



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 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
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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

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

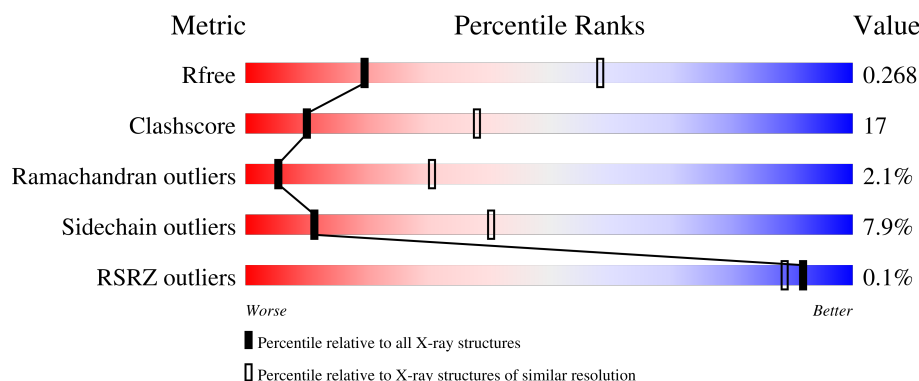
1 Overall quality at a glance

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% .
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 the smallest and is located at the far right of the bar. The bar is positioned within the 'Quality of chain' column of the table.

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:

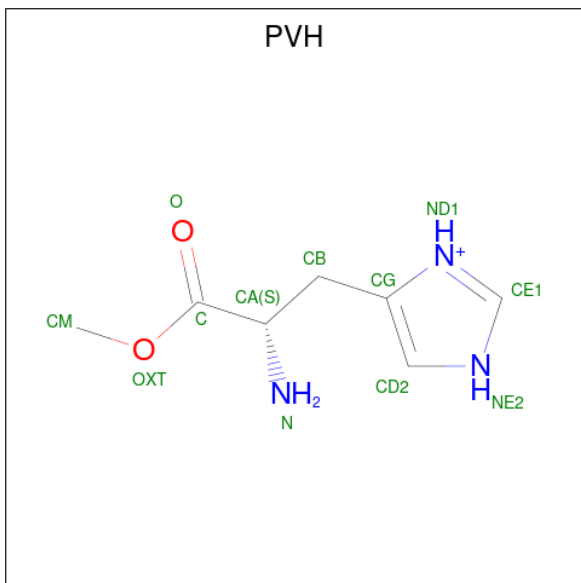
Chain	Residue	Modelled	Actual	Comment	Reference
B	82	PYR	SER	conflict	UNP P00862
D	82	PYR	SER	conflict	UNP P00862

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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: $C_7H_{12}N_3O_2$).



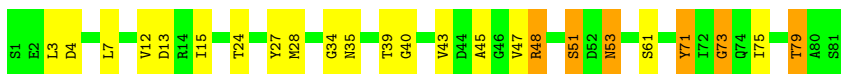
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			12	7	3	2		
3	D	1	Total	C	N	O	0	0
			12	7	3	2		
3	F	1	Total	C	N	O	0	0
			12	7	3	2		

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.

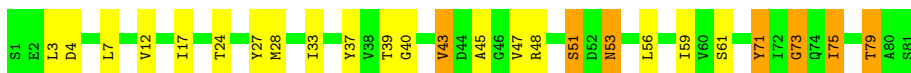
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain A: 



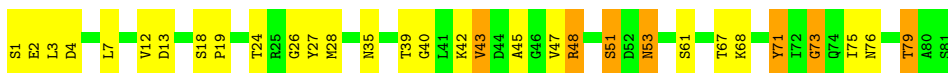
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain C: 



