Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:53 PM GMT

PDB ID	:	1HQ6
Title	:	STRUCTURE OF PYRUVOYL-DEPENDENT HISTIDINE DECARBOXY-LASE AT PH 8
Authors	:	Schelp, E.; Worley, S.; Monzingo, A.F.; Ernst, S.; Robertus, J.D.
Deposited on	:	2000-12-14
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

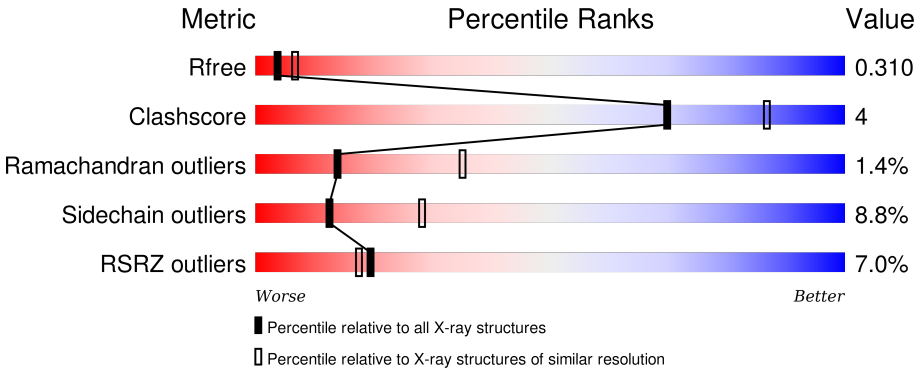
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	81	2% 64% 16% • 19%
1	C	81	4% 65% 15% • 19%
2	B	229	8% 77% 20% •
2	D	229	7% 77% 20% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4600 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 HISTIDINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			506	315	91	98	2			
1	C	66	Total	C	N	O	S	0	0	0
			506	315	91	98	2			

- Molecule 2 is a protein called HISTIDINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			
2	D	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	PYR	SER	MODIFIED RESIDUE	UNP P00862
D	82	PYR	SER	MODIFIED RESIDUE	UNP P00862

- Molecule 3 is water.

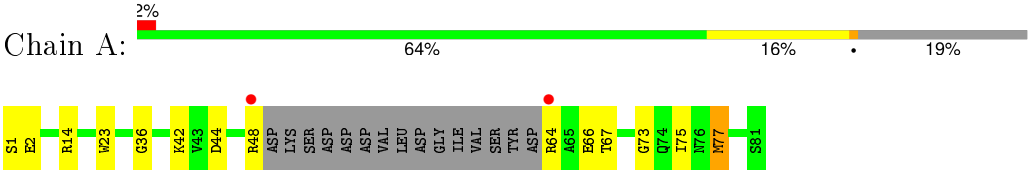
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	3	Total	O	0	0
			3	3		
3	C	10	Total	O	0	0
			10	10		
3	D	12	Total	O	0	0
			12	12		

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 errors 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.

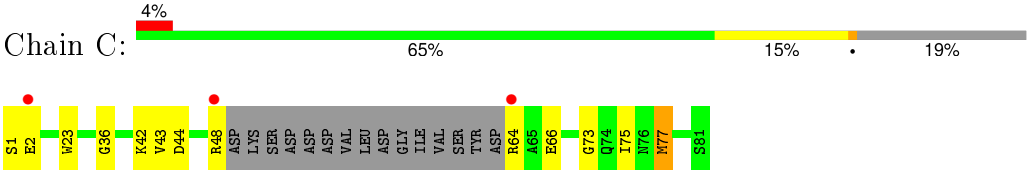
- Molecule 1: HISTIDINE DECARBOXYLASE

Chain A:



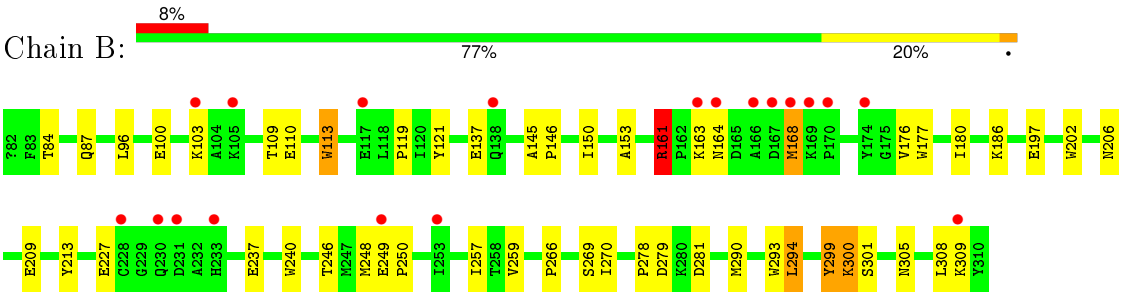
- Molecule 1: HISTIDINE DECARBOXYLASE

Chain C:



