Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:44 am BST

PDB ID	:	5J83
Title	:	Crystal structure of L-arabinonate dehydratase in apo-form
Authors	:	Rahman, M.M.; Rouvinen, J.; Hakulinen, N.
Deposited on	:	2016-04-07
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

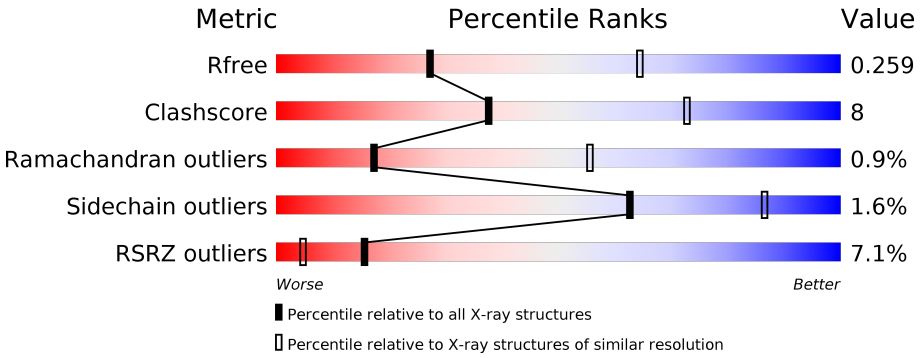
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 <=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	588	9% 76% 21%
1	B	588	5% 80% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8698 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 Dihydroxyacid dehydratase/phosphogluconate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			
1	B	575	Total	C	N	O	S	0	0	0
			4349	2724	766	825	34			

There are 20 discrepancies between the modelled and reference sequences:

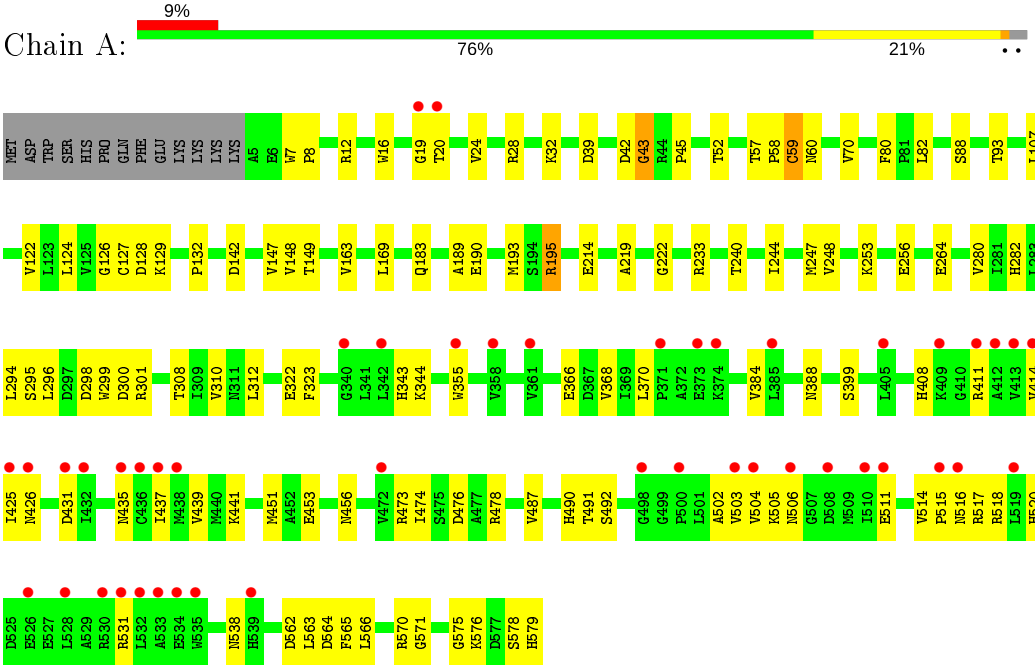
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP I9XDU6
A	-7	ASP	-	expression tag	UNP I9XDU6
A	-6	TRP	-	expression tag	UNP I9XDU6
A	-5	SER	-	expression tag	UNP I9XDU6
A	-4	HIS	-	expression tag	UNP I9XDU6
A	-3	PRO	-	expression tag	UNP I9XDU6
A	-2	GLN	-	expression tag	UNP I9XDU6
A	-1	PHE	-	expression tag	UNP I9XDU6
A	0	GLU	-	expression tag	UNP I9XDU6
A	1	LYS	-	expression tag	UNP I9XDU6
B	-8	MET	-	initiating methionine	UNP I9XDU6
B	-7	ASP	-	expression tag	UNP I9XDU6
B	-6	TRP	-	expression tag	UNP I9XDU6
B	-5	SER	-	expression tag	UNP I9XDU6
B	-4	HIS	-	expression tag	UNP I9XDU6
B	-3	PRO	-	expression tag	UNP I9XDU6
B	-2	GLN	-	expression tag	UNP I9XDU6
B	-1	PHE	-	expression tag	UNP I9XDU6
B	0	GLU	-	expression tag	UNP I9XDU6
B	1	LYS	-	expression tag	UNP I9XDU6

