



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:58 pm GMT

PDB ID : 2Q0I
Title : Structure of Pseudomonas Quinolone Signal Response Protein PqsE
Authors : Yu, S.; Jensen, V.; Feldmann, I.; Haussler, S.; Blankenfeldt, W.
Deposited on : 2007-05-22
Resolution : 1.57 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

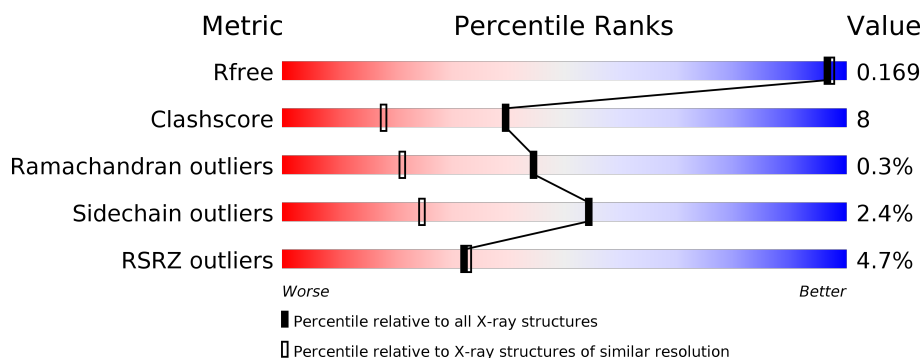
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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}	100719	4211 (1.60-1.56)
Clashscore	112137	4539 (1.60-1.56)
Ramachandran outliers	110173	4423 (1.60-1.56)
Sidechain outliers	110143	4420 (1.60-1.56)
RSRZ outliers	101464	4232 (1.60-1.56)

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 ≥ 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	303	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>5%</div> </div> </div>

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
3	BEZ	A	990	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2815 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 Quinolone signal response protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2458	1545	454	444	15	0	7	0

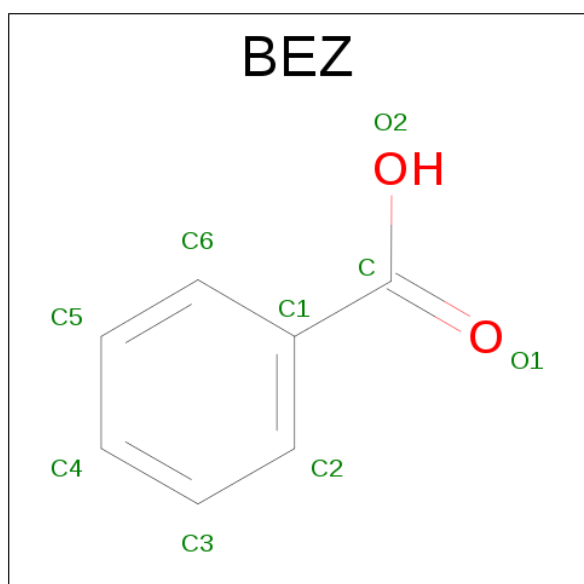
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	900	SER	-	EXPRESSION TAG	UNP Q02IG5
A	901	HIS	-	EXPRESSION TAG	UNP Q02IG5

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		

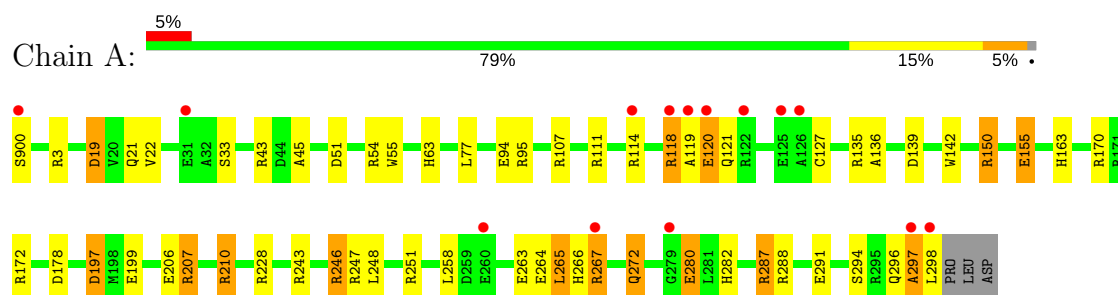
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	346	Total	O	0	0
			346	346		

