



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 AM UTC

PDB ID : 2Y4Y / pdb_00002y4y
Title : Structure of a domain from the type IV pilus biogenesis lipoprotein PilP, from *Pseudomonas aeruginosa*
Authors : Derrick, J.P.; Berry, J.
Deposited on : 2011-01-11
Resolution : 1.70 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

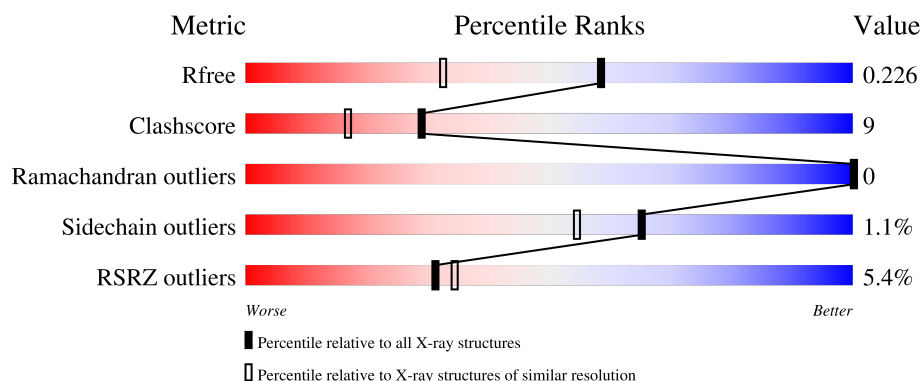
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	93	3% 75% 11% • 12%
1	B	93	4% 70% 10% •• 18%
1	C	93	6% 70% 11% • 15%
1	D	93	4% 76% 9% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2806 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 PILP PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	0	2	0
			648	414	114	118	2			
1	B	76	Total	C	N	O	S	0	1	0
			589	373	106	108	2			
1	C	79	Total	C	N	O	S	0	1	0
			621	395	112	111	3			
1	D	80	Total	C	N	O	S	0	0	0
			619	394	111	113	1			

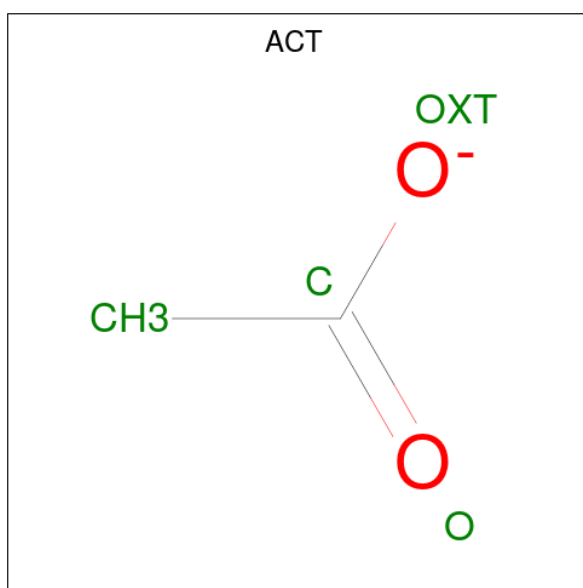
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	-	expression tag	UNP Q51354
A	80	SER	-	expression tag	UNP Q51354
A	81	HIS	-	expression tag	UNP Q51354
A	82	MET	-	expression tag	UNP Q51354
B	79	GLY	-	expression tag	UNP Q51354
B	80	SER	-	expression tag	UNP Q51354
B	81	HIS	-	expression tag	UNP Q51354
B	82	MET	-	expression tag	UNP Q51354
C	79	GLY	-	expression tag	UNP Q51354
C	80	SER	-	expression tag	UNP Q51354
C	81	HIS	-	expression tag	UNP Q51354
C	82	MET	-	expression tag	UNP Q51354
D	79	GLY	-	expression tag	UNP Q51354
D	80	SER	-	expression tag	UNP Q51354
D	81	HIS	-	expression tag	UNP Q51354
D	82	MET	-	expression tag	UNP Q51354

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

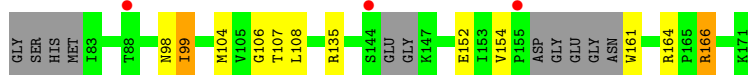


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total 89	O 89	0	0
4	B	69	Total 69	O 69	0	0
4	C	77	Total 77	O 77	0	0
4	D	64	Total 64	O 64	0	0

- Molecule 1: PILP PROTEIN

[illegible]

GLY	H81	M52	ILE	LYS	PRO	ASP	GLU	THR	R59	F103	M104	T107	G122	G134	D137	V141	S144	S145	G146	K147	I151	V154	PR0	ASP	GLY	GLU	GLY	ASN	L161	L162	K171
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GLY	SER	HIS	MET	ILE	K64	P95	D86	GLU	THR	R69	N98	I99	E100	L108	G113	R128	D131	E145	E152	A155	ASP	GLY	GLU	GLY	ASN	W161	R166	L170	LVS
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.20Å 74.51Å 74.18Å 90.00° 125.80° 90.00°	Depositor
Resolution (Å)	32.22 – 1.70 32.22 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.22-1.70) 94.4 (32.22-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.178 , 0.224 0.183 , 0.226	Depositor DCC
R_{free} test set	2424 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.0	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	0.95	EDS
Total number of atoms	2806	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, ZN

