



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4RBM / pdb_00004rbm
Title : Porphyromonas gingivalis gingipain K (Kgp) catalytic and immunoglobulin superfamily-like domains
Authors : de Diego, I.; Veillard, F.; Sztukowska, M.N.; Guevara, T.; Potempa, B.; Pomowski, A.; Huntington, J.A.; Potempa, J.; Gomis-Ruth, F.X.
Deposited on : 2014-09-12
Resolution : 1.75 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

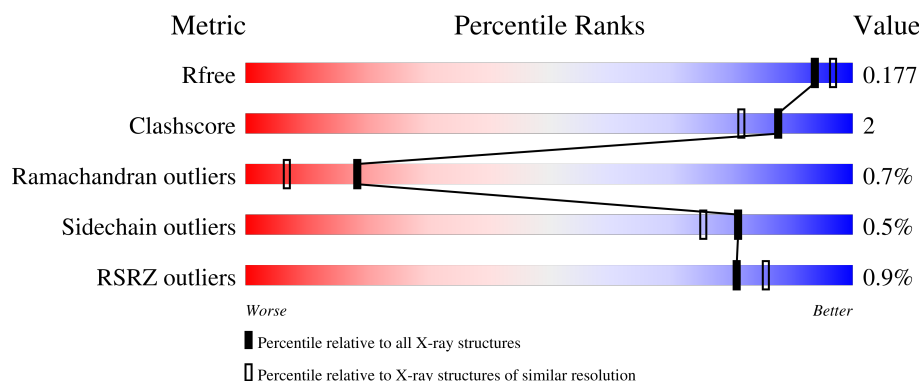
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	461	92% 6%

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
7	AZI	A	710	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	A	716	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4124 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 Lys-gingipain W83.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	1	0
			3524	2261	562	685	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	684	HIS	-	expression tag	UNP Q51817
A	685	HIS	-	expression tag	UNP Q51817
A	686	HIS	-	expression tag	UNP Q51817
A	687	HIS	-	expression tag	UNP Q51817
A	688	HIS	-	expression tag	UNP Q51817
A	689	HIS	-	expression tag	UNP Q51817

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

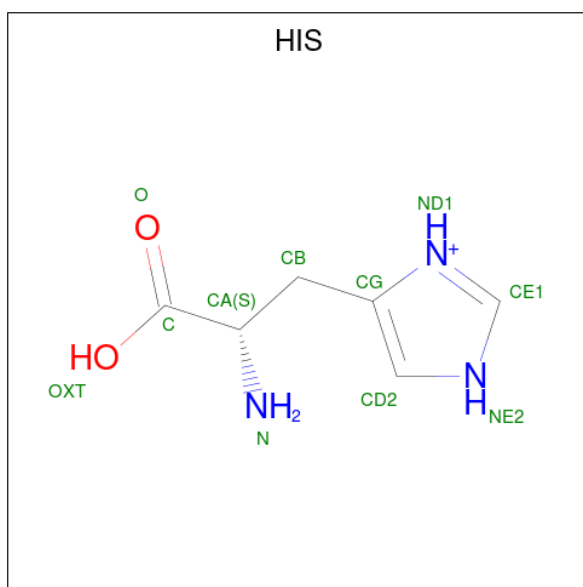
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 5 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



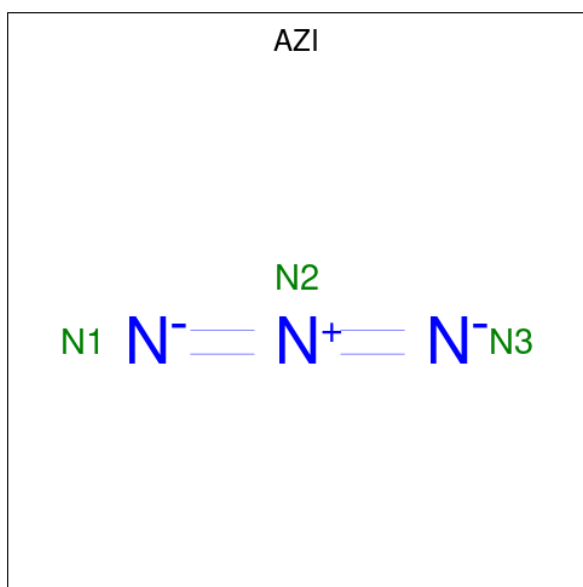
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is AZIDE ION (CCD ID: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total N 3 3	0	0
7	A	1	Total N 3 3	0	0
7	A	1	Total N 3 3	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