3 Residue-property plots [i](#)

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: Quinolone signal response protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 61.10Å 145.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.57 19.81 – 1.57	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-1.57) 98.8 (19.81-1.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.120 , 0.169 0.126 , 0.169	Depositor DCC
R_{free} test set	2236 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2815	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: BEZ, FE

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	1.32	12/2514 (0.5%)	1.29	31/3412 (0.9%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	GLU	CG-CD	8.53	1.64	1.51
1	A	54	ARG	CG-CD	-7.09	1.34	1.51
1	A	247	ARG	CB-CG	-6.97	1.33	1.52
1	A	251	ARG	CG-CD	-6.74	1.35	1.51
1	A	206	GLU	CB-CG	-6.64	1.39	1.52
1	A	272	GLN	CB-CG	-6.51	1.34	1.52
1	A	228	ARG	CB-CG	-6.14	1.35	1.52
1	A	263	GLU	CG-CD	5.96	1.60	1.51
1	A	3	ARG	CD-NE	-5.52	1.37	1.46
1	A	150	ARG	CG-CD	5.49	1.65	1.51
1	A	263	GLU	CB-CG	5.24	1.62	1.52
1	A	55	TRP	CB-CG	5.05	1.59	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	A	107	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	3	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	197	ASP	CB-CG-OD1	9.69	127.02	118.30
1	A	95[A]	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	95[B]	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	207	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	A	51	ASP	CB-CG-OD1	8.08	125.58	118.30
1	A	107	ARG	NE-CZ-NH1	8.07	124.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	172	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	A	246	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	95[A]	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	95[B]	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	265	LEU	CB-CG-CD1	7.58	123.89	111.00
1	A	247	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	3	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	135	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	170	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	243[A]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	243[B]	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	19[A]	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	19[B]	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	287	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	197	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	210	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	247	ARG	CG-CD-NE	-5.46	100.33	111.80
1	A	228	ARG	CG-CD-NE	-5.32	100.64	111.80
1	A	127[A]	CYS	CA-CB-SG	5.16	123.28	114.00
1	A	127[B]	CYS	CA-CB-SG	5.16	123.28	114.00
1	A	139	ASP	CB-CG-OD1	5.03	122.83	118.30

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	2458	0	2405	40	3
2	A	2	0	0	0	0
3	A	9	0	5	1	0
4	A	346	0	0	16	4
All	All	2815	0	2410	41	4

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.

