



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:08 AM UTC

PDB ID : 5IAO / pdb_00005iao
Title : Structure and mapping of spontaneous mutational sites of PyrR from Mycobacterium tuberculosis
Authors : Sivaraman, J.; Ghode, P.; Ramachandran, S.
Deposited on : 2016-02-21
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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<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

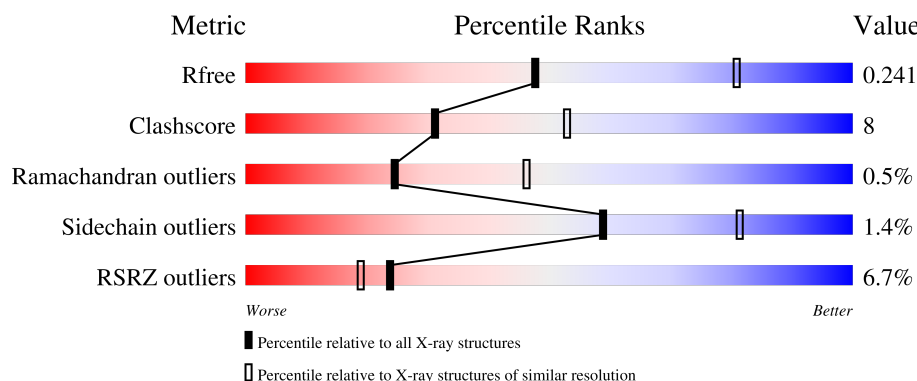
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	199	
1	B	199	
1	C	199	
1	D	199	
1	E	199	

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Mol	Chain	Length	Quality of chain
1	F	199	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URF	A	301	-	X	-	-
2	URF	C	301	-	X	-	-
2	URF	F	301	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8150 atoms, of which 9 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 Bifunctional protein PyrR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1296	798	250	247	1			
1	B	171	Total	C	N	O	S	0	0	0
			1295	798	250	246	1			
1	C	171	Total	C	N	O	S	0	0	0
			1296	798	250	247	1			
1	D	171	Total	C	N	O	S	0	0	0
			1295	798	250	246	1			
1	E	171	Total	C	N	O	S	0	0	0
			1296	798	250	247	1			
1	F	171	Total	C	N	O	S	0	0	0
			1295	798	250	246	1			

There are 36 discrepancies between the modelled and reference sequences:

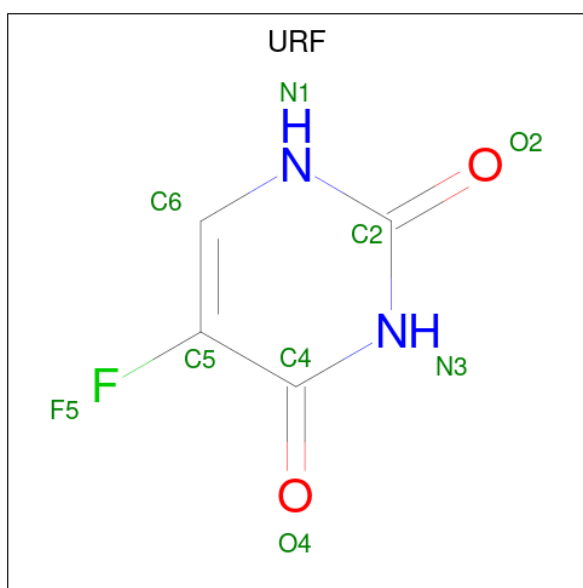
Chain	Residue	Modelled	Actual	Comment	Reference
A	194	HIS	-	expression tag	UNP A5U281
A	195	HIS	-	expression tag	UNP A5U281
A	196	HIS	-	expression tag	UNP A5U281
A	197	HIS	-	expression tag	UNP A5U281
A	198	HIS	-	expression tag	UNP A5U281
A	199	HIS	-	expression tag	UNP A5U281
B	194	HIS	-	expression tag	UNP A5U281
B	195	HIS	-	expression tag	UNP A5U281
B	196	HIS	-	expression tag	UNP A5U281
B	197	HIS	-	expression tag	UNP A5U281
B	198	HIS	-	expression tag	UNP A5U281
B	199	HIS	-	expression tag	UNP A5U281
C	194	HIS	-	expression tag	UNP A5U281
C	195	HIS	-	expression tag	UNP A5U281
C	196	HIS	-	expression tag	UNP A5U281
C	197	HIS	-	expression tag	UNP A5U281
C	198	HIS	-	expression tag	UNP A5U281

