



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 10:05 am GMT

PDB ID : 1IBW  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

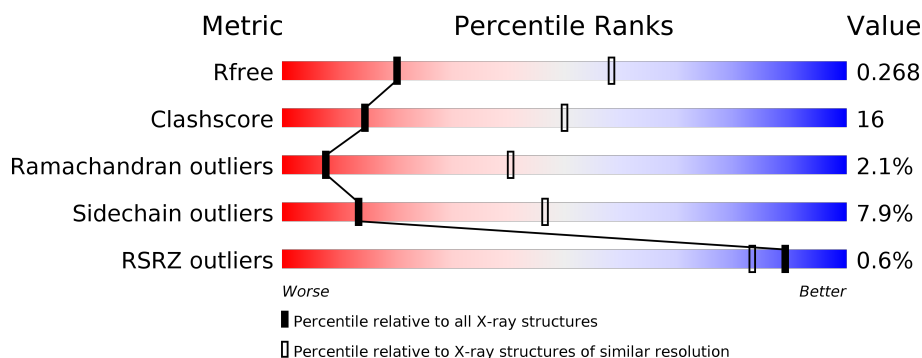
# 1 Overall quality at a glance

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))
$R_{free}$	111664	1121 (3.22-3.18)
Clashscore	122126	1091 (3.20-3.20)
Ramachandran outliers	120053	1074 (3.20-3.20)
Sidechain outliers	120020	1073 (3.20-3.20)
RSRZ outliers	108989	1083 (3.22-3.18)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>70%</div> <div>25%</div> <div>5%</div> </div>
1	C	81	<div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
1	E	81	<div> <div>63%</div> <div>31%</div> <div>6%</div> </div>
2	B	228	<div> <div>%</div> <div>63%</div> <div>34%</div> <div>•</div> </div>
2	D	228	<div> <div>%</div> <div>66%</div> <div>29%</div> <div>5%</div> </div>
2	F	228	<div> <div>%</div> <div>62%</div> <div>33%</div> <div>•</div> </div>

## 2 Entry composition

There are 4 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	UNP P00862
A	54	ASN	ASP	ENGINEERED	UNP P00862
C	53	ASN	ASP	ENGINEERED	UNP P00862
C	54	ASN	ASP	ENGINEERED	UNP P00862
E	53	ASN	ASP	ENGINEERED	UNP P00862
E	54	ASN	ASP	ENGINEERED	UNP P00862

- Molecule 2 is a protein called HISTIDINE DECARBOXYLASE ALPHA CHAIN.

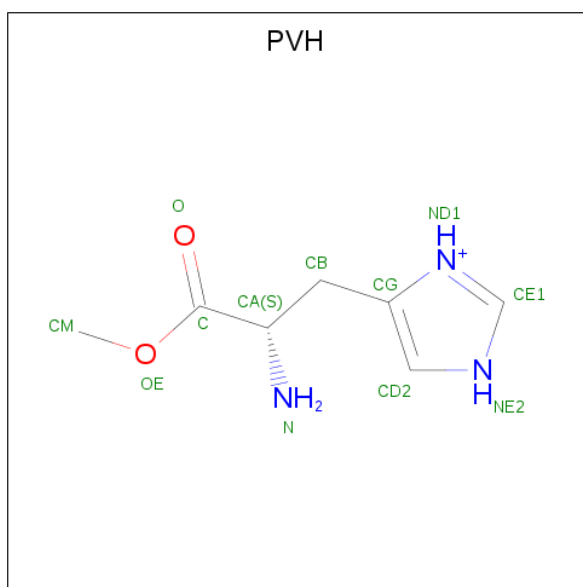
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	228	Total	C	N	O	S	0	0	0
			1771	1124	286	350	11			
2	D	228	Total	C	N	O	S	0	0	0
			1771	1124	286	350	11			
2	F	228	Total	C	N	O	S	0	0	0
			1770	1124	286	349	11			

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	3	1		
3	D	1	Total	C	O	0	0
			4	3	1		
3	F	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is HISTIDINE-METHYL-ESTER (three-letter code: PVH) (formula:  $C_7H_{12}N_3O_2$ ).



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

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

### 3 Residue-property plots

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.