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

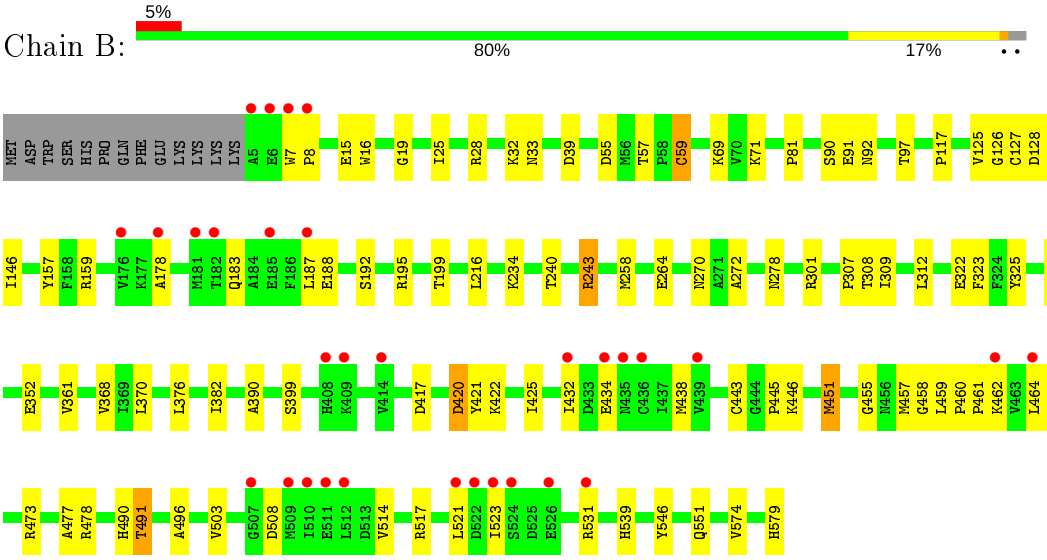
- Molecule 1: Dihydroxyacid dehydratase/phosphogluconate dehydratase

Chain A:



- Molecule 1: Dihydroxyacid dehydratase/phosphogluconate dehydratase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	161.13Å 161.13Å 114.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.91 – 3.00 47.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.91-3.00) 99.6 (47.91-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, R_{free}	0.208 , 0.259 0.208 , 0.259	Depositor DCC
R_{free} test set	1689 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 81.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8698	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: KCX

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	0.24	0/4422	0.43	0/5988
1	B	0.24	0/4422	0.43	0/5988
All	All	0.24	0/8844	0.43	0/11976

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4349	0	4320	82	1
1	B	4349	0	4320	61	1
All	All	8698	0	8640	134	1

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 8.

