



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:41 PM UTC

PDB ID : 1PVV / pdb_00001pvv
Title : Refined Structure of Pyrococcus furiosus Ornithine Carbamoyltransferase at 1.87 Å
Authors : Massant, J.; Wouters, J.; Glansdorff, N.
Deposited on : 2003-06-29
Resolution : 1.87 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

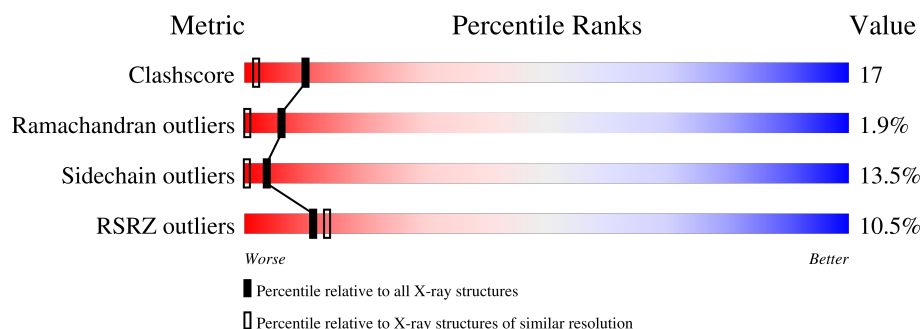
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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))
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	315	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2653 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 Ornithine carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2454	1559	425	457	13			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			3	2	1		

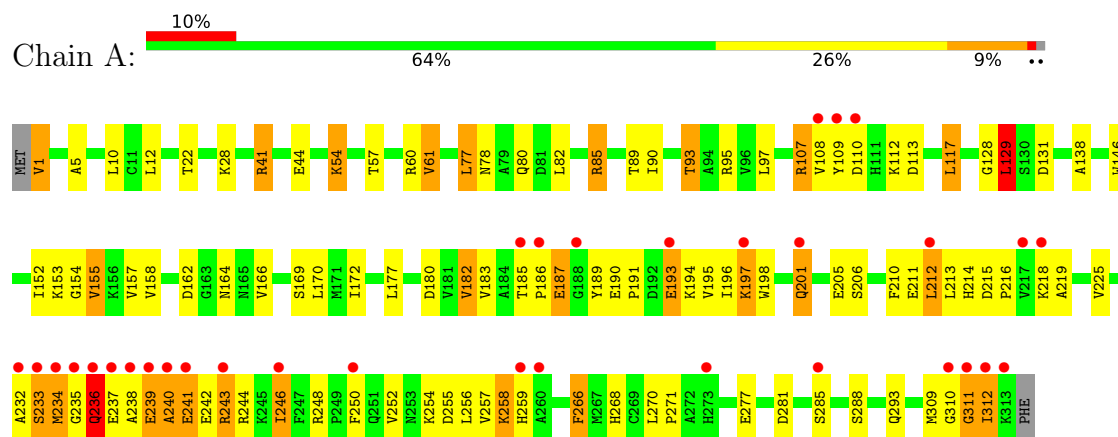
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total	O	0	0
			191	191		

3 Residue-property plots [i](#)

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: Ornithine carbamoyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	184.78Å 184.78Å 184.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 1.87 99.00 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.5 (99.00-1.87) 97.1 (99.00-1.87)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.86Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.213 , 0.269 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2653	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: SO4

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	0.48	0/2505	1.39	14/3394 (0.4%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	CD-NE-CZ	12.25	141.55	124.40
1	A	157	VAL	CA-C-N	-6.38	114.62	123.10
1	A	157	VAL	C-N-CA	-6.38	114.62	123.10
1	A	266	PHE	CA-CB-CG	-6.12	107.68	113.80
1	A	154	GLY	CA-C-N	-5.91	111.74	122.43
1	A	154	GLY	C-N-CA	-5.91	111.74	122.43
1	A	107	ARG	CA-C-N	5.41	131.22	122.68
1	A	107	ARG	C-N-CA	5.41	131.22	122.68
1	A	259	HIS	CA-CB-CG	-5.28	108.52	113.80
1	A	187	GLU	CA-C-N	-5.14	113.57	122.83
1	A	187	GLU	C-N-CA	-5.14	113.57	122.83
1	A	60	ARG	CA-C-N	-5.12	111.49	120.29
1	A	60	ARG	C-N-CA	-5.12	111.49	120.29
1	A	180	ASP	CA-CB-CG	-5.07	107.53	112.60

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	2454	0	2454	85	0
2	A	8	0	0	0	1
3	A	191	0	0	3	0
All	All	2653	0	2454	85	1