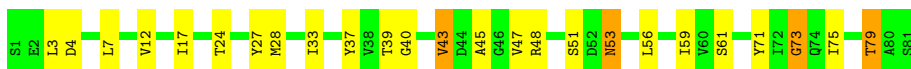
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain A: 



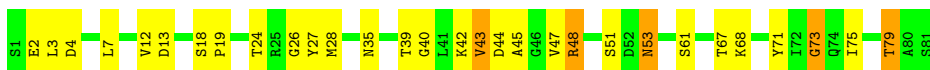
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain C: 



- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain E: 



- Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN

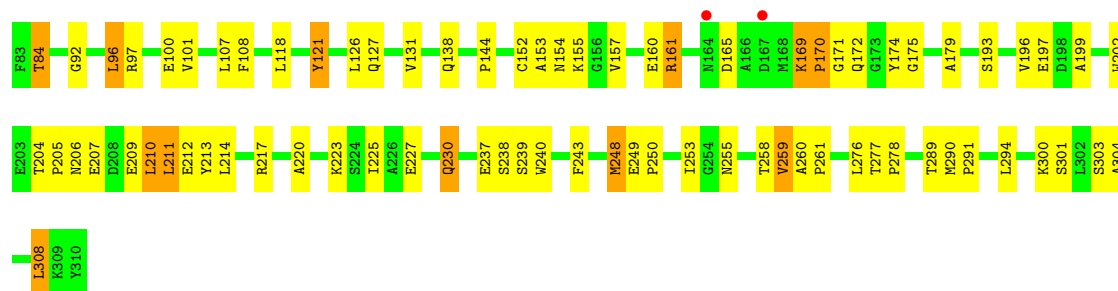
Chain B: 



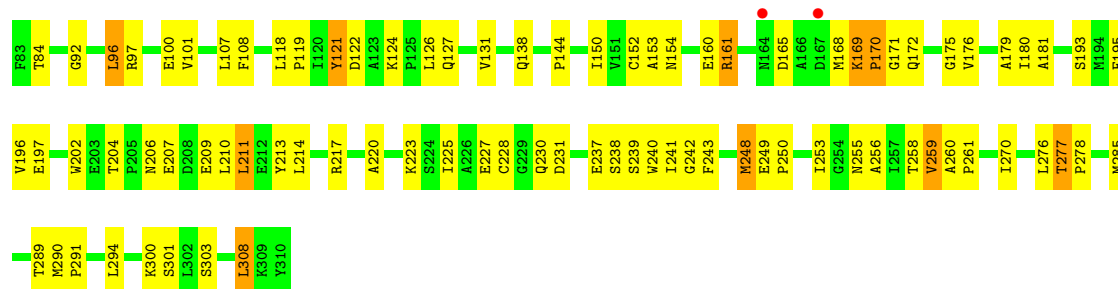
- Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN

Chain D: 





• Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.02Å 117.77Å 205.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.20) 77.7 (19.84-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.53	0/629	0.75	0/848
1	C	0.51	0/629	0.76	0/848
1	E	0.54	0/629	0.76	0/848
2	B	0.56	0/1816	0.71	1/2463 (0.0%)
2	D	0.55	0/1816	0.71	1/2463 (0.0%)
2	F	0.54	0/1815	0.72	1/2463 (0.0%)
All	All	0.54	0/7334	0.73	3/9933 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	153	ALA	N-CA-C	-5.67	95.69	111.00
2	F	153	ALA	N-CA-C	-5.57	95.96	111.00
2	B	153	ALA	N-CA-C	-5.54	96.03	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	621	0	615	20	0
1	C	621	0	615	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	621	0	615	24	0
2	B	1771	0	1703	64	0
2	D	1771	0	1703	62	0
2	F	1770	0	1703	70	0
3	B	4	0	3	1	0
3	D	4	0	3	1	0
3	F	4	0	3	1	0
4	B	12	0	10	1	0
4	D	12	0	10	1	0
4	F	12	0	10	1	0
All	All	7223	0	6993	233	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 16.