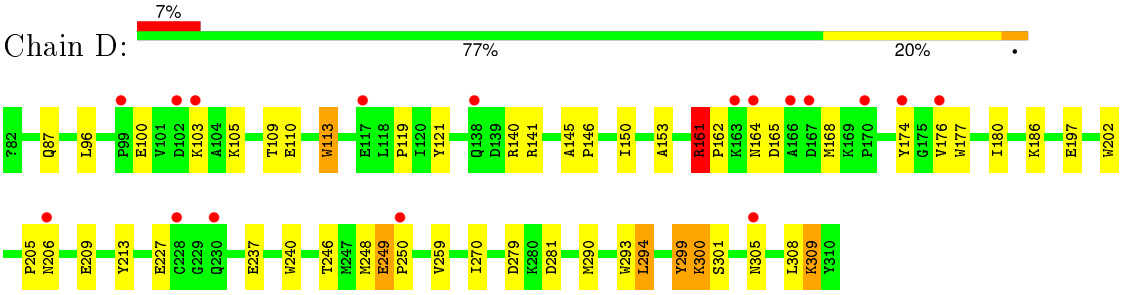
- Molecule 2: HISTIDINE DECARBOXYLASE

Chain B:



- Molecule 2: HISTIDINE DECARBOXYLASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	117.43Å 117.43Å 241.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-2.70) 97.5 (19.81-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.15 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.253 , 0.314 0.254 , 0.310	Depositor DCC
R_{free} test set	1717 reflections (9.84%)	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 17611 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PYR

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	0.79	0/512	1.52	7/687 (1.0%)
1	C	0.80	0/512	1.52	8/687 (1.2%)
2	B	0.77	0/1816	1.43	18/2463 (0.7%)
2	D	0.77	0/1816	1.43	21/2463 (0.9%)
All	All	0.77	0/4656	1.45	54/6300 (0.9%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	161	ARG	NE-CZ-NH2	9.11	124.86	120.30
1	C	23	TRP	CD1-CG-CD2	8.49	113.10	106.30
1	A	23	TRP	CD1-CG-CD2	8.37	112.99	106.30
2	D	202	TRP	CD1-CG-CD2	8.30	112.94	106.30
2	B	202	TRP	CD1-CG-CD2	8.22	112.88	106.30
2	B	177	TRP	CD1-CG-CD2	8.20	112.86	106.30
2	D	177	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	C	23	TRP	CE2-CD2-CG	-7.67	101.17	107.30
2	B	113	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	C	48	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	A	23	TRP	CE2-CD2-CG	-7.57	101.24	107.30
2	D	202	TRP	CE2-CD2-CG	-7.57	101.25	107.30
2	B	202	TRP	CE2-CD2-CG	-7.55	101.26	107.30
2	B	177	TRP	CE2-CD2-CG	-7.45	101.34	107.30
2	D	113	TRP	CD1-CG-CD2	7.44	112.25	106.30
2	B	299	TYR	CB-CG-CD2	-7.43	116.54	121.00
2	B	240	TRP	CE2-CD2-CG	-7.40	101.38	107.30
2	D	240	TRP	CE2-CD2-CG	-7.15	101.58	107.30
2	D	113	TRP	CE2-CD2-CG	-7.14	101.59	107.30
2	B	240	TRP	CD1-CG-CD2	7.08	111.97	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	177	TRP	CE2-CD2-CG	-6.90	101.78	107.30
2	D	240	TRP	CD1-CG-CD2	6.88	111.80	106.30
2	B	113	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	A	48	ARG	CA-CB-CG	6.50	127.69	113.40
2	B	293	TRP	CE2-CD2-CG	-6.49	102.11	107.30
2	B	293	TRP	CD1-CG-CD2	6.49	111.49	106.30
2	D	299	TYR	CB-CG-CD2	-6.48	117.11	121.00
2	B	213	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	C	48	ARG	CA-CB-CG	6.44	127.57	113.40
1	C	23	TRP	CG-CD2-CE3	6.19	139.47	133.90
2	D	213	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	A	23	TRP	CG-CD2-CE3	6.13	139.42	133.90
1	A	23	TRP	CG-CD1-NE1	-6.07	104.03	110.10
1	C	64	ARG	NE-CZ-NH1	-6.02	117.29	120.30
2	D	293	TRP	CE2-CD2-CG	-6.00	102.50	107.30
1	C	23	TRP	CG-CD1-NE1	-5.92	104.18	110.10
2	D	293	TRP	CD1-CG-CD2	5.88	111.01	106.30
2	B	161	ARG	NE-CZ-NH2	5.78	123.19	120.30
2	D	141	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	B	240	TRP	CG-CD2-CE3	5.66	138.99	133.90
2	D	240	TRP	CG-CD2-CE3	5.62	138.96	133.90
2	D	305	ASN	N-CA-C	-5.52	96.09	111.00
2	B	305	ASN	N-CA-C	-5.47	96.22	111.00
1	A	77	MET	CA-CB-CG	5.46	122.58	113.30
2	D	140	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	C	77	MET	CA-CB-CG	5.41	122.50	113.30
2	B	163	LYS	CA-C-N	-5.34	105.45	117.20
2	D	202	TRP	CB-CG-CD1	-5.27	120.15	127.00
2	D	202	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	A	14	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	B	84	THR	N-CA-C	-5.11	97.19	111.00
2	D	177	TRP	CG-CD1-NE1	-5.07	105.03	110.10
2	D	153	ALA	N-CA-C	-5.05	97.36	111.00
2	B	153	ALA	N-CA-C	-5.00	97.50	111.00

