Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 12:23 PM JST

PDB ID	:	7W6B
Title	:	Crystal Structure of PitA from pilus islet-2 of Streptococcus oralis
Authors	:	Yadav, R.K.; Krishnan, V.
Deposited on	:	2021-12-01
Resolution	:	2.98 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:

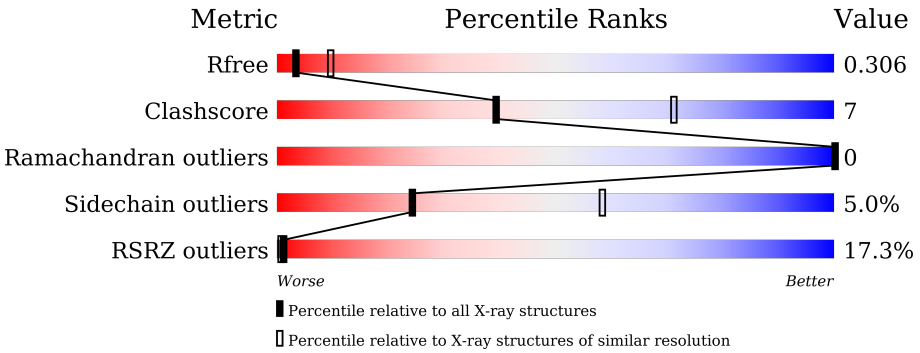
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	793	17% 81% 16%

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	IOD	A	911	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5925 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 von Willebrand factor type A domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	782	Total	C	N	O	S	0	0	0
			5877	3635	1022	1216	4			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	I	0	0
			15	15		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

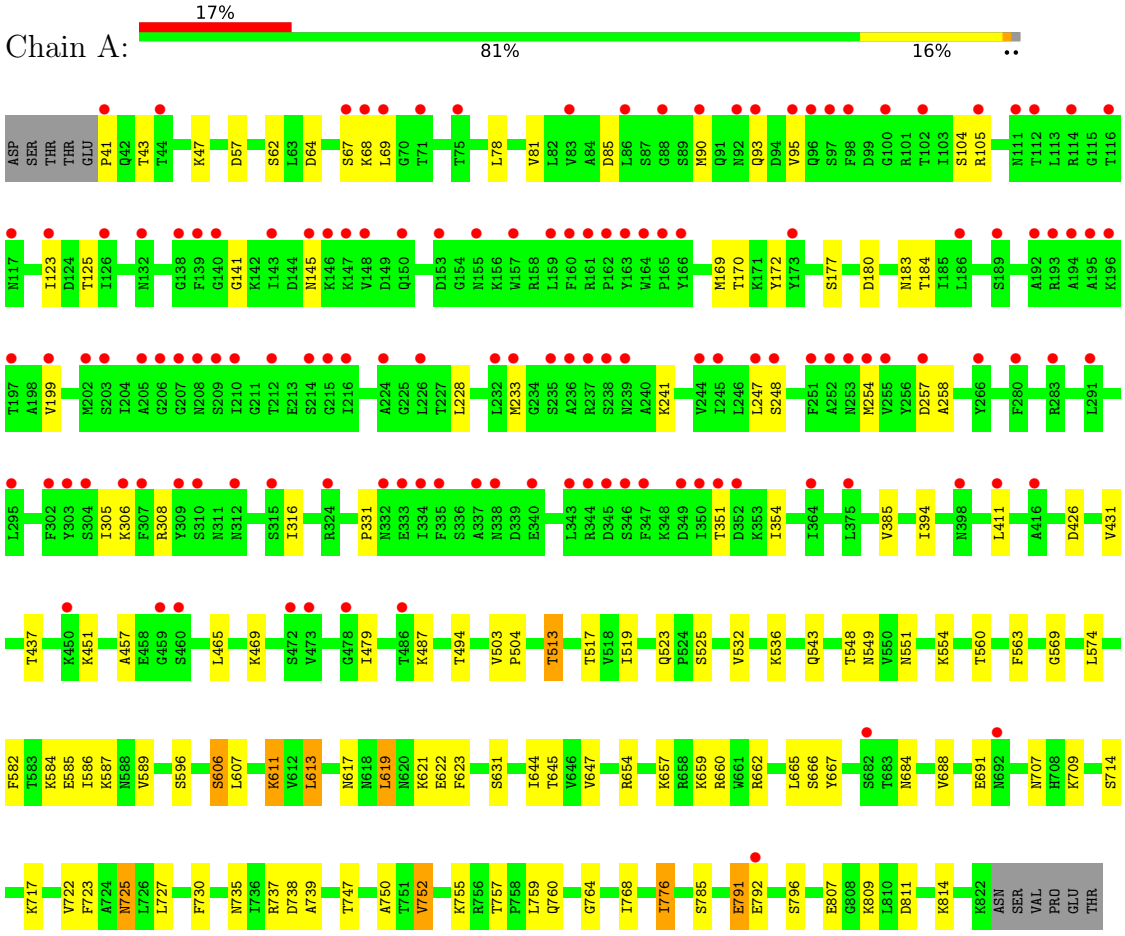
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		

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: von Willebrand factor type A domain protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	52.27Å 422.93Å 48.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.93 – 2.98 51.88 – 2.98	Depositor EDS
% Data completeness (in resolution range)	90.1 (51.93-2.98) 90.1 (51.88-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.253 , 0.305 0.254 , 0.306	Depositor DCC
R_{free} test set	1068 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 78.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5925	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, IOD, CA

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	0.44	2/5973 (0.0%)	0.82	0/8118

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	GLU	CD-OE1	6.77	1.33	1.25
1	A	691	GLU	CD-OE2	5.19	1.31	1.25

There are no bond angle outliers.