All (233) 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
1:A:75:ILE:HD11	2:B:144:PRO:HB2	1.60	0.82
2:B:92:GLY:O	2:B:97:ARG:HA	1.80	0.82
2:D:202:TRP:HZ2	2:D:209:GLU:HG3	1.47	0.78
2:F:169:LYS:HB3	2:F:170:PRO:HD2	1.63	0.78
2:B:169:LYS:HB3	2:B:170:PRO:HD2	1.64	0.77
2:D:169:LYS:HB3	2:D:170:PRO:CD	2.17	0.73
2:F:202:TRP:HZ2	2:F:209:GLU:HG3	1.52	0.73
2:B:202:TRP:HZ2	2:B:209:GLU:HG3	1.54	0.72
2:F:169:LYS:HB3	2:F:170:PRO:CD	2.22	0.70
1:A:79:THR:HG23	2:B:154:ASN:OD1	1.92	0.69
2:B:169:LYS:HB3	2:B:170:PRO:CD	2.24	0.68
1:C:79:THR:HG23	2:D:154:ASN:OD1	1.95	0.67
2:F:211:LEU:N	2:F:211:LEU:HD23	2.10	0.66
2:F:169:LYS:HE2	2:F:172:GLN:OE1	1.96	0.64
2:D:213:TYR:CE1	2:D:217:ARG:HD3	2.33	0.63
2:D:169:LYS:HE2	2:D:172:GLN:OE1	1.98	0.62
2:D:211:LEU:HD23	2:D:211:LEU:N	2.15	0.62
1:A:61:SER:HB2	2:B:255:ASN:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:GLU:HG3	2:B:250:PRO:HD2	1.82	0.61
2:F:118:LEU:HD11	2:F:238:SER:O	1.99	0.61
2:B:207:GLU:O	2:B:210:LEU:HB3	2.01	0.61
1:C:27:TYR:O	1:C:28:MET:HB2	2.02	0.60
1:E:61:SER:HB2	2:F:255:ASN:HB2	1.83	0.60
2:B:276:LEU:C	2:B:278:PRO:HD3	2.22	0.60
1:A:43:VAL:HG12	2:B:258:THR:HA	1.84	0.60
2:F:213:TYR:CE1	2:F:217:ARG:HD3	2.37	0.60
2:F:84:THR:HG23	2:F:193:SER:HB2	1.83	0.59
2:F:214:LEU:HA	2:F:217:ARG:HG2	1.84	0.59
1:A:3:LEU:HG	1:A:7:LEU:HD21	1.85	0.59
2:D:118:LEU:HD11	2:D:238:SER:O	2.03	0.58
2:B:211:LEU:HD23	2:B:211:LEU:N	2.18	0.58
1:A:27:TYR:O	1:A:28:MET:HB2	2.03	0.58
2:B:169:LYS:HB2	2:B:172:GLN:OE1	2.04	0.58
2:D:207:GLU:O	2:D:210:LEU:HB3	2.04	0.58
1:C:3:LEU:HG	1:C:7:LEU:HD21	1.86	0.58
1:E:27:TYR:O	1:E:28:MET:HB2	2.04	0.58
1:E:3:LEU:HG	1:E:7:LEU:HD21	1.86	0.57
2:F:227:GLU:O	2:F:230:GLN:HB3	2.04	0.57
2:F:207:GLU:O	2:F:210:LEU:HB3	2.05	0.57
2:B:213:TYR:CE1	2:B:217:ARG:HD3	2.40	0.57
2:B:84:THR:HG23	2:B:193:SER:HB2	1.86	0.57
2:F:169:LYS:HB2	2:F:172:GLN:OE1	2.05	0.57
2:D:227:GLU:O	2:D:230:GLN:HB3	2.06	0.56
1:C:4:ASP:HA	1:C:7:LEU:HD23	1.87	0.56
2:F:240:TRP:N	2:F:240:TRP:CD1	2.73	0.56
2:F:161:ARG:CD	2:F:250:PRO:HA	2.36	0.56
2:D:196:VAL:HG21	2:D:225:ILE:HG12	1.88	0.56
2:D:240:TRP:CD1	2:D:240:TRP:N	2.74	0.56
2:D:170:PRO:HG2	2:D:171:GLY:H	1.70	0.55
1:C:61:SER:HB2	2:D:255:ASN:HB2	1.88	0.55
2:B:118:LEU:HD11	2:B:238:SER:O	2.07	0.55
2:D:214:LEU:HA	2:D:217:ARG:HG2	1.88	0.55
2:B:169:LYS:HB2	2:B:172:GLN:CD	2.27	0.54
1:C:27:TYR:CD2	1:C:28:MET:HG3	2.42	0.54
2:F:127:GLN:O	2:F:131:VAL:HG23	2.08	0.54
2:D:169:LYS:HB2	2:D:172:GLN:OE1	2.07	0.54
2:B:240:TRP:N	2:B:240:TRP:CD1	2.74	0.54
1:E:4:ASP:HA	1:E:7:LEU:HD23	1.89	0.54