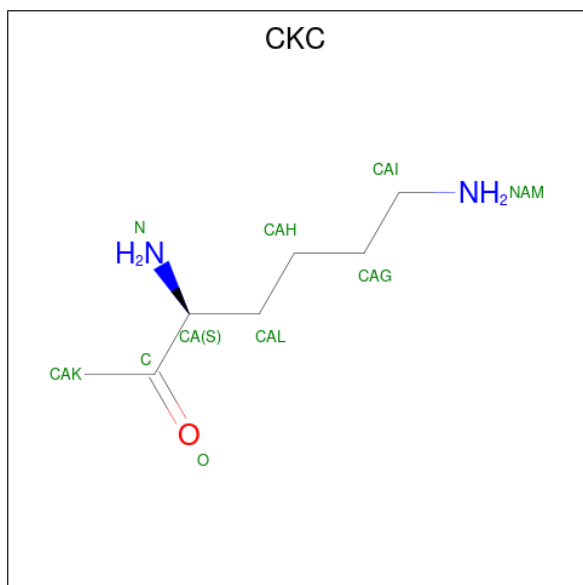
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

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

- Molecule 9 is (3S)-3,7-diaminoheptan-2-one (CCD ID: CKC) (formula: C₇H₁₆N₂O).

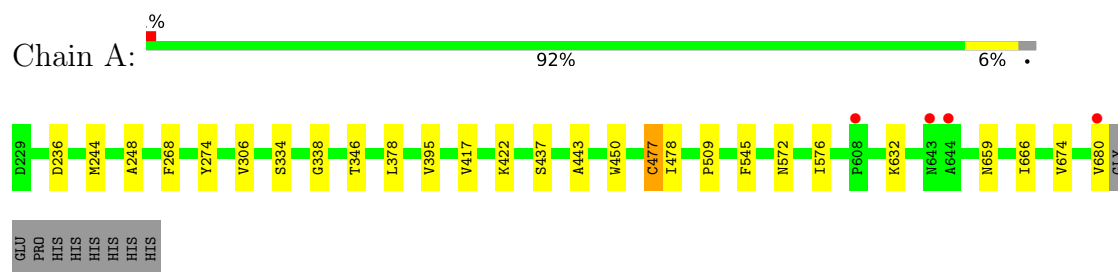


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			10	7	2	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	533	Total	O	0	0
			533	533		

- Molecule 1: Lys-gingipain W83



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.64Å 58.81Å 135.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.41 – 1.75 44.41 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.41-1.75) 99.5 (44.41-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.149 , 0.172 0.150 , 0.177	Depositor DCC
R_{free} test set	768 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4124	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: GOL, ACT, CA, CKC, NA, NI, AZI

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	0.79	1/3624 (0.0%)	1.02	9/4941 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	MET	SD-CE	-6.47	1.63	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	TRP	N-CA-C	-6.94	98.64	109.25
1	A	338	GLY	N-CA-C	6.84	122.19	114.67
1	A	477	CYS	CA-C-N	6.14	133.02	121.97
1	A	477	CYS	C-N-CA	6.14	133.02	121.97
1	A	572	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	268	PHE	CA-CB-CG	5.54	119.34	113.80
1	A	545	PHE	CA-CB-CG	-5.50	108.31	113.80
1	A	306	VAL	N-CA-C	-5.24	106.58	111.45
1	A	236	ASP	CA-CB-CG	5.13	117.73	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	3524	0	3372	11	0
2	A	2	0	0	0	0
3	A	3	0	0	0	0
4	A	1	0	0	0	0
5	A	10	0	6	0	0
6	A	8	0	6	0	0
7	A	9	0	0	1	0
8	A	24	0	32	4	0
9	A	10	0	8	2	0
10	A	533	0	0	5	0
All	All	4124	0	3424	14	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 2.

