



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:55 PM UTC

PDB ID : 8IVJ / pdb_00008ivj
Title : Candida boidinii Formate Dehydrogenase V120T Mutant
Authors : Gul, M.; Yuksel, B.; Bulut, H.; DeMirci, H.
Deposited on : 2023-03-28
Resolution : 1.90 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

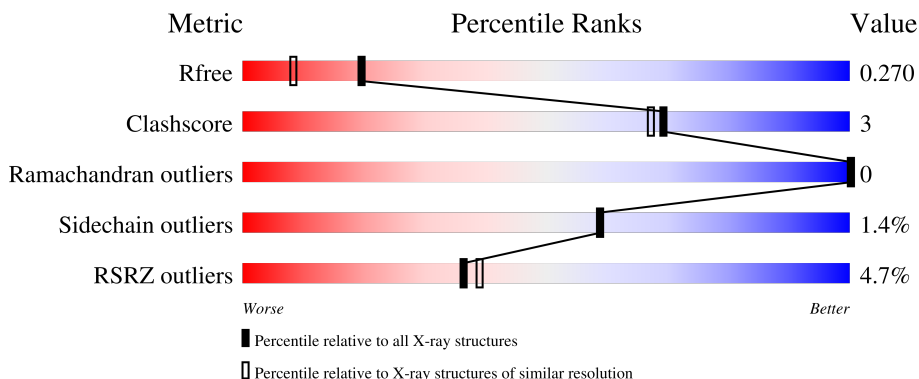
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	364	2% 90% 7%
1	B	364	6% 88% 9%
1	C	364	7% 88% 9%
1	D	364	3% 89% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23734 atoms, of which 11104 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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	356	Total	C	H	N	O	S	0	4	0
			5623	1791	2814	482	529	7			
1	B	353	Total	C	H	N	O	S	0	1	0
			5509	1759	2746	473	524	7			
1	C	354	Total	C	H	N	O	S	0	4	0
			5545	1780	2748	478	532	7			
1	D	356	Total	C	H	N	O	S	0	3	0
			5598	1785	2796	480	530	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	THR	VAL	engineered mutation	UNP A0A0A1EQY0
B	120	THR	VAL	engineered mutation	UNP A0A0A1EQY0
C	120	THR	VAL	engineered mutation	UNP A0A0A1EQY0
D	120	THR	VAL	engineered mutation	UNP A0A0A1EQY0

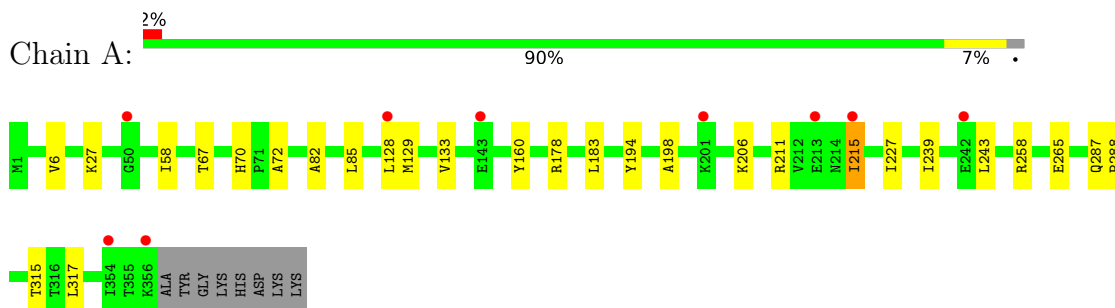
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	414	Total	O	0	0
			414	414		
2	B	308	Total	O	0	0
			308	308		
2	C	352	Total	O	0	0
			352	352		
2	D	385	Total	O	0	0
			385	385		