All (134) 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:A:60:ASN:ND2	1:A:127:CYS:SG	2.58	0.76
1:A:19:GLY:O	1:A:28:ARG:NH2	2.24	0.70
1:A:129:KCX:OQ1	1:A:478:ARG:NH1	2.27	0.68
1:B:19:GLY:O	1:B:28:ARG:NH2	2.28	0.67
1:B:461:PRO:HB2	1:B:465:LYS:HE2	1.75	0.66
1:B:434:GLU:HB3	1:B:468:ILE:HD13	1.77	0.66
1:A:163:VAL:HG11	1:A:193:MET:HG2	1.80	0.64
1:A:514:VAL:O	1:A:517:ARG:NH1	2.29	0.63
1:B:432:ILE:HG13	1:B:462:LYS:HD2	1.80	0.63
1:A:473:ARG:HB2	1:A:487:VAL:HG22	1.81	0.62
1:A:253:LYS:HE2	1:A:256:GLU:HG3	1.81	0.62
1:A:60:ASN:HD21	1:A:127:CYS:H	1.47	0.62
1:A:562:ASP:OD1	1:A:563:LEU:N	2.32	0.62
1:B:59:CYS:HB2	1:B:199:THR:HG22	1.83	0.61
1:A:42:ASP:OD1	1:A:43:GLY:N	2.34	0.60
1:B:334:LYS:NZ	1:B:361:VAL:O	2.26	0.60
1:A:264:GLU:OE1	1:A:343:HIS:NE2	2.33	0.60
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.84	0.59
1:A:16:TRP:CD2	1:A:117:PRO:HB3	2.37	0.59
1:A:129:KCX:OQ2	1:A:282:HIS:NE2	2.36	0.59
1:A:511:GLU:HB2	1:A:520:HIS:HB3	1.84	0.58
1:B:129:KCX:OQ2	1:B:278:ASN:ND2	2.35	0.58
1:B:69:LYS:HE3	1:B:234:LYS:HB3	1.86	0.56
1:A:441:LYS:NZ	1:A:502:ALA:O	2.38	0.56
1:A:114:ARG:NH1	1:A:571:GLY:O	2.38	0.56
1:A:264:GLU:OE2	1:A:301:ARG:NH2	2.35	0.56
1:B:457:MET:O	1:B:473:ARG:NH1	2.32	0.56
1:A:70:VAL:HG11	1:A:122:VAL:HG11	1.87	0.55
1:A:308:THR:HG21	1:A:399:SER:HB3	1.89	0.55
1:B:508:ASP:OD2	1:B:531:ARG:NH2	2.40	0.55
1:A:60:ASN:HD21	1:A:127:CYS:N	2.04	0.55
1:B:438:MET:HE1	1:B:459:LEU:HA	1.89	0.55
1:B:443:CYS:HB3	1:B:477:ALA:HB2	1.90	0.54
1:A:284:LEU:HD23	1:A:294:LEU:HD23	1.90	0.54
1:A:411:ARG:NH1	1:A:431:ASP:O	2.40	0.54
1:A:148:VAL:HG22	1:A:240:THR:HG21	1.90	0.53
1:A:408:HIS:HD2	1:A:437:ILE:HD11	1.73	0.53
1:B:57:THR:HG23	1:B:90:SER:HB2	1.90	0.53
1:B:417:ASP:OD1	1:B:420:ASP:N	2.40	0.53
1:B:178:ALA:HB2	1:B:464:LEU:HB3	1.90	0.53
1:A:566:LEU:O	1:A:570:ARG:NH2	2.41	0.53
1:B:461:PRO:O	1:B:465:LYS:N	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:NH2	1:A:114:ARG:O	2.37	0.52
1:B:128:ASP:OD2	1:B:129:KCX:HD2	2.09	0.52