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	1.52	2/662 (0.3%)	1.27	1/886 (0.1%)
1	B	1.55	3/597 (0.5%)	1.28	1/796 (0.1%)
1	C	1.70	6/631 (1.0%)	1.38	6/841 (0.7%)
1	D	1.46	1/627 (0.2%)	1.20	1/841 (0.1%)
All	All	1.56	12/2517 (0.5%)	1.28	9/3364 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	102	PHE	C-N	10.13	1.47	1.33
1	C	102	PHE	C-O	8.69	1.33	1.23
1	A	106	GLY	N-CA	7.71	1.52	1.45
1	A	99	ILE	N-CA	6.55	1.54	1.46
1	B	126	ARG	CG-CD	-5.71	1.35	1.52
1	C	141	VAL	CA-CB	5.51	1.60	1.54
1	B	90	VAL	N-CA	5.51	1.52	1.46
1	C	134	GLY	N-CA	5.48	1.52	1.45
1	B	126	ARG	CD-NE	5.46	1.53	1.46
1	D	113	GLY	N-CA	5.44	1.51	1.44
1	C	81	HIS	N-CA	5.29	1.56	1.46
1	C	102	PHE	N-CA	5.01	1.51	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	HIS	CB-CA-C	10.26	129.59	110.10
1	C	82	MET	CB-CG-SD	7.41	134.93	112.70
1	C	102	PHE	CA-C-O	-6.47	113.64	121.28
1	B	153	ILE	CB-CA-C	-6.44	101.62	110.77
1	A	166	ARG	CB-CA-C	-6.26	96.88	111.09
1	C	103	GLU	CA-C-N	-5.89	112.75	121.24
1	C	103	GLU	C-N-CA	-5.89	112.75	121.24
1	C	103	GLU	O-C-N	5.15	129.43	123.30
1	D	128	ARG	NE-CZ-NH2	5.04	123.74	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	81	HIS	Peptide

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	648	0	673	13	0
1	B	589	0	613	12	0
1	C	621	0	638	11	0
1	D	619	0	631	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	9	0	0
3	C	8	0	6	0	0
3	D	4	0	3	0	0
4	A	89	0	0	8	0
4	B	69	0	0	0	0
4	C	77	0	0	1	0
4	D	64	0	0	3	0
All	All	2806	0	2573	44	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 9.

All (44) 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:B:126:ARG:HH11	1:B:126:ARG:CG	1.64	1.07
1:B:126:ARG:HH11	1:B:126:ARG:HG2	0.86	1.02
1:B:126:ARG:HG2	1:B:126:ARG:NH1	1.55	0.99
1:C:82:MET:SD	1:C:137:ASP:OD2	2.26	0.92
1:A:161:TRP:N	4:A:2069:HOH:O	2.15	0.79
1:A:98:ASN:HB2	4:A:2051:HOH:O	1.88	0.73
1:C:82:MET:HE3	1:C:137:ASP:OD1	1.88	0.72
1:D:166:ARG:CG	4:D:2054:HOH:O	2.38	0.70
1:D:166:ARG:HG2	4:D:2054:HOH:O	1.90	0.70
1:C:104[B]:MET:SD	1:C:146:GLY:O	2.60	0.60
1:B:104[A]:MET:SD	1:B:146:GLY:O	2.60	0.60
1:C:161:TRP:N	4:C:2063:HOH:O	2.35	0.58
1:B:126:ARG:CG	1:B:126:ARG:NH1	2.32	0.58
1:A:166:ARG:HG2	4:A:2075:HOH:O	2.06	0.56
1:D:166:ARG:HG3	4:D:2054:HOH:O	2.08	0.53
1:A:161:TRP:CA	4:A:2069:HOH:O	2.59	0.51
1:B:116:ALA:HB1	1:B:148:ILE:HD11	1.95	0.49
1:A:161:TRP:HA	4:A:2069:HOH:O	2.13	0.49
1:C:104[A]:MET:HE1	1:C:107:THR:HG22	1.96	0.48
1:A:135:ARG:NH1	4:A:2051:HOH:O	2.39	0.47
1:A:99:ILE:HD13	1:A:166:ARG:HD3	1.95	0.47
1:A:152:GLU:CD	1:A:166:ARG:HD2	2.40	0.46
1:C:147:LYS:HB2	1:C:147:LYS:HE2	1.61	0.46
1:B:147:LYS:HE2	1:B:167:SER:HB2	1.97	0.46
1:B:104[A]:MET:SD	1:B:148:ILE:HG13	2.56	0.45
1:B:104[A]:MET:SD	1:B:168:LEU:O	2.73	0.45
1:B:104[B]:MET:SD	1:B:148:ILE:HD11	2.56	0.45
1:C:104[B]:MET:SD	1:C:146:GLY:C	3.00	0.45
1:A:107:THR:HG23	4:A:2024:HOH:O	2.17	0.44
1:C:82:MET:CE	1:C:137:ASP:OD1	2.62	0.44
1:D:152:GLU:CD	1:D:166:ARG:HD2	2.43	0.44
1:C:82:MET:SD	1:C:137:ASP:CG	2.99	0.43
1:A:108:LEU:C	1:A:108:LEU:HD23	2.43	0.43
1:D:128:ARG:HE	1:D:131:ASP:CG	2.24	0.43
1:B:104[A]:MET:CE	1:B:146:GLY:C	2.92	0.42
1:D:86:ASP:OD1	1:D:86:ASP:C	2.62	0.42
1:D:108:LEU:C	1:D:108:LEU:HD23	2.45	0.42
1:C:141:VAL:HG11	1:C:151:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HG2	4:A:2075:HOH:O	2.20	0.41
1:A:154:VAL:HG11	1:A:164:ARG:CZ	2.50	0.41
1:B:104[B]:MET:HE1	1:B:107:THR:HG22	2.02	0.41
1:D:98:ASN:OD1	1:D:100:GLU:OE1	2.38	0.41
1:A:104[A]:MET:HE1	1:A:107:THR:HG22	2.02	0.41