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Chain	Residue	Modelled	Actual	Comment	Reference
C	199	HIS	-	expression tag	UNP A5U281
D	194	HIS	-	expression tag	UNP A5U281
D	195	HIS	-	expression tag	UNP A5U281
D	196	HIS	-	expression tag	UNP A5U281
D	197	HIS	-	expression tag	UNP A5U281
D	198	HIS	-	expression tag	UNP A5U281
D	199	HIS	-	expression tag	UNP A5U281
E	194	HIS	-	expression tag	UNP A5U281
E	195	HIS	-	expression tag	UNP A5U281
E	196	HIS	-	expression tag	UNP A5U281
E	197	HIS	-	expression tag	UNP A5U281
E	198	HIS	-	expression tag	UNP A5U281
E	199	HIS	-	expression tag	UNP A5U281
F	194	HIS	-	expression tag	UNP A5U281
F	195	HIS	-	expression tag	UNP A5U281
F	196	HIS	-	expression tag	UNP A5U281
F	197	HIS	-	expression tag	UNP A5U281
F	198	HIS	-	expression tag	UNP A5U281
F	199	HIS	-	expression tag	UNP A5U281

- Molecule 2 is 5-FLUOROURACIL (CCD ID: URF) (formula: $C_4H_3FN_2O_2$).



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

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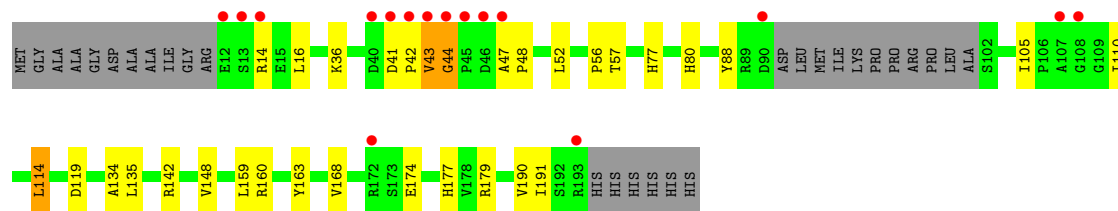
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	F	1	Total	C	F	H	N	O	0	0
			12	4	1	3	2	2		

- Molecule 3 is water.

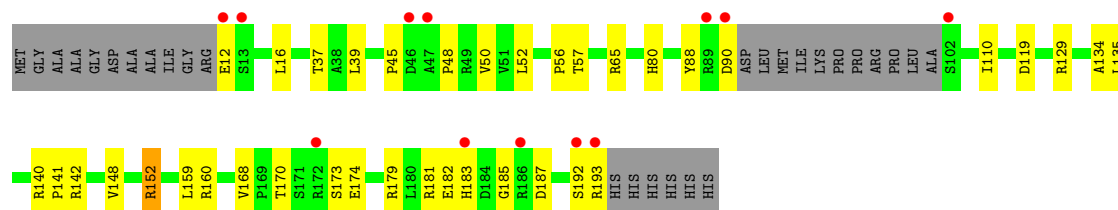
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	46	Total	O	0	0
			46	46		
3	C	80	Total	O	0	0
			80	80		
3	D	51	Total	O	0	0
			51	51		
3	E	46	Total	O	0	0
			46	46		
3	F	61	Total	O	0	0
			61	61		

- Molecule 1: Bifunctional protein PyrR

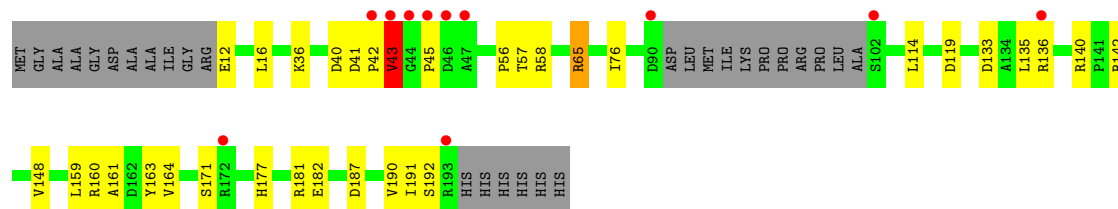




• Molecule 1: Bifunctional protein PyrR



• Molecule 1: Bifunctional protein PyrR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.84Å 127.77Å 90.78Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	42.24 – 2.60 42.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.24-2.60) 93.6 (42.24-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.195 , 0.238 0.204 , 0.241	Depositor DCC
R_{free} test set	2007 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8150	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: URF

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	0.36	0/1312	0.81	2/1780 (0.1%)
1	B	0.37	0/1311	0.76	0/1779
1	C	0.38	0/1312	0.84	2/1780 (0.1%)
1	D	0.37	0/1311	0.84	2/1779 (0.1%)
1	E	0.36	0/1312	0.81	0/1780
1	F	0.36	0/1311	0.80	0/1779
All	All	0.37	0/7869	0.81	6/10677 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	GLY	CA-C-N	8.78	128.10	118.97
1	D	44	GLY	C-N-CA	8.78	128.10	118.97
1	C	47	ALA	CA-C-N	6.84	127.02	120.31
1	C	47	ALA	C-N-CA	6.84	127.02	120.31
1	A	47	ALA	CA-C-N	6.48	126.66	120.31