1:A:456:ASN:O	1:A:456:ASN:ND2	2.42	0.52
1:A:190:GLU:HG3	1:B:25:ILE:HG23	1.92	0.52
1:B:312:LEU:HD11	1:B:323:PHE:HB2	1.92	0.52
1:A:59:CYS:C	1:A:60:ASN:HD22	2.14	0.52
1:A:107:LEU:HD21	1:B:546:TYR:HB2	1.92	0.52
1:A:344:LYS:HB3	1:A:355:TRP:HB2	1.92	0.51
1:A:132:PRO:HA	1:A:286:ILE:HD11	1.92	0.51
1:A:149:THR:O	1:A:233:ARG:NH1	2.43	0.51
1:A:564:ASP:OD1	1:A:565:PHE:N	2.44	0.51
1:A:7:TRP:CD2	1:A:8:PRO:HA	2.46	0.51
1:A:128:ASP:OD1	1:A:128:ASP:N	2.41	0.51
1:A:439:VAL:HG21	1:A:504:VAL:HG11	1.92	0.50
1:A:295:SER:OG	1:A:298:ASP:OD2	2.23	0.50
1:B:514:VAL:O	1:B:517:ARG:NH1	2.33	0.50
1:A:20:THR:HG22	1:B:187:LEU:HD11	1.93	0.50
1:B:216:LEU:HD22	1:B:258:MET:HG2	1.94	0.50
1:A:388:ASN:ND2	1:A:521:LEU:O	2.44	0.49
1:B:159:ARG:NH2	1:B:188:GLU:OE1	2.39	0.49
1:B:264:GLU:OE2	1:B:301:ARG:NH2	2.40	0.48
1:B:15:GLU:HG3	1:B:574:VAL:HG11	1.94	0.48
1:B:71:LYS:HG2	1:B:81:PRO:HB2	1.95	0.48
1:A:563:LEU:HB2	1:A:566:LEU:HD12	1.96	0.48
1:A:408:HIS:CD2	1:A:437:ILE:HD11	2.48	0.48
1:B:7:TRP:CD2	1:B:8:PRO:HA	2.49	0.48
1:B:432:ILE:HD12	1:B:460:PRO:HG3	1.96	0.47
1:A:366:GLU:O	1:A:370:LEU:HD23	2.14	0.47
1:A:57:THR:HG21	1:A:88:SER:HB3	1.96	0.47
1:A:425:ILE:HG23	1:A:426:ASN:OD1	2.14	0.47
1:A:490:HIS:O	1:A:492:SER:N	2.48	0.47
1:A:124:LEU:HD23	1:A:148:VAL:HB	1.96	0.47
1:A:414:VAL:HA	1:A:439:VAL:HG13	1.97	0.47
1:B:421:TYR:OH	1:B:458:GLY:N	2.49	0.46
1:A:453:GLU:OE1	1:B:579:HIS:NE2	2.40	0.46
1:A:45:PRO:HB3	1:A:248:VAL:HG11	1.96	0.46
1:B:125:VAL:HG21	1:B:131:THR:HG23	1.98	0.46
1:B:421:TYR:CE1	1:B:425:ILE:HG13	2.51	0.46
1:A:244:ILE:HA	1:A:247:MET:HB2	1.98	0.46
1:A:214:GLU:OE2	1:A:222:GLY:N	2.36	0.46
1:A:516:ASN:O	1:A:518:ARG:NE	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LEU:O	1:B:523:ILE:N	2.49	0.45
1:A:576:LYS:HA	1:A:576:LYS:HD3	1.74	0.45
1:A:253:LYS:HB2	1:A:253:LYS:HE3	1.81	0.45
1:A:578:SER:O	1:A:579:HIS:ND1	2.49	0.45
1:B:127:CYS:O	1:B:130:THR:OG1	2.31	0.45
1:B:308:THR:OG1	1:B:376:LEU:HB2	2.17	0.45