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 (85) 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:215:ASP:HB3	1:A:218:LYS:HE2	1.48	0.95
1:A:158:VAL:HG13	1:A:182:VAL:HG22	1.57	0.84
1:A:268:HIS:HD2	1:A:270:LEU:H	1.35	0.75
1:A:57:THR:O	1:A:61:VAL:HG13	1.89	0.73
1:A:232:ALA:O	1:A:243:ARG:HD3	1.89	0.72
1:A:110:ASP:OD2	1:A:112:LYS:HB3	1.90	0.72
1:A:77:LEU:HG	1:A:82:LEU:HD21	1.74	0.70
1:A:268:HIS:H	1:A:293:GLN:HE22	1.40	0.69
1:A:187:GLU:HB2	3:A:1157:HOH:O	1.94	0.67
1:A:78:ASN:OD1	1:A:80:GLN:HB2	1.94	0.67
1:A:197:LYS:O	1:A:201:GLN:HG3	1.95	0.66
1:A:152:ILE:HD13	1:A:177:LEU:HD13	1.78	0.65
1:A:213:LEU:HD13	1:A:218:LYS:HG2	1.77	0.65
1:A:234:MET:HE3	1:A:234:MET:H	1.62	0.64
1:A:152:ILE:O	1:A:155:VAL:HG13	1.98	0.64
1:A:268:HIS:CD2	1:A:270:LEU:H	2.16	0.63
1:A:185:THR:OG1	1:A:190:GLU:HG3	1.99	0.63
1:A:213:LEU:HD13	1:A:218:LYS:HE3	1.81	0.62
1:A:236:GLN:HA	1:A:236:GLN:NE2	2.10	0.61
1:A:213:LEU:HD22	1:A:218:LYS:HE3	1.83	0.61
1:A:242:GLU:O	1:A:246:ILE:HG12	2.01	0.60
1:A:187:GLU:HA	1:A:214:HIS:CD2	2.37	0.60
1:A:194:LYS:HD2	1:A:198:TRP:CZ2	2.38	0.58
1:A:215:ASP:OD2	1:A:218:LYS:HB2	2.04	0.58
1:A:254:LYS:HD2	1:A:254:LYS:H	1.69	0.58
1:A:213:LEU:HB3	1:A:218:LYS:HE3	1.87	0.57
1:A:237:GLU:OE2	1:A:243:ARG:HB3	2.05	0.56
1:A:110:ASP:O	1:A:113:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HG23	1:A:117:LEU:HD13	1.89	0.55
1:A:248:ARG:HG3	1:A:248:ARG:HH11	1.71	0.55
1:A:243:ARG:HH11	1:A:243:ARG:HG3	1.72	0.55
1:A:255:ASP:O	1:A:258:LYS:HB2	2.07	0.55
1:A:54:LYS:HD2	1:A:109:TYR:CE1	2.43	0.53
1:A:312:ILE:HG13	3:A:1132:HOH:O	2.10	0.52
1:A:234:MET:H	1:A:234:MET:CE	2.22	0.51
1:A:268:HIS:HE1	1:A:277:GLU:OE2	1.94	0.51
1:A:80:GLN:HE21	1:A:85:ARG:NH1	2.07	0.51
1:A:216:PRO:HD3	1:A:250:PHE:CE2	2.46	0.51
1:A:89:THR:O	1:A:93:THR:HG23	2.11	0.50
1:A:234:MET:HE3	1:A:234:MET:N	2.25	0.50
1:A:107:ARG:HD3	1:A:129:LEU:CB	2.43	0.49
1:A:5:ALA:HB1	1:A:311:GLY:O	2.13	0.49
1:A:213:LEU:HD13	1:A:218:LYS:CG	2.43	0.48
1:A:270:LEU:HB3	1:A:271:PRO:HA	1.95	0.48
1:A:213:LEU:HD12	1:A:219:ALA:HA	1.97	0.47
1:A:239:GLU:O	1:A:240:ALA:HB2	2.15	0.47
1:A:107:ARG:HD3	1:A:129:LEU:HB3	1.96	0.47
1:A:186:PRO:HG3	1:A:250:PHE:CE1	2.50	0.46
1:A:213:LEU:HD13	1:A:218:LYS:CE	2.46	0.46
1:A:183:VAL:O	1:A:212:LEU:HD23	2.16	0.46
1:A:190:GLU:HB3	1:A:191:PRO:HD2	1.95	0.46
1:A:266:PHE:HB3	1:A:288:SER:HA	1.96	0.46
1:A:185:THR:HG21	1:A:190:GLU:HA	1.98	0.46
1:A:193:GLU:HA	1:A:196:ILE:HD12	1.98	0.45
1:A:153:LYS:NZ	1:A:206:SER:O	2.50	0.45
1:A:218:LYS:HE2	1:A:218:LYS:HB3	1.76	0.45
1:A:235:GLY:O	1:A:237:GLU:N	2.50	0.45
1:A:213:LEU:HD22	1:A:218:LYS:CE	2.46	0.45
1:A:252:VAL:HA	1:A:256:LEU:HD23	1.97	0.45
1:A:233:SER:HA	1:A:236:GLN:HE22	1.82	0.45
1:A:128:GLY:O	1:A:129:LEU:HB2	2.16	0.44
1:A:196:ILE:HG23	1:A:210:PHE:HE2	1.81	0.44
1:A:281:ASP:O	1:A:285:SER:HB3	2.18	0.44
1:A:162:ASP:O	1:A:164:ASN:N	2.52	0.43
1:A:310:GLY:O	1:A:312:ILE:N	2.51	0.43
1:A:172:ILE:HD11	1:A:195:VAL:HG13	2.01	0.43
1:A:310:GLY:O	1:A:312:ILE:HG12	2.18	0.43
1:A:254:LYS:H	1:A:254:LYS:CD	2.24	0.43
1:A:1:VAL:HA	1:A:22:THR:OG1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NH1	1:A:44:GLU:OE1	2.52	0.42
1:A:196:ILE:HG23	1:A:210:PHE:CE2	2.54	0.42
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.33	0.41
1:A:281:ASP:OD1	1:A:281:ASP:N	2.53	0.41
1:A:182:VAL:HA	1:A:211:GLU:O	2.21	0.41
1:A:233:SER:CB	1:A:234:MET:HE3	2.51	0.41
1:A:80:GLN:NE2	1:A:85:ARG:HG3	2.35	0.41
1:A:311:GLY:HA3	3:A:1021:HOH:O	2.20	0.40
1:A:213:LEU:CD1	1:A:218:LYS:HG2	2.46	0.40
1:A:309:MET:O	1:A:312:ILE:HG23	2.21	0.40
1:A:80:GLN:NE2	1:A:85:ARG:NH1	2.70	0.40
1:A:185:THR:HB	1:A:189:TYR:O	2.22	0.40
1:A:138:ALA:HB2	1:A:169:SER:HB3	2.03	0.40
1:A:243:ARG:HG3	1:A:243:ARG:NH1	2.36	0.40
1:A:28:LYS:HE3	1:A:146:TRP:CZ3	2.56	0.40
1:A:197:LYS:NZ	1:A:201:GLN:NE2	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402:SO4:S	2:A:402:SO4:O2[9_555]	1.45	0.75