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	506	0	511	5	0
1	C	506	0	511	3	0
2	B	1776	0	1706	19	0
2	D	1776	0	1706	20	0
3	A	11	0	0	0	0
3	B	3	0	0	0	0
3	C	10	0	0	0	0
3	D	12	0	0	1	0
All	All	4600	0	4434	40	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 4.

All (40) 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)
2:D:96:LEU:HB3	2:D:290:MET:HE2	1.69	0.73
2:D:270:ILE:HD13	2:D:281:ASP:HB3	1.72	0.72
2:B:270:ILE:HD13	2:B:281:ASP:HB3	1.72	0.71
2:B:96:LEU:HB3	2:B:290:MET:HE2	1.74	0.70
2:B:161:ARG:HG2	2:B:250:PRO:HA	1.80	0.63
2:D:161:ARG:HG2	2:D:250:PRO:HA	1.81	0.63
2:D:180:ILE:HG13	2:D:197:GLU:HG2	1.82	0.62
2:D:105:LYS:HG3	3:D:18:HOH:O	2.01	0.60
2:B:180:ILE:HG13	2:B:197:GLU:HG2	1.84	0.58
1:C:36:GLY:HA2	2:D:87:GLN:HB3	1.89	0.54
1:A:42:LYS:HB3	2:B:259:VAL:HG13	1.89	0.53
1:C:42:LYS:HB3	2:D:259:VAL:HG13	1.91	0.52
1:A:36:GLY:HA2	2:B:87:GLN:HB3	1.91	0.52
2:B:206:ASN:HB3	2:B:209:GLU:HB2	1.90	0.52
2:D:294:LEU:HD12	2:D:299:TYR:HB2	1.94	0.49
2:D:206:ASN:HB3	2:D:209:GLU:HB2	1.94	0.48
2:D:96:LEU:HB3	2:D:290:MET:CE	2.43	0.48
2:D:100:GLU:HA	2:D:103:LYS:HD2	1.97	0.47
2:B:100:GLU:HA	2:B:103:LYS:HD2	1.99	0.45
2:D:300:LYS:NZ	2:D:300:LYS:H	2.13	0.45
2:B:294:LEU:HD12	2:B:299:TYR:HB2	1.99	0.44
2:B:300:LYS:H	2:B:300:LYS:NZ	2.15	0.44
2:B:109:THR:HG22	2:B:119:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:PRO:O	2:B:281:ASP:HB2	2.17	0.43
1:A:64:ARG:N	1:A:67:THR:HG1	2.16	0.43
2:B:96:LEU:HB3	2:B:290:MET:CE	2.44	0.43
2:D:109:THR:HG22	2:D:119:PRO:HA	2.00	0.43
2:D:119:PRO:HB2	2:D:121:TYR:CE1	2.53	0.43
1:A:42:LYS:HE3	2:B:257:ILE:HD11	2.01	0.43
1:C:77:MET:HA	2:D:150:ILE:O	2.20	0.42
2:B:119:PRO:HB2	2:B:121:TYR:CE1	2.55	0.42
2:D:161:ARG:HH11	2:D:249:GLU:HA	1.84	0.42
1:A:77:MET:HA	2:B:150:ILE:O	2.19	0.42
2:B:266:PRO:O	2:B:269:SER:HB2	2.20	0.42
2:D:162:PRO:HG2	2:D:165:ASP:HB3	2.03	0.41
2:D:174:TYR:CD1	2:D:205:PRO:HB3	2.56	0.41
2:B:168:MET:HG3	2:B:168:MET:H	1.68	0.41
2:D:145:ALA:HA	2:D:146:PRO:HD2	1.95	0.41
2:B:145:ALA:HA	2:B:146:PRO:HD2	1.93	0.40
2:D:309:LYS:O	2:D:309:LYS:HD3	2.21	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	62/81 (76%)	58 (94%)	3 (5%)	1 (2%)	12	30
1	C	62/81 (76%)	59 (95%)	2 (3%)	1 (2%)	12	30
2	B	226/229 (99%)	205 (91%)	18 (8%)	3 (1%)	15	37
2	D	226/229 (99%)	205 (91%)	18 (8%)	3 (1%)	15	37
All	All	576/620 (93%)	527 (92%)	41 (7%)	8 (1%)	14	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLY
2	B	113	TRP
1	C	73	GLY
2	D	113	TRP
2	B	164	ASN
2	B	301	SER
2	D	164	ASN
2	D	301	SER

