



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:20 AM UTC

PDB ID : 4K89 / pdb_00004k89
Title : Crystal structure of Pseudomonas aeruginosa strain K solvent tolerant elastase
Authors : Ali, M.S.M.; Said, Z.S.A.M.; Rahman, R.N.Z.R.A.; Basri, M.; Salleh, A.B.
Deposited on : 2013-04-18
Resolution : 1.39 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

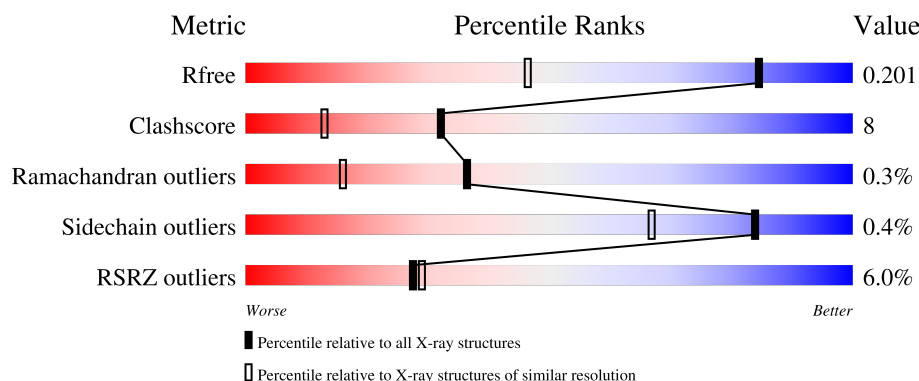
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	301	

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	PO4	A	406	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2542 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 Organic solvent tolerant elastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2315	1453	399	450	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ASP	GLY	engineered mutation	UNP A7LI11

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

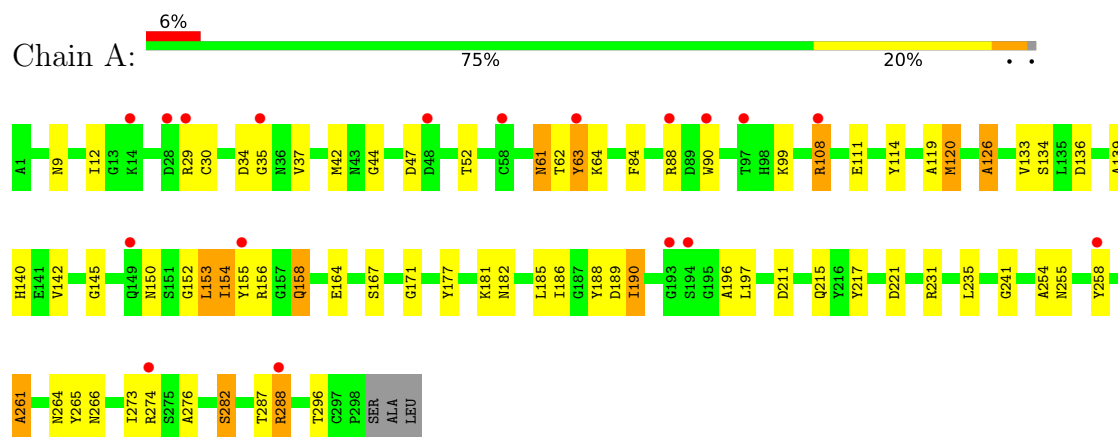
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total 186	O 186	0	0

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: Organic solvent tolerant elastase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.99Å 90.17Å 40.60Å 90.00° 113.81° 90.00°	Depositor
Resolution (Å)	45.09 – 1.39 45.09 – 1.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.09-1.39) 99.8 (45.09-1.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.167 , 0.191 0.175 , 0.201	Depositor DCC
R_{free} test set	2610 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2542	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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: ZN, CA, PO4, GOL