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	78/93 (84%)	76 (97%)	2 (3%)	0	100	100
1	B	73/93 (78%)	70 (96%)	3 (4%)	0	100	100
1	C	74/93 (80%)	71 (96%)	3 (4%)	0	100	100
1	D	74/93 (80%)	72 (97%)	2 (3%)	0	100	100
All	All	299/372 (80%)	289 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	71/76 (93%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	63/76 (83%)	60 (95%)	3 (5%)	23	8
1	C	66/76 (87%)	65 (98%)	1 (2%)	57	43
1	D	66/76 (87%)	66 (100%)	0	100	100
All	All	266/304 (88%)	262 (98%)	4 (2%)	65	43

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104[A]	MET
1	B	104[B]	MET
1	B	126	ARG
1	C	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	ACT	A	1174	-	3,3,3	1.28	1 (33%)	3,3,3	1.55	1 (33%)
3	ACT	C	1173	-	3,3,3	0.76	0	3,3,3	0.61	0
3	ACT	A	1176	2	3,3,3	0.96	0	3,3,3	0.81	0
3	ACT	D	1171	-	3,3,3	0.74	0	3,3,3	0.94	0
3	ACT	C	1174	-	3,3,3	1.03	0	3,3,3	2.04	1 (33%)
3	ACT	A	1173	-	3,3,3	0.48	0	3,3,3	1.10	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1174	ACT	O-C	2.19	1.31	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1174	ACT	OXT-C-CH3	2.83	126.91	115.05
3	A	1174	ACT	OXT-C-O	-2.16	114.00	122.03

There are no chirality outliers.

There are no torsion outliers.

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(Å ²)	Q < 0.9
1	A	82/93 (88%)	-0.14	3 (3%)	45	49	9, 17, 30, 44	2 (2%)
1	B	76/93 (81%)	-0.14	4 (5%)	32	35	9, 16, 27, 39	1 (1%)
1	C	79/93 (84%)	-0.11	6 (7%)	20	21	10, 17, 27, 39	1 (1%)
1	D	80/93 (86%)	-0.03	4 (5%)	34	38	13, 19, 32, 39	0
All	All	317/372 (85%)	-0.10	17 (5%)	31	34	9, 17, 29, 44	4 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	GLY	3.8
1	C	145	GLU	3.6
1	B	146	GLY	3.1
1	A	144	SER	3.0
1	B	145	GLU	2.8
1	A	155	PRO	2.6
1	A	88	THR	2.5
1	B	144	SER	2.4
1	D	155	PRO	2.3
1	C	122	GLY	2.3
1	B	154	VAL	2.3
1	C	162	LEU	2.2
1	C	144	SER	2.1
1	C	154	VAL	2.1
1	D	170	LEU	2.1
1	D	145	GLU	2.0
1	D	84	LYS	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
3	ACT	A	1174	4/4	0.87	0.11	25,25,28,29	0
3	ACT	C	1174	4/4	0.87	0.11	25,25,25,28	0
3	ACT	A	1176	4/4	0.92	0.10	22,22,23,24	0
3	ACT	C	1173	4/4	0.95	0.08	19,23,23,23	0
3	ACT	A	1173	4/4	0.96	0.09	20,22,23,24	0
2	ZN	B	1173	1/1	0.98	0.06	27,27,27,27	0
2	ZN	B	1172	1/1	0.98	0.04	25,25,25,25	1
3	ACT	D	1171	4/4	0.98	0.05	19,21,22,22	0
2	ZN	C	1172	1/1	1.00	0.01	15,15,15,15	0
2	ZN	D	1172	1/1	1.00	0.01	18,18,18,18	0
2	ZN	A	1172	1/1	1.00	0.01	16,16,16,16	0
2	ZN	A	1175	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.