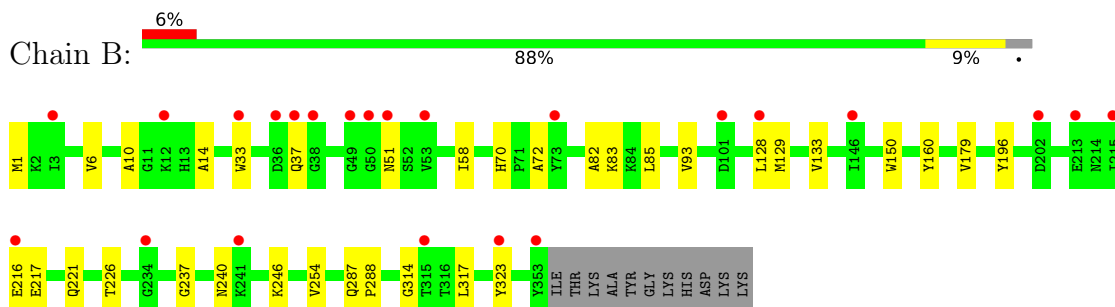
3 Residue-property plots

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.

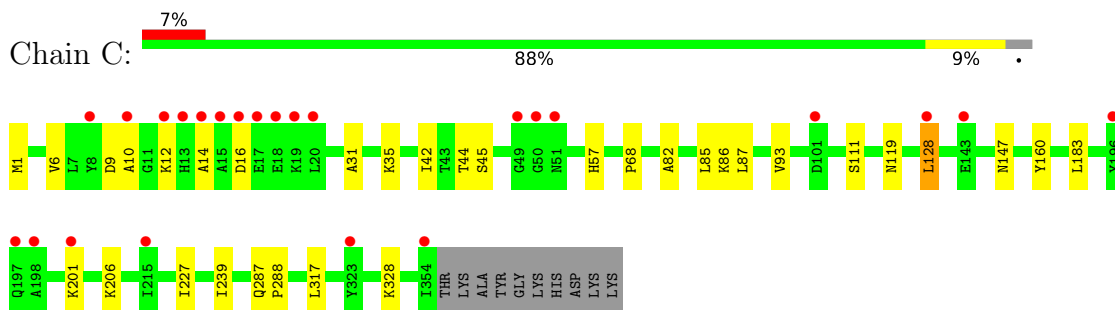
- Molecule 1: Formate dehydrogenase



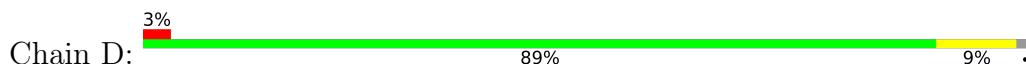
- Molecule 1: Formate dehydrogenase

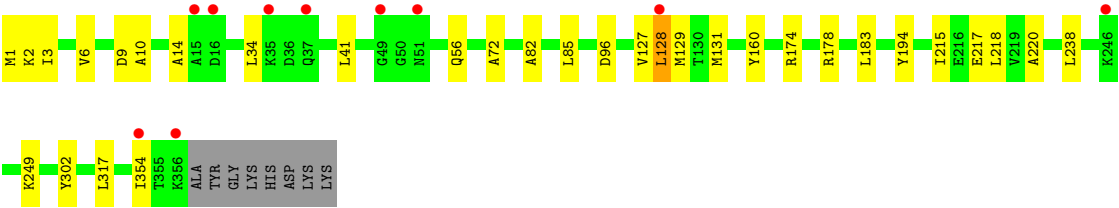


- Molecule 1: Formate dehydrogenase



- Molecule 1: Formate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.66Å 68.61Å 109.43Å 77.96° 89.63° 81.40°	Depositor
Resolution (Å)	24.30 – 1.90 24.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	80.8 (24.30-1.90) 80.8 (24.30-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.247 , 0.271 0.247 , 0.270	Depositor DCC
R_{free} test set	2000 reflections (1.68%)	wwPDB-VP
Wilson B-factor (Å ²)	8.2	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	23734	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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	0.12	0/2872	0.31	0/3894
1	B	0.10	0/2820	0.29	0/3826
1	C	0.15	0/2855	0.32	0/3874
1	D	0.12	0/2862	0.31	0/3881
All	All	0.12	0/11409	0.31	0/15475

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	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258[A]	ARG	Sidechain
1	A	258[B]	ARG	Sidechain

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	2809	2814	2828	17	0
1	B	2763	2746	2761	22	2
1	C	2797	2748	2781	20	3
1	D	2802	2796	2812	24	0
2	A	414	0	0	2	4
2	B	308	0	0	9	1
2	C	352	0	0	7	2
2	D	385	0	0	9	2
All	All	12630	11104	11182	78	7

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 3.