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	1.89	36/2377 (1.5%)	1.52	15/3221 (0.5%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	TYR	N-CA	8.54	1.56	1.45
1	A	177	TYR	C-O	8.30	1.33	1.24
1	A	261	ALA	N-CA	-7.66	1.36	1.46
1	A	30	CYS	CA-C	7.34	1.62	1.53
1	A	153	LEU	CA-C	-7.12	1.44	1.52
1	A	108	ARG	C-O	-6.99	1.16	1.24
1	A	119	ALA	CA-C	-6.94	1.44	1.52
1	A	63	TYR	C-O	-6.90	1.15	1.24
1	A	273	ILE	C-O	-6.73	1.16	1.24
1	A	255	ASN	CA-C	6.63	1.61	1.52
1	A	190	ILE	CA-CB	6.61	1.62	1.54
1	A	276	ALA	CA-C	6.50	1.61	1.52
1	A	114	TYR	CA-C	-6.17	1.45	1.52
1	A	155	TYR	N-CA	-6.09	1.39	1.46
1	A	156	ARG	C-O	-6.09	1.16	1.23
1	A	158	GLN	CA-C	-5.90	1.45	1.52
1	A	52	THR	CA-C	5.84	1.59	1.52
1	A	186	ILE	C-O	-5.71	1.17	1.24
1	A	287	THR	N-CA	-5.68	1.39	1.46
1	A	221	ASP	C-O	5.57	1.30	1.23
1	A	150	ASN	C-O	-5.51	1.16	1.25
1	A	114	TYR	N-CA	5.48	1.52	1.46
1	A	84	PHE	C-O	5.45	1.30	1.24
1	A	145	GLY	C-O	5.45	1.30	1.23
1	A	99	LYS	C-O	-5.42	1.17	1.23
1	A	61	ASN	CA-C	-5.41	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ALA	C-N	5.38	1.40	1.33
1	A	88	ARG	CD-NE	-5.34	1.38	1.46
1	A	62	THR	C-O	-5.32	1.16	1.24
1	A	185	LEU	C-O	5.28	1.30	1.24
1	A	186	ILE	CA-CB	5.25	1.60	1.54
1	A	90	TRP	CA-C	-5.19	1.45	1.52
1	A	235	LEU	C-O	5.18	1.30	1.24
1	A	182	ASN	CG-OD1	5.11	1.33	1.23
1	A	37	VAL	N-CA	5.09	1.52	1.46
1	A	196	ALA	CA-CB	5.06	1.61	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	SER	N-CA-C	7.29	120.29	108.63
1	A	29	ARG	NE-CZ-NH2	6.75	125.28	119.20
1	A	255	ASN	O-C-N	6.69	129.05	122.09
1	A	133	VAL	O-C-N	-6.47	115.40	122.64
1	A	154	ILE	CA-C-O	-6.28	115.16	122.13
1	A	120	MET	CG-SD-CE	-6.01	87.68	100.90
1	A	288	ARG	CB-CG-CD	5.69	124.39	111.30
1	A	273	ILE	CA-C-O	-5.68	115.15	121.17
1	A	136	ASP	CB-CA-C	-5.65	101.41	110.79
1	A	231	ARG	CA-C-O	-5.52	114.57	120.42
1	A	136	ASP	CA-C-O	-5.38	114.84	120.55
1	A	9	ASN	CA-C-O	-5.30	115.64	121.31
1	A	276	ALA	CA-C-O	-5.15	115.09	120.55
1	A	35	GLY	N-CA-C	5.13	120.92	114.25
1	A	164	GLU	CA-C-O	-5.07	115.50	120.82

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	2315	0	2142	36	0
2	A	24	0	32	2	0
3	A	15	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	186	0	0	2	0
All	All	2542	0	2174	36	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.

All (36) 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:44:GLY:HA3	1:A:108:ARG:NH2	1.66	1.09
1:A:44:GLY:HA3	1:A:108:ARG:HH22	1.34	0.91
1:A:241:GLY:H	2:A:403:GOL:H31	1.35	0.88
1:A:44:GLY:CA	1:A:108:ARG:NH2	2.37	0.88
1:A:120:MET:CE	1:A:142:VAL:HG23	2.07	0.83
1:A:44:GLY:CA	1:A:108:ARG:HH22	1.97	0.75
1:A:120:MET:HE1	1:A:142:VAL:HG23	1.67	0.74
1:A:282:SER:OG	2:A:404:GOL:H2	1.90	0.71
1:A:190:ILE:HD11	1:A:197:LEU:HD11	1.75	0.68
1:A:44:GLY:O	1:A:108:ARG:NH2	2.29	0.65
1:A:44:GLY:C	1:A:108:ARG:NH2	2.56	0.64
1:A:158:GLN:HE21	1:A:265:TYR:H	1.46	0.64
1:A:44:GLY:C	1:A:108:ARG:HH22	2.07	0.63
1:A:154:ILE:HG23	1:A:261:ALA:HB1	1.89	0.55
1:A:158:GLN:NE2	1:A:264:ASN:HB2	2.22	0.55
1:A:158:GLN:NE2	1:A:265:TYR:H	2.05	0.53
1:A:211:ASP:H	1:A:215:GLN:NE2	2.07	0.52
1:A:266:ASN:ND2	1:A:296:THR:H	2.08	0.51
1:A:158:GLN:HE21	1:A:264:ASN:HB2	1.76	0.51
1:A:211:ASP:H	1:A:215:GLN:HE22	1.59	0.51
1:A:61:ASN:HD21	1:A:63:TYR:HB3	1.76	0.50
1:A:134:SER:HB3	1:A:190:ILE:HG23	1.95	0.48
1:A:139:ALA:HB3	1:A:171:GLY:HA2	1.96	0.48
1:A:152:GLY:O	1:A:153:LEU:C	2.58	0.46
1:A:44:GLY:CA	1:A:108:ARG:HH21	2.25	0.46
1:A:34:ASP:OD1	1:A:34:ASP:C	2.60	0.45
1:A:111:GLU:CD	1:A:126:ALA:HB3	2.42	0.44
1:A:288:ARG:NE	6:A:520:HOH:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:MET:HE1	1:A:47:ASP:O	2.18	0.43
1:A:12:ILE:HG21	1:A:189:ASP:CG	2.44	0.43
1:A:120:MET:CE	1:A:142:VAL:CG2	2.90	0.43
1:A:258:TYR:CE1	1:A:274:ARG:HD2	2.54	0.42
1:A:140:HIS:CG	1:A:167:SER:HB3	2.55	0.42
1:A:288:ARG:O	1:A:288:ARG:HG2	2.19	0.42
1:A:188:TYR:N	6:A:643:HOH:O	2.53	0.41
1:A:63:TYR:HA	1:A:64:LYS:HA	1.88	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	296/301 (98%)	288 (97%)	7 (2%)	1 (0%)	36 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	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	238/240 (99%)	237 (100%)	1 (0%)	84 67