2:B:160:GLU:O	2:B:172:GLN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:LEU:C	2:D:278:PRO:HD3	2.28	0.53
2:F:169:LYS:HB2	2:F:172:GLN:CD	2.28	0.53
2:F:101:VAL:HG13	2:F:240:TRP:CH2	2.43	0.53
2:F:175:GLY:HA2	2:F:248:MET:SD	2.49	0.53
2:D:101:VAL:HG13	2:D:240:TRP:CH2	2.44	0.53
1:E:43:VAL:HG12	2:F:258:THR:HA	1.90	0.53
2:D:202:TRP:CZ2	2:D:209:GLU:HG3	2.38	0.53
2:D:84:THR:HG23	2:D:193:SER:HB2	1.90	0.53
2:F:127:GLN:OE1	2:F:242:GLY:HA3	2.08	0.53
2:F:276:LEU:C	2:F:278:PRO:HD3	2.29	0.53
1:A:4:ASP:HA	1:A:7:LEU:HD23	1.90	0.52
2:F:121:TYR:CD1	2:F:121:TYR:N	2.78	0.52
1:A:27:TYR:CD2	1:A:28:MET:HG3	2.44	0.52
2:B:169:LYS:HE2	2:B:172:GLN:OE1	2.08	0.52
2:D:169:LYS:HB2	2:D:172:GLN:CD	2.30	0.52
2:B:214:LEU:HA	2:B:217:ARG:HG2	1.92	0.52
2:D:249:GLU:HG3	2:D:250:PRO:HD2	1.90	0.52
2:B:198:ASP:HB2	1:C:56:LEU:HD21	1.92	0.52
2:B:217:ARG:NH1	1:C:53:ASN:OD1	2.43	0.51
2:B:303:SER:HA	2:B:308:LEU:HD22	1.92	0.51
2:F:202:TRP:CG	2:F:210:LEU:HD13	2.46	0.51
2:F:161:ARG:CZ	2:F:250:PRO:HG3	2.40	0.51
1:E:27:TYR:CD2	1:E:28:MET:HG3	2.45	0.51
2:F:196:VAL:HG21	2:F:225:ILE:HG12	1.92	0.51
2:D:96:LEU:O	2:D:290:MET:HB2	2.11	0.50
2:B:84:THR:O	2:B:84:THR:HG23	2.11	0.50
1:C:43:VAL:HG12	2:D:258:THR:HA	1.92	0.50
2:B:289:THR:OG1	2:B:291:PRO:HD2	2.12	0.50
2:F:84:THR:HG23	2:F:84:THR:O	2.12	0.50
2:D:161:ARG:CD	2:D:250:PRO:HA	2.42	0.49
1:A:3:LEU:O	1:A:7:LEU:HD22	2.13	0.49
2:F:249:GLU:HG3	2:F:250:PRO:HD2	1.94	0.49
2:B:170:PRO:HG2	2:B:171:GLY:H	1.77	0.49
2:F:303:SER:HA	2:F:308:LEU:HD22	1.95	0.49
2:B:181:ALA:CB	2:B:241:ILE:HG12	2.43	0.49
2:F:122:ASP:OD2	2:F:124:LYS:HB2	2.13	0.48
2:F:170:PRO:HG2	2:F:171:GLY:H	1.77	0.48
2:D:303:SER:HA	2:D:308:LEU:HD22	1.94	0.48
1:E:71:TYR:CZ	1:E:73:GLY:HA3	2.48	0.48
2:D:179:ALA:HB2	2:D:243:PHE:HD1	1.79	0.48
2:F:228:CYS:O	2:F:231:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:O	2:D:209:GLU:HB3	2.14	0.48
1:C:27:TYR:CD1	1:C:37:TYR:HB3	2.49	0.48
2:B:249:GLU:HG3	2:B:250:PRO:CD	2.44	0.48
2:F:160:GLU:O	2:F:172:GLN:HB3	2.13	0.48
2:D:152:CYS:HB3	2:D:259:VAL:HG23	1.95	0.48
2:F:303:SER:HA	2:F:308:LEU:CD2	2.43	0.47
1:A:51:SER:OG	1:A:53:ASN:ND2	2.47	0.47
2:B:161:ARG:CD	2:B:250:PRO:HA	2.43	0.47
3:F:82:PYR:H31	4:F:482:PVH:HA	1.52	0.47
1:C:7:LEU:HB3	1:C:12:VAL:HB	1.97	0.47
2:F:289:THR:OG1	2:F:291:PRO:HD2	2.15	0.47
1:E:47:VAL:HA	2:F:253:ILE:O	2.15	0.47
2:B:227:GLU:O	2:B:230:GLN:HB3	2.15	0.47
2:F:179:ALA:HB2	2:F:243:PHE:HD1	1.80	0.47
2:F:161:ARG:HD2	2:F:250:PRO:HA	1.96	0.47
2:B:197:GLU:HB3	2:B:258:THR:HG21	1.95	0.46
2:B:96:LEU:O	2:B:290:MET:HB2	2.15	0.46
