



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:16 AM UTC

PDB ID : 1IBW / pdb_00001ibw
Title : STRUCTURE OF THE D53,54N MUTANT OF HISTIDINE DECARBOXY-
LASE BOUND WITH HISTIDINE METHYL ESTER AT 25 C
Authors : Worley, S.; Schelp, E.; Monzingo, A.F.; Ernst, S.; Robertus, J.D.
Deposited on : 2001-03-29
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

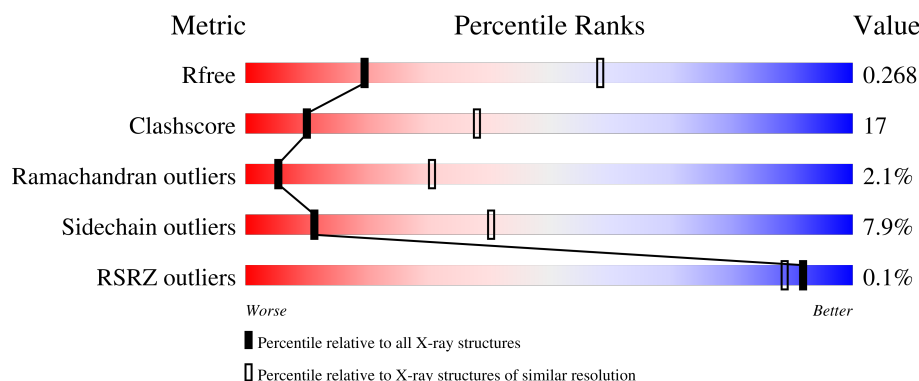
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	81	 70% 22% 7%
1	C	81	 69% 22% 9%
1	E	81	 62% 30% 9%
2	B	229	 58% 38% 4%
2	D	229	 61% 34% 5%

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Mol	Chain	Length	Quality of chain
2	F	229	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (58%), yellow (38%), and orange (4%). The green segment is labeled '58%' and the yellow segment is labeled '38%'. The orange segment is labeled with a period '.'.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7223 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 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	0	0	0
			621	384	109	126	2			
1	C	81	Total	C	N	O	S	0	0	0
			621	384	109	126	2			
1	E	81	Total	C	N	O	S	0	0	0
			621	384	109	126	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ASN	ASP	engineered mutation	UNP P00862
A	54	ASN	ASP	engineered mutation	UNP P00862
C	53	ASN	ASP	engineered mutation	UNP P00862
C	54	ASN	ASP	engineered mutation	UNP P00862
E	53	ASN	ASP	engineered mutation	UNP P00862
E	54	ASN	ASP	engineered mutation	UNP P00862

- Molecule 2 is a protein called Histidine decarboxylase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1775	1127	286	351	11			
2	D	229	Total	C	N	O	S	0	0	0
			1775	1127	286	351	11			
2	F	229	Total	C	N	O	S	0	0	0
			1774	1127	286	350	11			

There are 3 discrepancies between the modelled and reference sequences:

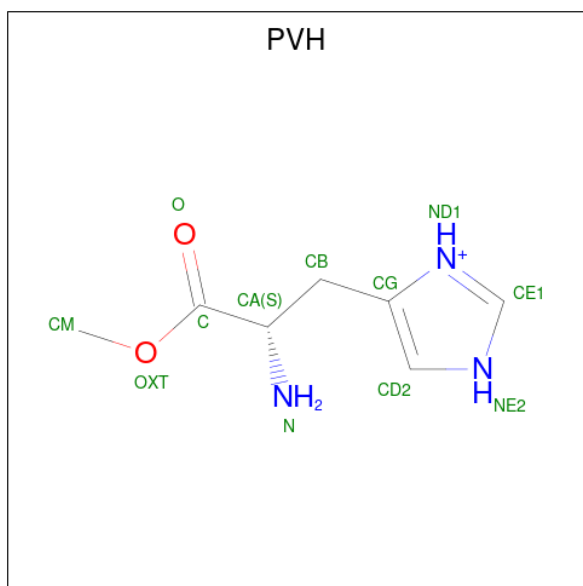
Chain	Residue	Modelled	Actual	Comment	Reference
B	82	PYR	SER	conflict	UNP P00862
D	82	PYR	SER	conflict	UNP P00862

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Chain	Residue	Modelled	Actual	Comment	Reference
F	82	PYR	SER	conflict	UNP P00862

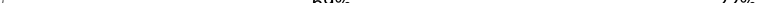
- Molecule 3 is HISTIDINE-METHYL-ESTER (CCD ID: PVH) (formula: $C_7H_{12}N_3O_2$).