1:B:272:ALA:HA	1:B:307:PRO:O	2.17	0.45
1:B:157:TYR:O	1:B:192:SER:OG	2.20	0.45
1:B:243:ARG:NE	1:B:349:VAL:O	2.39	0.45
1:A:322:GLU:HB3	1:A:368:VAL:HG21	1.99	0.44
1:A:441:LYS:HD2	1:A:502:ALA:HA	1.99	0.44
1:A:190:GLU:OE2	1:B:28:ARG:HD2	2.17	0.44
1:B:503:VAL:HB	1:B:531:ARG:HB3	2.00	0.44
1:B:91:GLU:OE2	1:B:97:THR:OG1	2.34	0.44
1:A:58:PRO:HB2	1:B:33:ASN:OD1	2.18	0.44
1:A:190:GLU:OE2	1:B:32:LYS:NZ	2.32	0.44
1:A:312:LEU:HD11	1:A:323:PHE:HB2	1.99	0.44
1:A:52:THR:OG1	1:A:60:ASN:OD1	2.31	0.44
1:B:348:THR:OG1	1:B:352:GLU:O	2.31	0.44
1:B:308:THR:HG21	1:B:399:SER:HB3	2.00	0.44
1:A:189:ALA:O	1:A:193:MET:HG3	2.18	0.44
1:A:93:THR:O	1:B:16:TRP:NE1	2.48	0.43
1:B:16:TRP:CD2	1:B:117:PRO:HB3	2.53	0.43
1:A:451:MET:HG2	1:A:478:ARG:HG3	2.01	0.43
1:A:439:VAL:HA	1:A:474:ILE:O	2.19	0.43
1:A:82:LEU:HD22	1:B:55:ASP:HB3	1.99	0.42
1:A:476:ASP:OD1	1:A:476:ASP:N	2.40	0.42
1:B:446:LYS:HE3	1:B:551:GLN:O	2.19	0.42
1:A:16:TRP:CG	1:A:117:PRO:HB3	2.54	0.42
1:B:523:ILE:HG13	1:B:531:ARG:HH12	1.84	0.42
1:B:90:SER:OG	1:B:92:ASN:OD1	2.34	0.42
1:A:280:VAL:HA	1:A:299:TRP:CZ2	2.55	0.42
1:B:496:ALA:HB1	1:B:539:HIS:CE1	2.55	0.42
1:A:505:LYS:HD2	1:A:506:ASN:H	1.84	0.42
1:B:455:GLY:N	1:B:478:ARG:O	2.49	0.41
1:A:411:ARG:O	1:A:437:ILE:N	2.42	0.41
1:B:7:TRP:CG	1:B:8:PRO:HA	2.55	0.41
1:A:147:VAL:HB	1:A:219:ALA:HB2	2.01	0.41
1:A:28:ARG:HG2	1:A:32:LYS:HE3	2.02	0.41
1:B:270:ASN:HD22	1:B:382:ILE:HD13	1.85	0.41
1:B:390:ALA:HB2	1:B:491:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:O	1:B:370:LEU:N	2.48	0.41
1:B:451:MET:O	1:B:478:ARG:NH2	2.40	0.41
1:A:20:THR:O	1:A:24:VAL:HB	2.21	0.41
1:A:408:HIS:NE2	1:A:435:ASN:O	2.46	0.41
1:B:322:GLU:HB3	1:B:368:VAL:HG21	2.03	0.41
1:A:514:VAL:HB	1:A:515:PRO:HD3	2.03	0.41
1:A:300:ASP:OD1	1:A:384:VAL:N	2.42	0.40
1:A:503:VAL:HB	1:A:531:ARG:HD3	2.04	0.40
1:A:296:LEU:O	1:A:384:VAL:HG21	2.22	0.40
1:B:146:ILE:HD13	1:B:240:THR:HG23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ARG:NH2	1:B:325:TYR:OH[4_455]	2.11	0.09