1:A:48:ARG:NH1	2:F:227:GLU:OE2	2.48	0.46
2:B:121:TYR:N	2:B:121:TYR:CD1	2.82	0.46
2:F:176:VAL:HG13	2:F:256:ALA:HB2	1.96	0.46
2:F:206:ASN:O	2:F:209:GLU:HB3	2.14	0.46
1:C:47:VAL:HA	2:D:253:ILE:O	2.15	0.46
1:C:71:TYR:CZ	1:C:73:GLY:HA3	2.50	0.46
2:D:290:MET:HB3	2:D:291:PRO:HD3	1.97	0.46
2:F:181:ALA:CB	2:F:241:ILE:HG12	2.46	0.46
2:B:179:ALA:HB2	2:B:243:PHE:HD1	1.80	0.46
2:B:217:ARG:O	2:B:220:ALA:HB3	2.14	0.46
2:B:101:VAL:HG13	2:B:240:TRP:CH2	2.51	0.46
1:C:39:THR:HA	2:D:261:PRO:O	2.16	0.46
2:D:213:TYR:CD1	2:D:217:ARG:HD3	2.51	0.46
2:F:213:TYR:CD1	2:F:217:ARG:HD3	2.51	0.46
2:F:211:LEU:CD2	2:F:211:LEU:N	2.79	0.46
2:F:202:TRP:CD2	2:F:210:LEU:HD13	2.51	0.45
2:D:289:THR:OG1	2:D:291:PRO:HD2	2.17	0.45
2:F:294:LEU:CD2	2:F:301:SER:HA	2.46	0.45
2:D:202:TRP:CG	2:D:210:LEU:HD13	2.51	0.45
2:F:290:MET:HB3	2:F:291:PRO:HD3	1.99	0.45
2:B:155:LYS:HE2	1:C:59:ILE:HD11	1.99	0.45
2:D:174:TYR:CE2	2:D:205:PRO:HD3	2.52	0.45
1:E:13:ASP:OD2	1:E:35:ASN:HB2	2.17	0.45
2:B:174:TYR:CE2	2:B:205:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:THR:HG23	2:F:154:ASN:OD1	2.16	0.45
2:B:206:ASN:O	2:B:209:GLU:HB3	2.17	0.45
1:A:71:TYR:CZ	1:A:73:GLY:HA3	2.52	0.45
1:C:51:SER:OG	1:C:53:ASN:ND2	2.51	0.44
2:D:160:GLU:O	2:D:172:GLN:HB3	2.18	0.44
2:D:290:MET:O	2:D:294:LEU:HD12	2.18	0.44
2:D:121:TYR:N	2:D:121:TYR:CD1	2.85	0.44
3:D:82:PYR:H31	4:D:482:PVH:HA	1.56	0.44
1:E:39:THR:HA	2:F:261:PRO:O	2.18	0.44
1:C:75:ILE:CD1	2:D:144:PRO:HB2	2.40	0.44
2:B:152:CYS:HB3	2:B:259:VAL:HG23	1.98	0.44
2:D:217:ARG:HA	2:D:217:ARG:HD2	1.83	0.44
2:B:181:ALA:O	2:B:195:PHE:HA	2.18	0.43
2:B:277:THR:N	2:B:278:PRO:HD3	2.32	0.43
2:F:211:LEU:H	2:F:211:LEU:HD23	1.81	0.43
2:D:107:LEU:O	2:D:108:PHE:HB3	2.18	0.43
2:D:294:LEU:CD2	2:D:301:SER:HA	2.48	0.43
3:B:82:PYR:H31	4:B:482:PVH:HA	1.53	0.43
2:F:107:LEU:O	2:F:108:PHE:HB3	2.18	0.43
1:A:13:ASP:OD2	1:A:35:ASN:HB2	2.19	0.43
2:B:175:GLY:HA2	2:B:248:MET:SD	2.58	0.43
2:D:175:GLY:HA2	2:D:248:MET:SD	2.58	0.43
2:F:290:MET:O	2:F:294:LEU:HD12	2.17	0.43
1:A:47:VAL:HA	2:B:253:ILE:O	2.19	0.43
1:E:3:LEU:HG	1:E:7:LEU:CD2	2.49	0.43
2:F:96:LEU:O	2:F:290:MET:HB2	2.19	0.43
1:C:17:ILE:HB	1:C:33:ILE:HB	1.99	0.43
2:F:119:PRO:HB2	2:F:121:TYR:CE1	2.53	0.43
2:D:157:VAL:CG1	2:D:199:ALA:HB1	2.48	0.43
2:F:152:CYS:HB3	2:F:259:VAL:HG23	2.00	0.43
1:E:7:LEU:HB3	1:E:12:VAL:HB	2.01	0.43
2:F:180:ILE:HB	2:F:258:THR:OG1	2.19	0.43
2:F:270:ILE:HG23	2:F:285:MET:SD	2.59	0.43
2:F:197:GLU:HB3	2:F:258:THR:HG21	2.00	0.43
2:F:277:THR:N	2:F:278:PRO:HD3	2.34	0.43
1:A:7:LEU:HB3	1:A:12:VAL:HB	2.00	0.42