All (78) 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:1:MET:SD	2:D:798:HOH:O	2.19	0.98
1:B:1:MET:SD	2:B:760:HOH:O	2.22	0.96
1:A:265:GLU:OE1	2:A:501:HOH:O	1.97	0.81
1:D:220:ALA:O	2:D:502:HOH:O	1.99	0.81
1:C:68:PRO:O	2:C:401:HOH:O	2.00	0.78
1:C:10:ALA:HB3	1:C:14:ALA:HB2	1.64	0.78
1:B:240:ASN:OD1	2:B:501:HOH:O	2.01	0.77
1:A:128:LEU:HD11	1:A:183:LEU:HG	1.72	0.71
1:B:93:VAL:O	2:B:502:HOH:O	2.09	0.70
1:C:119:ASN:ND2	2:C:404:HOH:O	2.20	0.70
1:C:82:ALA:O	2:C:403:HOH:O	2.11	0.69
1:D:9:ASP:OD2	2:D:503:HOH:O	2.11	0.67
1:A:198:ALA:HB2	1:A:211:ARG:NH1	2.10	0.66
1:D:56[B]:GLN:OE1	2:D:504:HOH:O	2.14	0.65
1:A:317:LEU:HD12	1:B:160:TYR:CZ	2.32	0.65
1:A:82:ALA:HB1	1:A:85:LEU:HB2	1.82	0.61
1:C:42:ILE:HG21	1:C:57:HIS:CD2	2.42	0.54
1:D:128:LEU:HD21	1:D:183:LEU:HG	1.87	0.54
1:D:128:LEU:HD11	1:D:183:LEU:HD23	1.89	0.54
1:B:70:HIS:ND1	2:B:506:HOH:O	2.22	0.53
1:B:314:GLY:O	1:B:323:TYR:OH	2.14	0.53
1:C:128:LEU:HD11	1:C:183:LEU:HD23	1.89	0.53
1:D:82:ALA:HB1	1:D:85:LEU:HB2	1.90	0.52
1:D:2:LYS:NZ	2:D:509:HOH:O	2.25	0.52
1:C:16:ASP:HB3	1:D:302:TYR:OH	2.09	0.51
1:D:127:VAL:CG1	1:D:131:MET:HE3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LYS:NZ	2:B:523:HOH:O	2.39	0.50
1:C:317:LEU:HD12	1:D:160:TYR:CZ	2.47	0.50
1:B:6:VAL:HG11	1:B:72:ALA:HB2	1.94	0.50
1:B:82:ALA:HB1	1:B:85:LEU:HB2	1.95	0.49
1:D:215:ILE:HD13	1:D:238:LEU:HD21	1.95	0.49
1:C:227:ILE:HD11	1:C:239:ILE:HG13	1.94	0.49
1:B:150:TRP:NE1	2:B:518:HOH:O	2.37	0.48
1:B:221:GLN:OE1	2:B:503:HOH:O	2.20	0.48
1:C:1:MET:HE2	1:C:86:LYS:HE3	1.95	0.47
1:D:217:GLU:OE1	2:D:505:HOH:O	2.20	0.47
1:B:237:GLY:O	2:B:504:HOH:O	2.20	0.46
1:A:160:TYR:CZ	1:B:317:LEU:HD12	2.51	0.46