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	1296	0	1321	24	0
1	B	1295	0	1321	21	0
1	C	1296	0	1321	14	0
1	D	1295	0	1321	29	0
1	E	1296	0	1321	30	0
1	F	1295	0	1321	25	0
2	A	9	3	3	0	0
2	C	9	3	3	0	0
2	F	9	3	3	1	0
3	A	57	0	0	1	0
3	B	46	0	0	1	0
3	C	80	0	0	0	0
3	D	51	0	0	0	0
3	E	46	0	0	2	0
3	F	61	0	0	0	0
All	All	8141	9	7935	129	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 8.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:HG23	1:A:183:HIS:HE1	1.45	0.82
1:A:159:LEU:HD23	1:B:159:LEU:HD23	1.61	0.81
1:F:16:LEU:HD11	1:F:191:ILE:HG22	1.64	0.80
1:C:159:LEU:HD23	1:D:159:LEU:HD23	1.63	0.80
1:B:16:LEU:HD21	1:B:191:ILE:HB	1.67	0.77

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	167/199 (84%)	165 (99%)	2 (1%)	0	100	100
1	B	167/199 (84%)	164 (98%)	3 (2%)	0	100	100
1	C	167/199 (84%)	164 (98%)	1 (1%)	2 (1%)	10	23
1	D	167/199 (84%)	165 (99%)	1 (1%)	1 (1%)	21	42
1	E	167/199 (84%)	166 (99%)	1 (1%)	0	100	100
1	F	167/199 (84%)	164 (98%)	1 (1%)	2 (1%)	10	23
All	All	1002/1194 (84%)	988 (99%)	9 (1%)	5 (0%)	24	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	43	VAL
1	C	43	VAL
1	F	43	VAL
1	C	42	PRO
1	F	42	PRO

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	140/160 (88%)	138 (99%)	2 (1%)	59	81
1	B	140/160 (88%)	138 (99%)	2 (1%)	59	81
1	C	140/160 (88%)	139 (99%)	1 (1%)	76	89
1	D	140/160 (88%)	138 (99%)	2 (1%)	59	81
1	E	140/160 (88%)	138 (99%)	2 (1%)	59	81
1	F	140/160 (88%)	137 (98%)	3 (2%)	47	73
All	All	840/960 (88%)	828 (99%)	12 (1%)	59	81

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	152	ARG
1	E	183	HIS
1	F	171	SER
1	F	43	VAL
1	B	114	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	B	69	ASN
1	C	167	ASN
1	C	69	ASN
1	A	167	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	URF	F	301	-	9,9,9	4.62	5 (55%)	12,12,12	4.05	7 (58%)
2	URF	A	301	-	9,9,9	4.66	5 (55%)	12,12,12	4.08	8 (66%)
2	URF	C	301	-	9,9,9	4.67	5 (55%)	12,12,12	4.14	8 (66%)

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
2	URF	F	301	-	-	-	0/1/1/1
2	URF	A	301	-	-	-	0/1/1/1
2	URF	C	301	-	-	-	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	URF	C6-C5	9.37	1.41	1.33
2	F	301	URF	C6-C5	9.21	1.41	1.33
2	A	301	URF	C6-C5	9.17	1.41	1.33
2	A	301	URF	C2-N1	7.62	1.46	1.36
2	F	301	URF	C2-N1	7.59	1.46	1.36

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	URF	C5-C4-N3	7.91	119.88	112.64
2	C	301	URF	C5-C4-N3	7.80	119.78	112.64
2	F	301	URF	C5-C4-N3	7.69	119.67	112.64
2	F	301	URF	O4-C4-C5	-6.74	119.95	125.69
2	A	301	URF	O4-C4-C5	-6.35	120.28	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	URF	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/199 (85%)	-0.09	7 (4%) 41 36	20, 29, 56, 97	0
1	B	171/199 (85%)	0.15	12 (7%) 22 18	22, 32, 69, 103	0
1	C	171/199 (85%)	0.05	11 (6%) 25 20	19, 29, 67, 102	0
1	D	171/199 (85%)	0.33	16 (9%) 14 11	20, 32, 69, 110	0
1	E	171/199 (85%)	0.16	12 (7%) 22 18	20, 32, 66, 105	0
1	F	171/199 (85%)	0.05	11 (6%) 25 20	21, 29, 68, 94	0
All	All	1026/1194 (85%)	0.11	69 (6%) 24 19	19, 31, 68, 110	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	45	PRO	7.8
1	D	44	GLY	7.5
1	D	43	VAL	7.1
1	B	90	ASP	6.5
1	B	45	PRO	6.5

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
2	URF	F	301	9/9	0.77	0.18	51,64,78,81	0
2	URF	A	301	9/9	0.84	0.13	50,57,79,95	0
2	URF	C	301	9/9	0.85	0.14	48,58,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.