2:B:196:VAL:HG21	2:B:225:ILE:HG12	2.00	0.42
2:D:217:ARG:O	2:D:220:ALA:HB3	2.19	0.42
1:E:40:GLY:O	2:F:261:PRO:HD2	2.18	0.42
2:D:227:GLU:OE2	1:E:48:ARG:NH1	2.51	0.42
2:B:127:GLN:O	2:B:131:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:ARG:NH1	2:F:248:MET:O	2.51	0.42
1:A:39:THR:HA	2:B:261:PRO:O	2.19	0.42
2:D:127:GLN:O	2:D:131:VAL:HG23	2.19	0.42
2:F:217:ARG:O	2:F:220:ALA:HB3	2.18	0.42
2:B:294:LEU:CD2	2:B:301:SER:HA	2.49	0.42
2:D:209:GLU:O	2:D:212:GLU:N	2.51	0.42
1:E:40:GLY:O	2:F:260:ALA:HA	2.20	0.42
2:F:202:TRP:CE3	2:F:202:TRP:HA	2.54	0.42
2:B:154:ASN:O	2:B:155:LYS:HG3	2.20	0.42
1:C:3:LEU:O	1:C:7:LEU:HD22	2.19	0.42
1:E:42:LYS:NZ	1:E:68:LYS:O	2.52	0.42
1:E:26:GLY:CA	2:F:150:ILE:HD13	2.50	0.42
2:B:217:ARG:HD2	2:B:217:ARG:HA	1.82	0.42
2:D:197:GLU:HB3	2:D:258:THR:HG21	2.01	0.41
2:D:169:LYS:CB	2:D:170:PRO:CD	2.95	0.41
2:B:107:LEU:O	2:B:108:PHE:HB3	2.20	0.41
2:B:213:TYR:O	2:B:217:ARG:HG2	2.20	0.41
2:D:211:LEU:CD2	2:D:211:LEU:N	2.83	0.41
1:C:40:GLY:O	2:D:260:ALA:HA	2.20	0.41
2:D:213:TYR:O	2:D:217:ARG:HG2	2.20	0.41
2:D:161:ARG:NH1	2:D:248:MET:O	2.51	0.41
2:B:209:GLU:O	2:B:212:GLU:N	2.52	0.41
2:D:96:LEU:HD12	2:D:96:LEU:HA	1.87	0.41
2:B:122:ASP:OD2	2:B:124:LYS:HB2	2.19	0.41
2:B:290:MET:HB3	2:B:291:PRO:HD3	2.03	0.41
1:A:45:ALA:HA	2:B:255:ASN:O	2.20	0.41
2:B:181:ALA:HB2	2:B:241:ILE:HG12	2.03	0.41
1:E:18:SER:HA	1:E:19:PRO:HD2	1.93	0.41
1:E:3:LEU:O	1:E:7:LEU:HD22	2.21	0.41
2:B:280:LYS:O	2:B:284:ILE:HG13	2.21	0.41
2:F:168:MET:O	2:F:169:LYS:O	2.38	0.41
2:B:213:TYR:CD1	2:B:217:ARG:HD3	2.56	0.40
2:B:130:LEU:HD11	2:B:134:PHE:CE1	2.57	0.40
2:D:157:VAL:HG12	2:D:199:ALA:HB1	2.04	0.40
1:E:51:SER:OG	1:E:53:ASN:ND2	2.54	0.40
2:F:181:ALA:O	2:F:195:PHE:HA	2.20	0.40
1:A:15:ILE:O	1:A:34:GLY:HA3	2.21	0.40
1:A:3:LEU:HG	1:A:7:LEU:CD2	2.50	0.40
1:A:40:GLY:O	2:B:261:PRO:HD2	2.21	0.40
1:C:45:ALA:HA	2:D:255:ASN:O	2.22	0.40
2:D:154:ASN:O	2:D:155:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ALA:HA	2:F:255:ASN:O	2.21	0.40
1:E:7:LEU:HD22	1:E:7:LEU:N	2.37	0.40
2:B:202:TRP:CG	2:B:210:LEU:HD13	2.56	0.40
2:B:161:ARG:NH1	2:B:248:MET:O	2.52	0.40
2:D:202:TRP:HA	2:D:202:TRP:CE3	2.56	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	79/81 (98%)	68 (86%)	10 (13%)	1 (1%)	13	52
1	C	79/81 (98%)	68 (86%)	10 (13%)	1 (1%)	13	52
1	E	79/81 (98%)	68 (86%)	9 (11%)	2 (2%)	6	36
2	B	226/228 (99%)	197 (87%)	24 (11%)	5 (2%)	7	39
2	D	226/228 (99%)	195 (86%)	25 (11%)	6 (3%)	5	34
2	F	226/228 (99%)	195 (86%)	27 (12%)	4 (2%)	9	45
All	All	915/927 (99%)	791 (86%)	105 (12%)	19 (2%)	8	40