All (41) 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:118:ARG:H	1:A:121:GLN:HE21	1.06	0.94
1:A:297:ALA:HB3	4:A:1259:HOH:O	1.78	0.83
1:A:266:HIS:HD2	1:A:282:HIS:HD2	1.27	0.82
1:A:19[B]:ASP:OD1	4:A:1081:HOH:O	2.00	0.80
1:A:142:TRP:CZ3	4:A:1330:HOH:O	2.36	0.77
1:A:19[B]:ASP:CG	1:A:21:GLN:HG2	2.06	0.76
1:A:266:HIS:HD2	1:A:282:HIS:CD2	2.05	0.73
1:A:163:HIS:HE1	1:A:178:ASP:H	1.34	0.73
1:A:266:HIS:HE1	4:A:1280:HOH:O	1.71	0.72
1:A:120:GLU:O	1:A:120:GLU:HG2	1.90	0.70
1:A:19[B]:ASP:OD1	1:A:21:GLN:HG2	1.94	0.67
1:A:118:ARG:H	1:A:121:GLN:NE2	1.89	0.65
1:A:266:HIS:CD2	1:A:282:HIS:HD2	2.14	0.63
1:A:118:ARG:N	1:A:121:GLN:HE21	1.89	0.63
1:A:142:TRP:HZ3	4:A:1330:HOH:O	1.77	0.62
1:A:163:HIS:CE1	1:A:178:ASP:H	2.16	0.62
1:A:155:GLU:OE1	4:A:1187:HOH:O	2.16	0.60
1:A:287:ARG:NH1	1:A:291:GLU:OE2	2.35	0.59
1:A:19[B]:ASP:OD2	1:A:21:GLN:NE2	2.37	0.57
1:A:282:HIS:HE1	4:A:1041:HOH:O	1.88	0.57
1:A:207:ARG:HG2	1:A:210:ARG:NH1	2.20	0.57
1:A:288:ARG:NH1	4:A:1132:HOH:O	2.37	0.56
1:A:119:ALA:O	4:A:1123:HOH:O	2.17	0.56
1:A:142:TRP:CH2	4:A:1330:HOH:O	2.59	0.55
1:A:294:SER:OG	1:A:298:LEU:CD1	2.58	0.52
1:A:33:SER:OG	1:A:63:HIS:HD2	1.94	0.50
1:A:900:SER:N	4:A:1294:HOH:O	2.45	0.50
1:A:114:ARG:HD3	4:A:1304:HOH:O	2.15	0.46
1:A:197:ASP:HA	1:A:296:GLN:HE22	1.80	0.45
1:A:120:GLU:C	4:A:1123:HOH:O	2.55	0.45
1:A:118:ARG:HD2	1:A:121:GLN:NE2	2.32	0.45
1:A:246:ARG:HD3	4:A:1253:HOH:O	2.17	0.44
1:A:19[B]:ASP:OD2	1:A:21:GLN:HG2	2.17	0.44
1:A:94:GLU:HG2	1:A:136:ALA:HB1	2.00	0.43
3:A:990:BEZ:O2	4:A:1001:HOH:O	2.21	0.43
1:A:45:ALA:HA	1:A:77:LEU:HD22	2.01	0.43
1:A:21:GLN:HG3	1:A:22[A]:VAL:HG23	2.01	0.43
1:A:264:GLU:OE1	1:A:267:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TRP:CE3	1:A:150:ARG:HG2	2.55	0.42
1:A:111:ARG:HD3	4:A:1279:HOH:O	2.20	0.41
1:A:248:LEU:HD11	1:A:258:LEU:CD2	2.51	0.40

All (4) 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)
1:A:280[B]:GLU:OE1	4:A:1152:HOH:O[4_565]	1.55	0.65
1:A:199:GLU:OE2	4:A:1147:HOH:O[4_555]	2.03	0.17
1:A:280[B]:GLU:CD	4:A:1152:HOH:O[4_565]	2.06	0.14
4:A:1117:HOH:O	4:A:1287:HOH:O[6_454]	2.16	0.04

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	305/303 (101%)	295 (97%)	9 (3%)	1 (0%)	44 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ALA

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	259/256 (101%)	252 (97%)	7 (3%)	50 20

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	118	ARG
1	A	120	GLU
1	A	265	LEU
1	A	272	GLN
1	A	280[A]	GLU
1	A	280[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	89	GLN
1	A	121	GLN
1	A	163	HIS
1	A	266	HIS
1	A	282	HIS
1	A	296	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	BEZ	A	990	2	6,9,9	1.13	0	8,11,11	1.74	3 (37%)

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	BEZ	A	990	2	-	0/0/4/4	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	990	BEZ	C2-C1-C	-2.66	116.87	120.45
3	A	990	BEZ	C3-C2-C1	-2.37	117.57	120.57
3	A	990	BEZ	C6-C1-C2	2.53	122.61	117.59

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
3	A	990	BEZ	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	300/303 (99%)	0.09	14 (4%) 32 33	11, 20, 37, 59	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	LEU	9.9
1	A	119	ALA	6.8
1	A	297	ALA	4.5
1	A	122	ARG	3.9
1	A	31	GLU	3.6
1	A	120	GLU	3.5
1	A	118	ARG	3.5
1	A	125	GLU	3.1
1	A	267	ARG	3.0
1	A	114	ARG	2.8
1	A	260	GLU	2.7
1	A	279	GLY	2.2
1	A	126	ALA	2.1
1	A	900	SER	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	BEZ	A	990	9/9	0.96	0.15	6.51	13,15,19,25	9
2	FE	A	998	1/1	1.00	0.04	-3.76	15,15,15,15	0
2	FE	A	999	1/1	1.00	0.03	-3.91	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.