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	572/588 (97%)	529 (92%)	38 (7%)	5 (1%)	17	55
1	B	572/588 (97%)	539 (94%)	28 (5%)	5 (1%)	17	55
All	All	1144/1176 (97%)	1068 (93%)	66 (6%)	10 (1%)	17	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	491	THR
1	A	491	THR
1	B	126	GLY

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Mol	Chain	Res	Type
1	A	126	GLY
1	B	422	LYS
1	B	451	MET
1	A	422	LYS
1	A	575	GLY
1	B	445	PRO
1	A	43	GLY

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	460/473 (97%)	452 (98%)	8 (2%)	60	85
1	B	460/473 (97%)	453 (98%)	7 (2%)	65	87
All	All	920/946 (97%)	905 (98%)	15 (2%)	62	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	59	CYS
1	A	80	PHE
1	A	142	ASP
1	A	169	LEU
1	A	183	GLN
1	A	195	ARG
1	A	538	ASN
1	B	39	ASP
1	B	59	CYS
1	B	183	GLN
1	B	195	ARG
1	B	243	ARG
1	B	420	ASP
1	B	490	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	223	ASN
1	A	538	ASN
1	A	572	ASN
1	B	270	ASN
1	B	278	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	A	129	1	7,11,12	0.72	0	4,12,14	1.28	1 (25%)
1	KCX	B	129	1	7,11,12	0.82	0	4,12,14	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	129	1	-	3/7/10/12	-
1	KCX	B	129	1	-	2/7/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	KCX	CE-NZ-CX	-2.41	118.87	122.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	129	KCX	N-CA-CB-CG
1	A	129	KCX	C-CA-CB-CG
1	B	129	KCX	C-CA-CB-CG
1	A	129	KCX	CA-CB-CG-CD
1	B	129	KCX	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	129	KCX	2	0
1	B	129	KCX	2	0

5.5 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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	574/588 (97%)	0.38	50 (8%)	10	3	34, 68, 103, 122	0
1	B	574/588 (97%)	0.06	32 (5%)	24	8	21, 56, 98, 118	0
All	All	1148/1176 (97%)	0.22	82 (7%)	16	5	21, 63, 100, 122	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	ASP	4.7
1	B	526	GLU	4.2
1	A	528	LEU	4.0
1	B	187	LEU	3.9
1	A	503	VAL	3.9
1	B	436	CYS	3.9
1	B	185	GLU	3.7
1	B	409	LYS	3.7
1	B	432	ILE	3.6
1	B	507	GLY	3.5
1	A	373	GLU	3.5
1	B	512	LEU	3.5
1	A	374	LYS	3.4
1	A	340	GLY	3.4
1	B	509	MET	3.4
1	A	19	GLY	3.3
1	A	371	PRO	3.3
1	A	522	ASP	3.3
1	B	435	ASN	3.3
1	B	414	VAL	3.2
1	B	523	ILE	3.1
1	A	524	SER	3.1
1	A	533	ALA	3.0
1	A	532	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	535	TRP	3.0
1	A	531	ARG	3.0
1	A	526	GLU	3.0
1	A	437	ILE	3.0
1	A	426	ASN	2.9
1	A	515	PRO	2.9
1	B	181	MET	2.9
1	A	412	ALA	2.8
1	B	5	ALA	2.8
1	B	176	VAL	2.7
1	B	511	GLU	2.7
1	A	414	VAL	2.7
1	A	405	LEU	2.6
1	B	8	PRO	2.6
1	B	466	LYS	2.6
1	A	436	CYS	2.6
1	A	539	HIS	2.6
1	A	530	ARG	2.6
1	A	413	VAL	2.6
1	A	504	VAL	2.6
1	A	432	ILE	2.5
1	B	510	ILE	2.5
1	A	409	LYS	2.5
1	A	431	ASP	2.5
1	B	178	ALA	2.5
1	B	7	TRP	2.4
1	B	462	LYS	2.4
1	B	521	LEU	2.4
1	A	361	VAL	2.4
1	A	355	TRP	2.4
1	B	6	GLU	2.4
1	A	472	VAL	2.4
1	A	425	ILE	2.4
1	A	438	MET	2.4
1	B	182	THR	2.4
1	B	464	LEU	2.3
1	B	439	VAL	2.3
1	A	385	LEU	2.3
1	A	516	ASN	2.3
1	A	424	LYS	2.3
1	A	20	THR	2.3
1	A	358	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	531	ARG	2.3
1	A	523	ILE	2.2
1	A	511	GLU	2.2
1	A	508	ASP	2.2
1	A	435	ASN	2.2
1	A	498	GLY	2.2
1	A	510	ILE	2.1
1	A	506	ASN	2.1
1	A	411	ARG	2.1
1	A	342	LEU	2.1
1	B	524	SER	2.1
1	A	519	LEU	2.1
1	B	434	GLU	2.0
1	A	500	PRO	2.0
1	A	534	GLU	2.0
1	B	408	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	A	129	12/13	0.90	0.30	50,61,85,88	0
1	KCX	B	129	12/13	0.90	0.25	48,66,76,100	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.