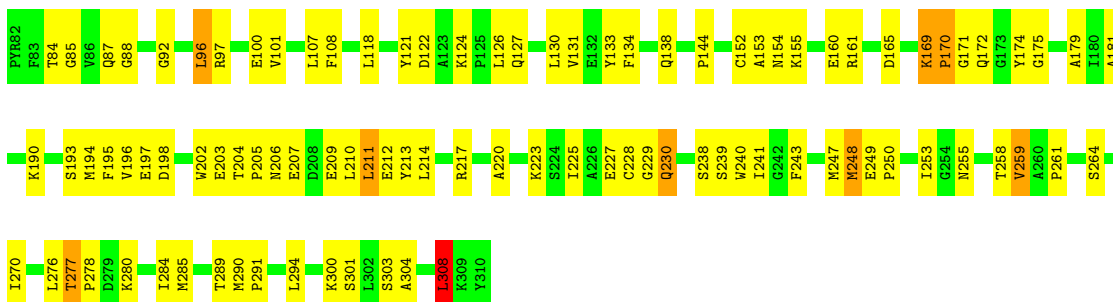
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN

Chain E: 



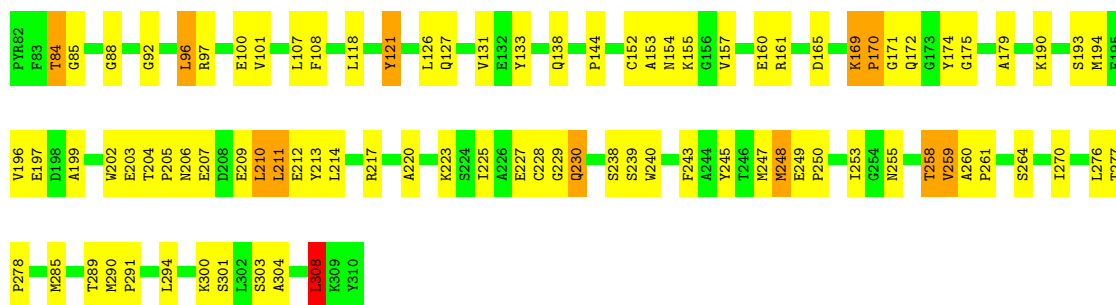
- Molecule 2: Histidine decarboxylase alpha chain

Chain B: 



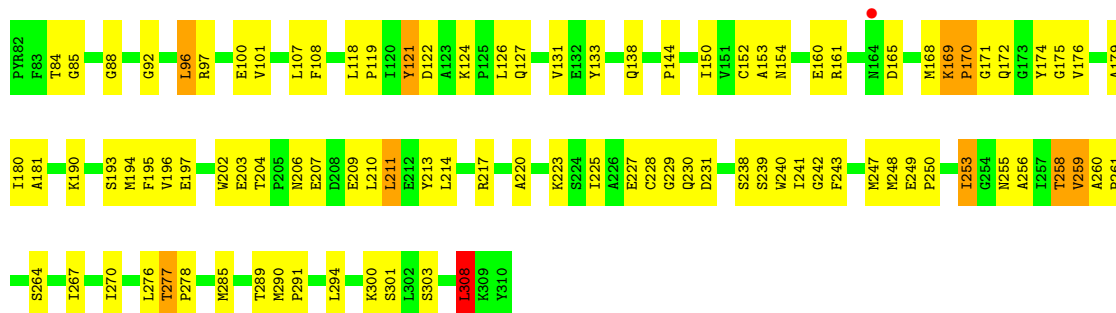
- Molecule 2: Histidine decarboxylase alpha chain

Chain D: 



• Molecule 2: Histidine decarboxylase alpha chain

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.

