1
1	A	213	GLY	3.1
1	D	251	LEU	3.1
1	A	389	PRO	3.1
1	A	27	LEU	3.1
1	A	285	LEU	3.1
1	A	377	ALA	3.1
1	B	463	PHE	3.1
1	C	410	GLU	3.1
1	A	260	GLY	3.0
1	A	190	LEU	3.0
1	A	376	THR	3.0
1	D	216	ILE	3.0
1	D	413	LEU	3.0
1	A	312	VAL	2.9
1	D	420	ARG	2.9
1	A	463	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	131	GLU	2.9
1	B	387	PHE	2.9
1	B	409	SER	2.9
1	C	213	GLY	2.9
1	C	243	ARG	2.8
1	B	156	ASN	2.8
1	D	157	PHE	2.8
1	C	26	ARG	2.8
1	A	373	GLY	2.8
1	D	156	ASN	2.8
1	A	99	SER	2.8
1	A	349	ALA	2.8
1	A	156	ASN	2.7
1	A	383	ARG	2.7
1	B	188	GLY	2.7
1	C	98	GLY	2.7
1	D	260	GLY	2.7
1	A	153	SER	2.7
1	A	252	LYS	2.7
1	B	5	ARG	2.7
1	A	93	ILE	2.7
1	A	155	TRP	2.7
1	A	433	ARG	2.6
1	C	248	GLY	2.6
1	B	99	SER	2.6
1	A	309	ALA	2.6
1	B	362	VAL	2.6
1	A	345	LYS	2.6
1	B	103	LYS	2.6
1	A	183	ASP	2.6
1	A	117	GLU	2.6
1	A	284	PHE	2.6
1	A	214	SER	2.6
1	D	214	SER	2.6
1	D	136	GLY	2.6
1	B	95	ARG	2.6
1	A	18	TRP	2.5
1	A	353	GLY	2.5
1	A	28	LYS	2.5
1	A	257	GLU	2.5
1	A	351	GLN	2.5
1	A	407	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	84	ARG	2.5
1	A	272	LEU	2.5
1	A	95	ARG	2.5
1	C	131	GLU	2.5
1	A	378	THR	2.5
1	C	412	GLY	2.5
1	C	463	PHE	2.5
1	A	253	HIS	2.4
1	A	237	VAL	2.4
1	B	294	ILE	2.4
1	A	337	ARG	2.4
1	B	441	ASP	2.4
1	A	209	VAL	2.4
1	A	41	ILE	2.4
1	A	43	GLN	2.4
1	B	94	ILE	2.4
1	D	189	GLY	2.4
1	A	32	PRO	2.4
1	C	442	ILE	2.4
1	A	364	GLY	2.4
1	B	413	LEU	2.3
1	A	23	ALA	2.3
1	B	246	SER	2.3
1	A	98	GLY	2.3
1	A	259	GLY	2.3
1	D	285	LEU	2.3
1	A	234	SER	2.3
1	A	157	PHE	2.3
1	A	307	PHE	2.3
1	D	436	MET	2.3
1	C	84	ARG	2.3
1	B	245	ALA	2.3
1	D	249	ALA	2.3
1	A	217	GLY	2.3
1	C	189	GLY	2.3
1	C	260	GLY	2.3
1	B	214	SER	2.2
1	C	261	ASN	2.2
1	B	299	VAL	2.2
1	C	247	GLY	2.2
1	D	465	GLY	2.2
1	A	372	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	318	LEU	2.2
1	C	413	LEU	2.2
1	B	427	ARG	2.2
1	D	4	SER	2.2
1	A	367	LEU	2.1
1	A	390	LEU	2.1
1	A	436	MET	2.1
1	A	25	ARG	2.1
1	A	101	ARG	2.1
1	A	154	PRO	2.1
1	A	356	PRO	2.1
1	A	338	GLN	2.1
1	C	80	GLU	2.1
1	A	371	VAL	2.1
1	B	433	ARG	2.1
1	C	319	ARG	2.1
1	A	182	SER	2.1
1	B	212	PRO	2.1
1	D	234	SER	2.1
1	C	28	LYS	2.1
1	A	29	VAL	2.1
1	A	37	LEU	2.1
1	B	131	GLU	2.1
1	D	410	GLU	2.1
1	C	384	ASP	2.1
1	A	39	LEU	2.1
1	A	393	LEU	2.1
1	B	483	ALA	2.1
1	C	350	ARG	2.1
1	D	188	GLY	2.1
1	A	17	GLU	2.1
1	B	340	GLU	2.1
1	A	297	ILE	2.1
1	C	386	ILE	2.1
1	A	343	LEU	2.0
1	A	462	ARG	2.0
1	A	100	THR	2.0
1	D	409	SER	2.0
1	B	102	LEU	2.0
1	C	252	LYS	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 monosaccharides 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.