All (14) 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)
7:A:711:AZI:N3	10:A:1327:HOH:O	2.25	0.69
1:A:477:CYS:H	9:A:717:CKC:CAK	2.09	0.65
1:A:417:VAL:H	8:A:716:GOL:H11	1.66	0.60
8:A:716:GOL:H32	10:A:1317:HOH:O	2.02	0.58
1:A:422:LYS:HE2	10:A:1032:HOH:O	2.04	0.57
8:A:716:GOL:H12	10:A:904:HOH:O	2.07	0.53
1:A:395:VAL:HG11	10:A:929:HOH:O	2.10	0.51
1:A:378:LEU:HA	1:A:437:SER:HB3	1.96	0.46
1:A:334:SER:HB3	1:A:346:THR:OG1	2.16	0.46
1:A:666:ILE:HB	1:A:674:VAL:HB	1.97	0.46
1:A:659:ASN:HA	1:A:680:VAL:HG13	2.01	0.43
1:A:477:CYS:N	9:A:717:CKC:CAK	2.80	0.42
1:A:417:VAL:H	8:A:716:GOL:C1	2.33	0.41
1:A:248:ALA:O	1:A:274:TYR:HA	2.21	0.41

There are no symmetry-related clashes.

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	451/461 (98%)	436 (97%)	12 (3%)	3 (1%)	18 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	ALA
1	A	478	ILE
1	A	576	ILE

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	371/378 (98%)	369 (100%)	2 (0%)	81 75

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	509	PRO
1	A	632	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	394	GLN
1	A	405	GLN
1	A	410	GLN
1	A	554	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 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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$
6	ACT	A	708	4	3,3,3	1.00	0	3,3,3	0.80	0
9	CKC	A	717	1	8,9,9	0.52	0	6,10,10	0.97	0
7	AZI	A	712	-	2,2,2	1.82	0	0,1,1	-	-
7	AZI	A	711	-	2,2,2	1.85	1 (50%)	0,1,1	-	-
5	HIS	A	707	4	9,10,11	0.46	0	8,12,14	0.18	0
6	ACT	A	709	-	3,3,3	0.97	0	3,3,3	1.02	0
8	GOL	A	716	-	5,5,5	0.07	0	5,5,5	0.39	0
8	GOL	A	715	-	5,5,5	0.06	0	5,5,5	0.18	0
8	GOL	A	714	-	5,5,5	0.13	0	5,5,5	0.31	0
8	GOL	A	713	-	5,5,5	0.07	0	5,5,5	0.29	0
7	AZI	A	710	-	2,2,2	2.25	2 (100%)	0,1,1	-	-

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
9	CKC	A	717	1	-	3/8/9/9	-
5	HIS	A	707	4	-	0/5/6/8	0/1/1/1
8	GOL	A	716	-	-	0/4/4/4	-
8	GOL	A	715	-	-	1/4/4/4	-
8	GOL	A	714	-	-	2/4/4/4	-
8	GOL	A	713	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	710	AZI	N3-N2	-2.39	1.18	1.23
7	A	711	AZI	N1-N2	-2.13	1.18	1.23
7	A	710	AZI	N1-N2	-2.09	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	714	GOL	C1-C2-C3-O3
9	A	717	CKC	CAK-C-CA-CAL
9	A	717	CKC	O-C-CA-N
9	A	717	CKC	O-C-CA-CAL
8	A	714	GOL	O2-C2-C3-O3
8	A	715	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	717	CKC	2	0
7	A	711	AZI	1	0
8	A	716	GOL	4	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	452/461 (98%)	-0.52	4 (0%) 81 86	8, 13, 41, 77	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	VAL	6.2
1	A	644	ALA	2.5
1	A	608	PRO	2.1
1	A	643	ASN	2.1

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
8	GOL	A	716	6/6	0.63	0.23	50,51,53,55	0
9	CKC	A	717	10/10	0.76	0.19	16,30,41,43	0
7	AZI	A	712	3/3	0.79	0.20	42,42,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	A	708	4/4	0.82	0.17	23,24,27,36	0
7	AZI	A	710	3/3	0.83	0.15	44,44,44,44	0
8	GOL	A	713	6/6	0.83	0.14	34,40,43,49	0
7	AZI	A	711	3/3	0.85	0.18	31,31,33,35	0
8	GOL	A	714	6/6	0.87	0.14	23,39,42,44	0
6	ACT	A	709	4/4	0.89	0.12	42,43,44,44	0
8	GOL	A	715	6/6	0.91	0.13	23,27,29,30	0
5	HIS	A	707	10/11	0.93	0.10	21,24,37,56	0
3	NA	A	706	1/1	0.98	0.04	16,16,16,16	0
3	NA	A	703	1/1	1.00	0.02	10,10,10,10	0
3	NA	A	704	1/1	1.00	0.02	12,12,12,12	0
2	CA	A	701	1/1	1.00	0.01	11,11,11,11	0
4	NI	A	705	1/1	1.00	0.02	12,12,12,12	0
2	CA	A	702	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.