All (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
2	B	153	ALA	N-CA-C	-7.69	96.03	108.41
1	A	51	SER	N-CA-C	-6.98	99.22	109.63
1	A	71	TYR	N-CA-C	6.72	118.83	109.15
2	F	194	MET	N-CA-C	6.72	120.47	109.24
2	F	203	GLU	N-CA-C	6.64	121.67	113.50
1	C	51	SER	N-CA-C	-6.62	99.77	109.63
2	D	194	MET	N-CA-C	6.57	120.21	109.24
2	B	194	MET	N-CA-C	6.50	120.10	109.24
2	F	308	LEU	N-CA-C	6.36	119.31	109.07
2	D	203	GLU	N-CA-C	6.30	121.25	113.50
2	D	308	LEU	N-CA-C	6.25	119.14	109.07
1	E	71	TYR	N-CA-C	6.25	118.77	109.59
1	C	71	TYR	N-CA-C	6.10	117.94	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	GLU	N-CA-C	6.01	120.89	113.50
2	B	308	LEU	N-CA-C	6.00	119.02	109.24
1	E	51	SER	N-CA-C	-5.86	100.74	109.94
2	B	85	GLY	N-CA-C	5.63	119.67	112.13
2	D	133	TYR	N-CA-C	5.57	117.21	111.03
2	D	85	GLY	N-CA-C	5.55	119.57	112.13
2	F	267	ILE	N-CA-C	5.43	115.52	110.42
2	F	258	THR	N-CA-C	-5.40	100.10	108.90
2	D	264	SER	N-CA-C	-5.32	101.21	109.72
2	F	264	SER	N-CA-C	-5.27	101.28	109.72
2	B	264	SER	N-CA-C	-5.20	101.40	109.72
2	B	133	TYR	N-CA-C	5.20	116.80	111.03
1	E	76	ASN	N-CA-C	-5.13	100.16	108.41
2	F	85	GLY	N-CA-C	5.12	118.99	112.13
2	F	133	TYR	N-CA-C	5.07	116.62	111.14
1	C	75	ILE	N-CA-C	5.01	115.79	108.53
2	D	258	THR	N-CA-C	-5.00	100.74	108.90

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.

All (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
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:HD23	2:F:211:LEU:N	2.10	0.66
2:B:276:LEU:C	2:B:278:PRO:HD3	2.22	0.65
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
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
2:F:270:ILE:HG12	2:F:285:MET:HE2	1.82	0.60
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
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:B:169:LYS:HB2	2:B:172:GLN:CD	2.27	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:N	2:B:211:LEU:HD23	2.18	0.58