5.3.2 Protein sidechains (i)

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	52/66 (79%)	47 (90%)	5 (10%)	10	24
1	C	52/66 (79%)	46 (88%)	6 (12%)	7	16
2	B	188/188 (100%)	172 (92%)	16 (8%)	13	30
2	D	188/188 (100%)	173 (92%)	15 (8%)	15	33
All	All	480/508 (94%)	438 (91%)	42 (9%)	12	28

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	GLU
1	A	44	ASP
1	A	66	GLU
1	A	75	ILE
2	B	110	GLU
2	B	137	GLU
2	B	161	ARG
2	B	168	MET
2	B	176	VAL
2	B	186	LYS
2	B	227	GLU
2	B	237	GLU
2	B	246	THR

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Mol	Chain	Res	Type
2	B	248	MET
2	B	249	GLU
2	B	279	ASP
2	B	294	LEU
2	B	300	LYS
2	B	308	LEU
2	B	309	LYS
1	C	1	SER
1	C	2	GLU
1	C	43	VAL
1	C	44	ASP
1	C	66	GLU
1	C	75	ILE
2	D	110	GLU
2	D	161	ARG
2	D	168	MET
2	D	176	VAL
2	D	186	LYS
2	D	227	GLU
2	D	237	GLU
2	D	246	THR
2	D	248	MET
2	D	249	GLU
2	D	279	ASP
2	D	294	LEU
2	D	300	LYS
2	D	308	LEU
2	D	309	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	255	ASN
2	D	255	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 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	66/81 (81%)	-0.10	2 (3%)	54	54	10, 23, 49, 80	0
1	C	66/81 (81%)	-0.11	3 (4%)	37	36	8, 24, 49, 81	0
2	B	228/229 (99%)	0.45	19 (8%)	14	11	13, 37, 61, 73	0
2	D	228/229 (99%)	0.43	17 (7%)	17	15	12, 38, 61, 73	0
All	All	588/620 (94%)	0.32	41 (6%)	19	17	8, 34, 61, 81	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	167	ASP	8.6
2	D	167	ASP	8.3
2	B	166	ALA	6.5
2	D	166	ALA	6.4
2	B	164	ASN	4.8
1	C	64	ARG	4.0
2	D	305	ASN	3.8
2	D	99	PRO	3.8
2	B	117	GLU	3.4
2	B	169	LYS	3.4
1	C	48	ARG	3.4
2	B	103	LYS	3.4
2	D	230	GLN	3.4
2	B	231	ASP	3.3
1	A	48	ARG	3.3
2	B	230	GLN	3.2
2	B	309	LYS	3.1
2	B	249	GLU	3.0
2	D	176	VAL	3.0
1	C	2	GLU	3.0
2	D	164	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	163	LYS	2.9
2	B	170	PRO	2.9
2	B	168	MET	2.8
2	D	138	GLN	2.7
2	D	174	TYR	2.7
2	D	117	GLU	2.7
2	B	174	TYR	2.6
2	D	250	PRO	2.6
2	D	163	LYS	2.6
2	D	103	LYS	2.5
2	B	228	CYS	2.4
2	D	102	ASP	2.3
2	B	105	LYS	2.3
1	A	64	ARG	2.2
2	B	253	ILE	2.2
2	B	233	HIS	2.2
2	D	170	PRO	2.1
2	D	228	CYS	2.1
2	D	206	ASN	2.0
2	B	138	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 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.