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	43	ASN
1	A	61	ASN
1	A	74	ASN
1	A	150	ASN
1	A	158	GLN
1	A	182	ASN
1	A	215	GLN
1	A	266	ASN

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	PO4	A	406	-	4,4,4	2.12	1 (25%)	6,6,6	4.37	3 (50%)
2	GOL	A	403	-	5,5,5	0.67	0	5,5,5	1.40	0
3	PO4	A	405	-	4,4,4	0.95	0	6,6,6	0.97	0
3	PO4	A	407	-	4,4,4	2.20	2 (50%)	6,6,6	1.58	1 (16%)
2	GOL	A	401	-	5,5,5	0.59	0	5,5,5	1.27	1 (20%)
2	GOL	A	404	-	5,5,5	0.32	0	5,5,5	0.77	0
2	GOL	A	402	-	5,5,5	0.57	0	5,5,5	1.06	0

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	GOL	A	403	-	-	4/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	A	404	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	406	PO4	P-O2	-3.83	1.43	1.54
3	A	407	PO4	P-O1	3.23	1.58	1.50
3	A	407	PO4	P-O2	-2.94	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	PO4	O3-P-O2	-8.07	82.79	107.91
3	A	406	PO4	O4-P-O2	5.12	123.84	107.91
3	A	406	PO4	O4-P-O3	-4.07	95.25	107.91
3	A	407	PO4	O4-P-O2	3.40	118.50	107.91
2	A	401	GOL	C3-C2-C1	-2.11	104.05	111.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	GOL	O1-C1-C2-C3
2	A	403	GOL	C1-C2-C3-O3
2	A	402	GOL	O1-C1-C2-C3
2	A	403	GOL	O1-C1-C2-O2
2	A	402	GOL	O1-C1-C2-O2
2	A	403	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	GOL	1	0
2	A	404	GOL	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	298/301 (99%)	0.27	18 (6%) 27 29	5, 12, 23, 28	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	TYR	5.5
1	A	155	TYR	4.1
1	A	35	GLY	4.0
1	A	88	ARG	3.8
1	A	28	ASP	3.7
1	A	29	ARG	3.7
1	A	193	GLY	3.7
1	A	58	CYS	3.6
1	A	274	ARG	3.6
1	A	258	TYR	2.9
1	A	194	SER	2.9
1	A	288	ARG	2.8
1	A	14	LYS	2.5
1	A	149	GLN	2.4
1	A	97	THR	2.4
1	A	48	ASP	2.4
1	A	108	ARG	2.2
1	A	90	TRP	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(Å ²)	Q<0.9
2	GOL	A	404	6/6	0.77	0.15	35,40,42,43	0
2	GOL	A	403	6/6	0.80	0.15	33,36,37,37	0
2	GOL	A	401	6/6	0.88	0.11	22,26,29,31	0
2	GOL	A	402	6/6	0.89	0.12	16,20,27,31	0
3	PO4	A	405	5/5	0.89	0.10	48,48,50,50	0
3	PO4	A	406	5/5	0.96	0.09	17,19,26,28	0
3	PO4	A	407	5/5	0.97	0.09	16,18,20,22	0
4	CA	A	408	1/1	0.99	0.07	13,13,13,13	0
5	ZN	A	409	1/1	1.00	0.04	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.