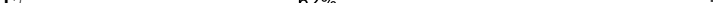
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			12	7	3	2		
3	D	1	Total	C	N	O	0	0
			12	7	3	2		
3	F	1	Total	C	N	O	0	0
			12	7	3	2		

● Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

S1	E2	L3	D4		L7	V12	D13	R14	I15		T24	Y27	M28		G34	N35		T39	G40	V43	D44	A45	G46	V47		R48	S51	D52	N53		S61		Y71	I72	G73	G74	I75		T79	A80	S81
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Chain C:  69% 22% 9%

S1	E2	L3	D4		L7		V12		I17		T24		Y27	M28		I33		Y37	P38		T39	G40		V43	D44	A45	G46	V47		R48		S51	D52	M53		L56		I59	V60		S61		Y71		I72	G73	Q74		I75		T79		A80		S81
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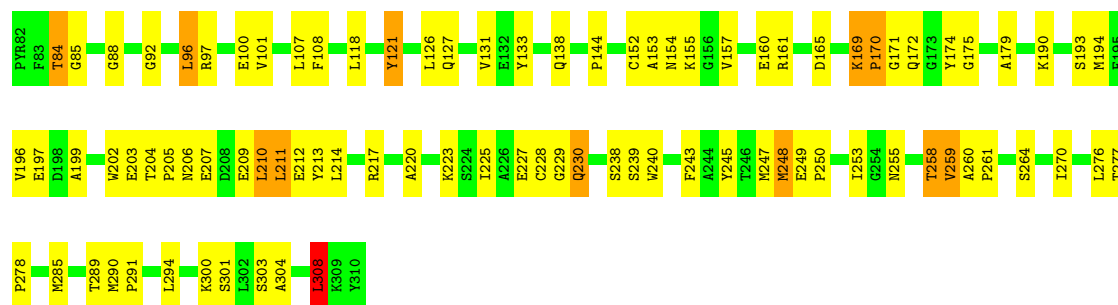
Chain E:  62% 30% 9%

S1	S2	L3	D4	L7	V12	D13	S18	P19	T24	R25	G26	Y27	M28	N35	T39	G40	L41	K42	V43	D44	A45	G46	V47	R48	S51	D52	M53	S61	T67	K68	Y71	IT2	G73	Q74	IT5	N76	T79	A80	S81
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Chain B: 58% 38% .

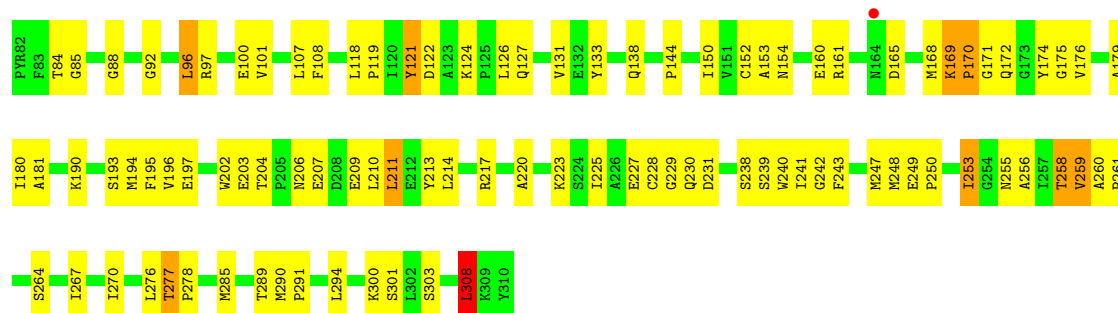
T270	K190	F182
T276		F83
T277	S193	T84
T278	M194	G85
D279	F195	V86
K280	V196	Q87
	E197	G88
T284	D198	G92
M285		
	W202	L96
T289	E203	R97
M290	T204	
P291	P205	E100
	N206	E101
L294	E207	
	D208	L107
K300	E209	F108
S301	L210	
L302	L211	L118
S303	E212	
A304	Y213	Y121
	L214	D122
L308		A123
K309	R217	K124
Y310		P125
	A320	L126
		Q127
	K223	L130
	S224	V131
	L225	E132
	A226	Y133
	E227	F134
	C228	
	G229	
	Q230	Q138
	S238	P144
	S239	
	T240	C152
	L241	A153
	G242	N154
	F243	K155
	M247	E160
	N248	R161
	E249	
	P250	D165
	L253	K169
	G254	P170
	N255	Q171
		G172
	T258	G173
	V259	Y174
	A260	G175
	P261	
		A179
	S264	L180
		A181

Chain D: 61% 34% 5%



• Molecule 2: Histidine decarboxylase alpha chain

Chain F: 58% 38% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.02Å 117.77Å 205.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.20) 77.3 (20.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.22Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.269 0.208 , 0.268	Depositor DCC
R_{free} test set	1606 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 51.5	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	0.92	EDS
Total number of atoms	7223	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PVH, 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	0.69	0/629	1.14	2/848 (0.2%)
1	C	0.62	0/629	1.14	3/848 (0.4%)
1	E	0.65	0/629	1.14	3/848 (0.4%)
2	B	0.60	0/1816	1.04	8/2463 (0.3%)
2	D	0.58	0/1816	1.06	9/2463 (0.4%)
2	F	0.62	0/1815	1.05	10/2463 (0.4%)
All	All	0.62	0/7334	1.07	35/9933 (0.4%)

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	88	GLY	N-CA-C	9.34	124.88	110.96
2	B	88	GLY	N-CA-C	8.76	123.88	111.10
2	D	88	GLY	N-CA-C	8.66	123.74	111.10
2	D	153	ALA	N-CA-C	-7.90	95.69	108.41
2	F	153	ALA	N-CA-C	-7.73	95.96	108.41

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	621	0	615	20	0
1	C	621	0	615	22	0
1	E	621	0	615	25	0
2	B	1775	0	1704	68	0
2	D	1775	0	1704	68	0
2	F	1774	0	1704	75	0
3	B	12	0	7	0	0
3	D	12	0	7	0	0
3	F	12	0	7	0	0
All	All	7223	0	6978	246	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 17.