All (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
1	E	73	GLY
2	F	165	ASP

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Mol	Chain	Res	Type
2	F	169	LYS
2	B	165	ASP
2	D	165	ASP
2	D	170	PRO
2	F	170	PRO
2	B	304	ALA
2	F	239	SER
2	B	239	SER
2	D	239	SER
2	D	210	LEU
2	D	304	ALA
1	E	2	GLU

### 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%)	20	58
1	C	66/66 (100%)	61 (92%)	5 (8%)	14	49
1	E	66/66 (100%)	59 (89%)	7 (11%)	7	30
2	B	188/188 (100%)	176 (94%)	12 (6%)	19	56
2	D	188/188 (100%)	171 (91%)	17 (9%)	10	38
2	F	188/188 (100%)	173 (92%)	15 (8%)	13	46
All	All	762/762 (100%)	702 (92%)	60 (8%)	13	46

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	48	ARG
1	A	53	ASN
1	A	79	THR
2	B	100	GLU
2	B	126	LEU

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Mol	Chain	Res	Type
2	B	138	GLN
2	B	161	ARG
2	B	204	THR
2	B	223	LYS
2	B	230	GLN
2	B	237	GLU
2	B	248	MET
2	B	259	VAL
2	B	300	LYS
2	B	308	LEU
1	C	24	THR
1	C	43	VAL
1	C	48	ARG
1	C	53	ASN
1	C	79	THR
2	D	84	THR
2	D	96	LEU
2	D	100	GLU
2	D	121	TYR
2	D	126	LEU
2	D	138	GLN
2	D	161	ARG
2	D	204	THR
2	D	211	LEU
2	D	223	LYS
2	D	230	GLN
2	D	237	GLU
2	D	248	MET
2	D	259	VAL
2	D	277	THR
2	D	300	LYS
2	D	308	LEU
1	E	24	THR
1	E	43	VAL
1	E	44	ASP
1	E	48	ARG
1	E	53	ASN
1	E	67	THR
1	E	79	THR
2	F	96	LEU
2	F	100	GLU
2	F	121	TYR