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	311/315 (99%)	292 (94%)	13 (4%)	6 (2%)	6 0

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	LEU
1	A	236	GLN
1	A	238	ALA
1	A	240	ALA
1	A	241	GLU
1	A	311	GLY

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	259/261 (99%)	224 (86%)	35 (14%)	4 0

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	10	LEU
1	A	12	LEU
1	A	54	LYS
1	A	61	VAL
1	A	77	LEU
1	A	85	ARG
1	A	93	THR
1	A	95	ARG
1	A	97	LEU
1	A	108	VAL
1	A	117	LEU
1	A	129	LEU
1	A	131	ASP
1	A	155	VAL
1	A	166	VAL
1	A	170	LEU
1	A	182	VAL
1	A	193	GLU
1	A	197	LYS
1	A	201	GLN

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Mol	Chain	Res	Type
1	A	205	GLU
1	A	212	LEU
1	A	225	VAL
1	A	233	SER
1	A	234	MET
1	A	236	GLN
1	A	239	GLU
1	A	241	GLU
1	A	243	ARG
1	A	244	ARG
1	A	246	ILE
1	A	257	VAL
1	A	258	LYS
1	A	312	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	69	HIS
1	A	80	GLN
1	A	201	GLN
1	A	236	GLN
1	A	259	HIS
1	A	268	HIS
1	A	293	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](#)

2 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	SO4	A	402	-	2,2,4	1.45	0	1,1,6	0.78	0
2	SO4	A	401	-	4,4,4	0.37	0	6,6,6	0.25	0

There are no bond length outliers.

There are no bond angle outliers.

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	A	402	SO4	0	1

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	313/315 (99%)	0.42	33 (10%)	11 14	13, 30, 69, 158	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	GLY	9.4
1	A	312	ILE	9.4
1	A	235	GLY	7.3
1	A	237	GLU	6.7
1	A	238	ALA	6.6
1	A	310	GLY	6.3
1	A	234	MET	5.8
1	A	240	ALA	5.7
1	A	236	GLN	5.6
1	A	313	LYS	5.3
1	A	239	GLU	5.0
1	A	233	SER	4.7
1	A	232	ALA	3.5
1	A	109	TYR	3.4
1	A	218	LYS	3.4
1	A	243	ARG	3.1
1	A	241	GLU	3.1
1	A	250	PHE	3.0
1	A	246	ILE	2.9
1	A	188	GLY	2.9
1	A	197	LYS	2.8
1	A	186	PRO	2.7
1	A	217	VAL	2.6
1	A	110	ASP	2.5
1	A	285	SER	2.3
1	A	212	LEU	2.3
1	A	260	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	193	GLU	2.3
1	A	108	VAL	2.2
1	A	185	THR	2.2
1	A	259	HIS	2.1
1	A	201	GLN	2.1
1	A	273	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	SO4	A	401	5/5	0.98	0.10	18,20,25,25	0
2	SO4	A	402	3/5	0.99	0.05	18,18,20,25	2

6.5 Other polymers [i](#)

There are no such residues in this entry.