The worst 5 of 246 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:F:92:GLY:O	2:F:97:ARG:HA	1.71	0.89
1:C:75:ILE:HD11	2:D:144:PRO:HB2	1.58	0.84
2:D:169:LYS:HB3	2:D:170:PRO:HD2	1.59	0.84
2:D:92:GLY:O	2:D:97:ARG:HA	1.76	0.83
1:E:75:ILE:HD11	2:F:144:PRO:HB2	1.59	0.83

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	79/81 (98%)	68 (86%)	10 (13%)	1 (1%)	9	40
1	C	79/81 (98%)	68 (86%)	10 (13%)	1 (1%)	9	40
1	E	79/81 (98%)	68 (86%)	9 (11%)	2 (2%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	227/229 (99%)	198 (87%)	24 (11%)	5 (2%)	5	29
2	D	227/229 (99%)	196 (86%)	25 (11%)	6 (3%)	4	26
2	F	227/229 (99%)	196 (86%)	27 (12%)	4 (2%)	6	34
All	All	918/930 (99%)	794 (86%)	105 (11%)	19 (2%)	5	31

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLY
2	B	169	LYS
2	B	170	PRO
1	C	73	GLY
2	D	169	LYS

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	66/66 (100%)	62 (94%)	4 (6%)	17	49
1	C	66/66 (100%)	61 (92%)	5 (8%)	12	42
1	E	66/66 (100%)	60 (91%)	6 (9%)	9	34
2	B	188/188 (100%)	173 (92%)	15 (8%)	11	40
2	D	188/188 (100%)	172 (92%)	16 (8%)	10	37
2	F	188/188 (100%)	174 (93%)	14 (7%)	13	43
All	All	762/762 (100%)	702 (92%)	60 (8%)	11	40

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	126	LEU
2	F	253	ILE
2	D	248	MET
2	F	223	LYS

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Mol	Chain	Res	Type
2	F	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	306	ASN
1	E	8	ASN
2	F	255	ASN
2	F	164	ASN
2	F	230	GLN

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](#)

3 ligands 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	$\# Z > 2$
3	PVH	D	482	2	12,12,12	0.71	1 (8%)	15,15,15	1.87	4 (26%)
3	PVH	B	482	2	12,12,12	0.68	0	15,15,15	1.86	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PVH	F	482	2	12,12,12	0.88	1 (8%)	15,15,15	1.81	3 (20%)

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
3	PVH	D	482	2	-	2/10/10/10	0/1/1/1
3	PVH	B	482	2	-	2/10/10/10	0/1/1/1
3	PVH	F	482	2	-	2/10/10/10	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	482	PVH	OXT-C	2.69	1.39	1.33
3	D	482	PVH	OXT-C	2.03	1.38	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	482	PVH	OXT-C-CA	4.03	121.75	111.50
3	B	482	PVH	OXT-C-CA	3.94	121.51	111.50
3	F	482	PVH	OXT-C-CA	3.79	121.15	111.50
3	B	482	PVH	OXT-C-O	-3.60	116.84	123.85
3	D	482	PVH	OXT-C-O	-3.33	117.36	123.85

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	482	PVH	CA-C-OXT-CM
3	D	482	PVH	CA-C-OXT-CM
3	F	482	PVH	CA-C-OXT-CM
3	D	482	PVH	O-C-OXT-CM
3	B	482	PVH	O-C-OXT-CM

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	81/81 (100%)	-0.24	0	100	100	13, 35, 70, 81	0
1	C	81/81 (100%)	-0.19	0	100	100	13, 36, 68, 82	0
1	E	81/81 (100%)	-0.21	0	100	100	15, 36, 69, 82	0
2	B	228/229 (99%)	-0.06	0	100	100	13, 48, 80, 99	0
2	D	228/229 (99%)	-0.04	0	100	100	13, 48, 80, 99	0
2	F	228/229 (99%)	-0.07	1 (0%)	88	79	12, 48, 79, 99	0
All	All	927/930 (99%)	-0.10	1 (0%)	92	89	12, 44, 79, 99	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	164	ASN	2.3

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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
3	PVH	D	482	12/12	0.90	0.14	36,38,44,45	0
3	PVH	B	482	12/12	0.91	0.11	35,39,42,49	0
3	PVH	F	482	12/12	0.91	0.11	36,39,42,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.