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Mol	Chain	Res	Type
2	F	126	LEU
2	F	138	GLN
2	F	161	ARG
2	F	204	THR
2	F	211	LEU
2	F	223	LYS
2	F	237	GLU
2	F	248	MET
2	F	259	VAL
2	F	277	THR
2	F	300	LYS
2	F	308	LEU

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

Mol	Chain	Res	Type
1	A	8	ASN
2	B	87	GLN
2	D	87	GLN
2	F	138	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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
4	PVH	B	482	3	8,12,12	0.82	0	8,15,15	2.20	4 (50%)
3	PYR	B	82	2,4	3,3,5	1.97	1 (33%)	2,2,6	2.13	1 (50%)
4	PVH	D	482	3	8,12,12	0.84	1 (12%)	8,15,15	2.18	4 (50%)
3	PYR	D	82	2,4	3,3,5	1.50	1 (33%)	2,2,6	2.17	1 (50%)
4	PVH	F	482	3	8,12,12	1.07	1 (12%)	8,15,15	2.06	3 (37%)
3	PYR	F	82	2,4	3,3,5	1.61	1 (33%)	2,2,6	2.11	1 (50%)

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
4	PVH	B	482	3	-	0/10/10/10	0/1/1/1
3	PYR	B	82	2,4	-	0/0/1/4	0/0/0/0
4	PVH	D	482	3	-	0/10/10/10	0/1/1/1
3	PYR	D	82	2,4	-	0/0/1/4	0/0/0/0
4	PVH	F	482	3	-	0/10/10/10	0/1/1/1
3	PYR	F	82	2,4	-	0/0/1/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	82	PYR	C2-C1	-3.34	1.40	1.49
3	F	82	PYR	C2-C1	-2.70	1.42	1.49
3	D	82	PYR	C2-C1	-2.46	1.42	1.49
4	D	482	PVH	OE-C	2.01	1.38	1.33
4	F	482	PVH	OE-C	2.65	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	482	PVH	OE-C-O	-3.52	116.84	123.82
4	D	482	PVH	OE-C-O	-3.25	117.36	123.82
4	F	482	PVH	OE-C-O	-3.12	117.63	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	482	PVH	CD2-NE2-CE1	2.04	108.96	105.78
4	D	482	PVH	CM-OE-C	2.07	120.75	115.97
4	D	482	PVH	CD2-NE2-CE1	2.10	109.05	105.78
4	F	482	PVH	CD2-NE2-CE1	2.15	109.14	105.78
4	B	482	PVH	CM-OE-C	2.25	121.15	115.97
3	B	82	PYR	C3-C2-C1	2.26	119.43	113.06
3	F	82	PYR	C3-C2-C1	2.37	119.73	113.06
3	D	82	PYR	C3-C2-C1	2.42	119.89	113.06
4	F	482	PVH	OE-C-CA	3.73	121.15	111.52
4	B	482	PVH	OE-C-CA	3.87	121.51	111.52
4	D	482	PVH	OE-C-CA	3.96	121.75	111.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	482	PVH	1	0
3	B	82	PYR	1	0
4	D	482	PVH	1	0
3	D	82	PYR	1	0
4	F	482	PVH	1	0
3	F	82	PYR	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	81/81 (100%)	-0.73	0 100 100	13, 35, 70, 81	0
1	C	81/81 (100%)	-0.69	0 100 100	13, 36, 68, 82	0
1	E	81/81 (100%)	-0.72	0 100 100	15, 36, 69, 82	0
2	B	228/228 (100%)	-0.51	2 (0%) 84 76	13, 48, 80, 99	0
2	D	228/228 (100%)	-0.48	2 (0%) 84 76	13, 48, 80, 99	0
2	F	228/228 (100%)	-0.49	2 (0%) 84 76	12, 48, 79, 99	0
All	All	927/927 (100%)	-0.55	6 (0%) 89 83	12, 44, 79, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	164	ASN	3.3
2	B	167	ASP	2.7
2	F	167	ASP	2.6
2	D	167	ASP	2.4
2	B	164	ASN	2.4
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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PYR	F	82	4/6	0.91	0.18	36,37,37,38	0
4	PVH	D	482	12/12	0.94	0.19	36,38,44,45	0
4	PVH	B	482	12/12	0.94	0.17	35,39,42,49	0
4	PVH	F	482	12/12	0.95	0.16	36,39,42,47	0
3	PYR	D	82	4/6	0.96	0.11	37,38,38,40	0
3	PYR	B	82	4/6	0.98	0.12	36,37,38,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.