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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	0.58
1:A:27:TYR:O	1:A:28:MET:HB2	2.03	0.58
2:F:169:LYS:HB2	2:F:172:GLN:CD	2.28	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:276:LEU:C	2:F:278:PRO:HD3	2.29	0.57
2:F:174:TYR:O	2:F:247:MET:HE3	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:D:169:LYS:HB2	2:D:172:GLN:CD	2.30	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:D:270:ILE:HG12	2:D:285:MET:HE2	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:N	2:D:240:TRP:CD1	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
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:CD1	2:B:240:TRP:N	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
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:B:270:ILE:HG12	2:B:285:MET:HE2	1.89	0.53
2:F:127:GLN:OE1	2:F:242:GLY:HA3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASP:HA	1:A:7:LEU:HD23	1.90	0.52
2:F:121:TYR:N	2:F:121:TYR:CD1	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: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:161:ARG:CZ	2:F:250:PRO:HG3	2.40	0.51
2:F:202:TRP:CG	2:F:210:LEU:HD13	2.46	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:HG23	2:B:84:THR:O	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:48:ARG:NH1	2:F:227:GLU:OE2	2.48	0.46
2:B:96:LEU:O	2:B:290:MET:HB2	2.15	0.46
2:B:197:GLU:HB3	2:B:258:THR:HG21	1.95	0.46
2:B:121:TYR:CD1	2:B:121:TYR:N	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:101:VAL:HG13	2:B:240:TRP:CH2	2.51	0.46
2:B:217:ARG:O	2:B:220:ALA:HB3	2.14	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:N	2:F:211:LEU:CD2	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
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:CD1	2:D:121:TYR:N	2.85	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:D:209:GLU:O	2:D:210:LEU:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	2:F:211:LEU:H	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
2:F:161:ARG:C	2:F:161:ARG:HD3	2.43	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
2:D:174:TYR:O	2:D:247:MET:HE3	2.18	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:B:209:GLU:O	2:B:210:LEU:C	2.61	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
2:D:227:GLU:OE2	1:E:48:ARG:NH1	2.51	0.42
1:E:40:GLY:O	2:F:261:PRO:HD2	2.18	0.42
2:B:127:GLN:O	2:B:131:VAL:HG23	2.19	0.42
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:174:TYR:O	2:B:247:MET:HE3	2.19	0.42
2:B:228:CYS:O	2:B:229:GLY:C	2.63	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:HA	2:F:202:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:GLY:CA	2:F:150:ILE:HD13	2.50	0.42
2:B:217:ARG:HA	2:B:217:ARG:HD2	1.82	0.42
1:E:42:LYS:NZ	1:E:68:LYS:O	2.52	0.42
2:F:168:MET:O	2:F:169:LYS:C	2.63	0.41
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
1:E:1:SER:C	1:E:3:LEU:N	2.78	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:N	2:D:211:LEU:CD2	2.83	0.41
1:C:40:GLY:O	2:D:260:ALA:HA	2.20	0.41
2:D:161:ARG:NH1	2:D:248:MET:O	2.51	0.41
2:D:213:TYR:O	2:D:217:ARG:HG2	2.20	0.41
2:D:228:CYS:O	2:D:229:GLY:C	2.63	0.41
2:B:209:GLU:O	2:B:212:GLU:N	2.52	0.41
2:D:96:LEU:HA	2:D:96:LEU:HD12	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
2:F:228:CYS:O	2:F:229:GLY:C	2.63	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
2:D:161:ARG:HD3	2:D:161:ARG:C	2.45	0.41
1:E:3:LEU:O	1:E:7:LEU:HD22	2.21	0.41
1:E:18:SER:HA	1:E:19:PRO:HD2	1.93	0.41
2:B:280:LYS:O	2:B:284:ILE:HG13	2.21	0.41
2:D:245:TYR:CD2	2:D:245:TYR:C	2.99	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
1:E:7:LEU:HD22	1:E:7:LEU:N	2.37	0.40
1:E:45:ALA:HA	2:F:255:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ARG:NH1	2:B:248:MET:O	2.52	0.40
2:B:202:TRP:CG	2:B:210:LEU:HD13	2.56	0.40
2:D:202:TRP:CE3	2:D:202:TRP:HA	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%)	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
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

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
2	F	169	LYS
2	B	165	ASP

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Mol	Chain	Res	Type
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 [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	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

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	87	GLN
2	B	96	LEU
2	B	100	GLU
2	B	126	LEU

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Mol	Chain	Res	Type
2	B	138	GLN
2	B	190	LYS
2	B	204	THR
2	B	211	LEU
2	B	223	LYS
2	B	230	GLN
2	B	248	MET
2	B	259	VAL
2	B	277	THR
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	190	LYS
2	D	204	THR
2	D	211	LEU
2	D	223	LYS
2	D	230	GLN
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	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
2	F	126	LEU

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Mol	Chain	Res	Type
2	F	138	GLN
2	F	190	LYS
2	F	204	THR
2	F	211	LEU
2	F	223	LYS
2	F	253	ILE
2	F	259	VAL
2	F	277	THR
2	F	300	LYS
2	F	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
2	B	87	GLN
2	B	138	GLN
1	C	8	ASN
2	D	87	GLN
2	D	164	ASN
2	D	230	GLN
2	D	306	ASN
1	E	8	ASN
2	F	87	GLN
2	F	164	ASN
2	F	230	GLN
2	F	255	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

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%)
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

All (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
3	F	482	PVH	OXT-C-O	-3.19	117.63	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	482	PVH	CB-CA-C	-2.97	101.72	110.46
3	B	482	PVH	CB-CA-C	-2.83	102.13	110.46
3	D	482	PVH	CB-CA-C	-2.69	102.54	110.46
3	B	482	PVH	CM-OXT-C	2.31	121.15	115.92
3	D	482	PVH	CM-OXT-C	2.13	120.75	115.92

There are no chirality outliers.

All (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
3	F	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.