1:C:119:ASN:OD1	2:C:405:HOH:O	2.20	0.46
1:C:9:ASP:OD2	1:C:45:SER:OG	2.31	0.46
1:A:198:ALA:HB2	1:A:211:ARG:HH11	1.79	0.44
1:D:354:ILE:C	1:D:354:ILE:HD12	2.42	0.44
1:C:6:VAL:HA	1:C:44:THR:O	2.18	0.44
1:D:34:LEU:HD12	1:D:41:LEU:HD22	2.00	0.44
1:A:6:VAL:HG11	1:A:72:ALA:HB2	1.99	0.44
1:A:67:THR:HG23	1:A:70:HIS:H	1.83	0.44
1:B:216[A]:GLU:OE1	2:B:505:HOH:O	2.21	0.44
1:A:287:GLN:HA	1:A:288:PRO:C	2.42	0.44
1:A:215:ILE:CG2	1:A:243:LEU:HD11	2.49	0.43
1:C:160:TYR:CZ	1:D:317:LEU:HD12	2.53	0.43
1:D:56[A]:GLN:O	2:D:506:HOH:O	2.20	0.43
1:A:194:TYR:CD1	1:A:194:TYR:C	2.96	0.43
1:C:82:ALA:HB1	1:C:85:LEU:HB2	2.00	0.43
1:C:93:VAL:HG11	2:C:405:HOH:O	2.18	0.43
1:A:227:ILE:HD11	1:A:239:ILE:HG13	2.01	0.42
1:D:10:ALA:HB3	1:D:14:ALA:HB2	2.01	0.42
1:D:129:MET:HE3	2:D:649:HOH:O	2.19	0.42
1:D:56[B]:GLN:O	2:D:506:HOH:O	2.21	0.42
1:B:33:TRP:CD1	1:B:37:GLN:HE22	2.36	0.42
1:A:315:THR:O	1:A:315:THR:HG23	2.18	0.42
1:B:33:TRP:NE1	1:B:37:GLN:HE22	2.17	0.42
1:C:111:SER:CB	2:C:409:HOH:O	2.67	0.42
1:B:10:ALA:HB3	1:B:14:ALA:HB2	2.02	0.42
1:B:128:LEU:HD11	1:B:179:VAL:HA	2.02	0.42
1:A:129:MET:O	1:A:133:VAL:HG23	2.20	0.41
1:A:27:LYS:NZ	2:A:508:HOH:O	2.38	0.41
1:D:174:ARG:O	1:D:178:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:TYR:HB3	1:D:218:LEU:HD22	2.02	0.41
1:D:3:ILE:HD13	1:D:34:LEU:HD22	2.02	0.41
1:D:6:VAL:HG11	1:D:72:ALA:HB2	2.02	0.41
1:B:129:MET:O	1:B:133:VAL:HG23	2.21	0.41
1:B:217:GLU:O	1:B:221:GLN:NE2	2.46	0.41
1:B:287:GLN:HA	1:B:288:PRO:C	2.45	0.41
1:C:287:GLN:HA	1:C:288:PRO:C	2.46	0.41
1:C:128:LEU:HD21	1:C:183:LEU:HG	2.02	0.41
1:C:87:LEU:HD13	2:C:409:HOH:O	2.22	0.40
1:A:194:TYR:CD1	1:A:215:ILE:HD11	2.57	0.40
1:B:226:THR:HA	1:B:254:VAL:O	2.22	0.40

All (7) 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:C:35:LYS:H	2:A:913:HOH:O[1_464]	1.09	0.51
1:C:35:LYS:N	2:A:913:HOH:O[1_464]	1.79	0.41
1:C:31:ALA:O	2:A:913:HOH:O[1_464]	1.79	0.41
1:B:221:GLN:OE1	2:A:914:HOH:O[1_565]	1.93	0.27
2:B:711:HOH:O	2:D:718:HOH:O[1_646]	1.98	0.22
2:C:498:HOH:O	2:D:738:HOH:O[1_655]	1.98	0.22
1:B:196:TYR:O	2:C:402:HOH:O[1_656]	2.01	0.19

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	358/364 (98%)	351 (98%)	7 (2%)	0	100	100
1	B	352/364 (97%)	345 (98%)	7 (2%)	0	100	100
1	C	356/364 (98%)	348 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	357/364 (98%)	351 (98%)	6 (2%)	0	100	100
All	All	1423/1456 (98%)	1395 (98%)	28 (2%)	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	296/298 (99%)	292 (99%)	4 (1%)	59	59
1	B	290/298 (97%)	287 (99%)	3 (1%)	68	70
1	C	293/298 (98%)	286 (98%)	7 (2%)	43	38
1	D	295/298 (99%)	292 (99%)	3 (1%)	68	70
All	All	1174/1192 (98%)	1157 (99%)	17 (1%)	59	59

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ILE
1	A	178	ARG
1	A	206	LYS
1	A	215	ILE
1	B	51	ASN
1	B	58	ILE
1	B	83	LYS
1	C	12	LYS
1	C	128	LEU
1	C	147[A]	ASN
1	C	147[B]	ASN
1	C	201	LYS
1	C	206	LYS
1	C	328	LYS
1	D	96	ASP
1	D	128	LEU

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Mol	Chain	Res	Type
1	D	249	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	B	37	GLN
1	B	228	ASN
1	C	26	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	356/364 (97%)	0.52	9 (2%) 58 62	11, 22, 35, 45	4 (1%)
1	B	353/364 (96%)	0.73	23 (6%) 25 26	15, 25, 37, 73	1 (0%)
1	C	354/364 (97%)	0.64	24 (6%) 23 24	10, 23, 40, 66	4 (1%)
1	D	356/364 (97%)	0.57	10 (2%) 55 59	14, 23, 36, 53	3 (0%)
All	All	1419/1456 (97%)	0.62	66 (4%) 36 39	10, 23, 37, 73	12 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	ALA	6.4
1	C	16	ASP	5.0
1	C	196	TYR	4.9
1	C	17	GLU	4.5
1	C	354	ILE	4.5
1	B	50	GLY	4.4
1	C	18	GLU	4.2
1	B	37	GLN	3.9
1	C	323[A]	TYR	3.8
1	C	143[A]	GLU	3.7
1	B	36	ASP	3.6
1	A	215	ILE	3.3
1	A	128	LEU	3.3
1	C	14	ALA	3.3
1	B	49	GLY	3.2
1	A	143[A]	GLU	3.1
1	D	15	ALA	3.0
1	B	51	ASN	3.0
1	C	12	LYS	3.0
1	C	51	ASN	3.0
1	B	234	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	356	LYS	2.9
1	A	50	GLY	2.9
1	C	198	ALA	2.9
1	B	53	VAL	2.8
1	D	51	ASN	2.8
1	B	128	LEU	2.8
1	C	50	GLY	2.6
1	D	35	LYS	2.6
1	C	10	ALA	2.6
1	D	49	GLY	2.6
1	B	12	LYS	2.6
1	A	354	ILE	2.5
1	C	197	GLN	2.5
1	B	323	TYR	2.5
1	A	356	LYS	2.5
1	C	20	LEU	2.4
1	A	242	GLU	2.4
1	B	216[A]	GLU	2.4
1	C	201	LYS	2.4
1	B	101	ASP	2.4
1	D	16	ASP	2.4
1	D	246	LYS	2.4
1	D	354	ILE	2.3
1	B	353	TYR	2.3
1	B	215	ILE	2.3
1	C	128	LEU	2.3
1	A	201[A]	LYS	2.2
1	D	128	LEU	2.2
1	C	215	ILE	2.2
1	B	33	TRP	2.2
1	C	101	ASP	2.2
1	B	38	GLY	2.2
1	B	73	TYR	2.1
1	B	241	LYS	2.1
1	C	19	LYS	2.1
1	B	202	ASP	2.1
1	C	13	HIS	2.1
1	A	213	GLU	2.0
1	B	146	ILE	2.0
1	B	213	GLU	2.0
1	C	8	TYR	2.0
1	B	315	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	3	ILE	2.0
1	C	49	GLY	2.0
1	D	37	GLN	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.