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	5877	0	5528	84	0
2	A	1	0	0	0	0
3	A	15	0	0	6	0
4	A	1	0	0	0	0
5	A	31	0	0	0	0
All	All	5925	0	5528	84	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 7.

All (84) 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:611:LYS:NZ	1:A:707:ASN:CG	1.70	1.42
1:A:551:ASN:OD1	3:A:911:IOD:I	2.24	1.26
1:A:611:LYS:HZ3	1:A:707:ASN:CG	1.41	1.01
1:A:611:LYS:HZ2	1:A:707:ASN:CG	1.50	0.92
1:A:611:LYS:CE	1:A:707:ASN:CG	2.47	0.83
1:A:684:ASN:O	1:A:684:ASN:OD1	2.00	0.79
1:A:717:LYS:HE2	1:A:730:PHE:CG	2.23	0.74
1:A:727:LEU:HA	3:A:912:IOD:I	2.60	0.72
1:A:622:GLU:OE1	1:A:654:ARG:HD2	1.88	0.72
1:A:331:PRO:HG3	1:A:479:ILE:CG2	2.20	0.71
1:A:738:ASP:OD1	1:A:739:ALA:N	2.23	0.70
1:A:81:VAL:HG23	1:A:233:MET:HE1	1.74	0.69
1:A:735:ASN:HA	1:A:764:GLY:O	1.93	0.68
1:A:81:VAL:HG23	1:A:233:MET:CE	2.25	0.66
1:A:331:PRO:HG3	1:A:479:ILE:HG22	1.78	0.65
1:A:717:LYS:HE2	1:A:730:PHE:CD2	2.32	0.65
1:A:41:PRO:HG2	1:A:69:LEU:HG	1.80	0.64
1:A:644:ILE:HG21	1:A:665:LEU:HD21	1.81	0.61
1:A:606:SER:HB3	1:A:666:SER:HA	1.83	0.61
1:A:525:SER:O	3:A:911:IOD:I	2.91	0.59
1:A:644:ILE:HB	1:A:665:LEU:HD23	1.86	0.58
1:A:257:ASP:OD1	1:A:258:ALA:N	2.31	0.58
1:A:722:VAL:CG2	1:A:725:ASN:HD22	2.16	0.58
1:A:536:LYS:HE3	1:A:569:GLY:O	2.05	0.57
1:A:81:VAL:CG2	1:A:233:MET:HE2	2.35	0.57
1:A:607:LEU:HD23	1:A:665:LEU:HD12	1.86	0.57
1:A:809:LYS:O	1:A:814:LYS:HE3	2.06	0.56
1:A:141:GLY:HA3	1:A:254:MET:SD	2.45	0.55
1:A:722:VAL:HA	3:A:915:IOD:I	2.76	0.55
1:A:411:LEU:CD1	1:A:469:LYS:HD2	2.37	0.54
1:A:123:ILE:HD11	1:A:199:VAL:HG21	1.89	0.54
1:A:714:SER:HA	1:A:776:ILE:O	2.08	0.54
1:A:532:VAL:HG22	1:A:543:GLN:HA	1.89	0.53
1:A:688:VAL:HG22	1:A:707:ASN:OD1	2.09	0.53
1:A:644:ILE:CG2	1:A:665:LEU:HD21	2.41	0.51
1:A:606:SER:HB3	1:A:667:TYR:H	1.77	0.50
1:A:791:GLU:HG2	1:A:796:SER:OG	2.12	0.50
1:A:64:ASP:HB3	1:A:431:VAL:HB	1.94	0.50
1:A:606:SER:CB	1:A:666:SER:HA	2.41	0.50
1:A:613:LEU:HD21	1:A:623:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:CG2	1:A:233:MET:CE	2.90	0.49
1:A:619:LEU:HB3	1:A:657:LYS:HD2	1.95	0.49
1:A:563:PHE:HA	3:A:905:IOD:I	2.82	0.48
1:A:57:ASP:O	1:A:437:THR:HA	2.13	0.48
1:A:90:MET:HA	1:A:105:ARG:HD2	1.94	0.48
1:A:385:VAL:HB	1:A:431:VAL:HG13	1.96	0.48
1:A:747:THR:HG22	1:A:760:GLN:OE1	2.15	0.47
1:A:750:ALA:HB1	1:A:776:ILE:HD11	1.96	0.46
1:A:589:VAL:N	1:A:596:SER:O	2.48	0.46
1:A:768:ILE:CD1	1:A:776:ILE:HG21	2.46	0.46
1:A:811:ASP:OD1	1:A:814:LYS:HE2	2.16	0.46
1:A:465:LEU:O	1:A:494:THR:HA	2.16	0.45
1:A:659:LYS:O	1:A:660:ARG:HB2	2.16	0.45
1:A:177:SER:OG	1:A:180:ASP:OD2	2.34	0.45
1:A:247:LEU:HD12	1:A:305:ILE:O	2.18	0.45
1:A:513:THR:OG1	1:A:517:THR:HG21	2.17	0.45
1:A:606:SER:HB3	1:A:667:TYR:N	2.32	0.44
1:A:43:THR:HG1	1:A:487:LYS:HZ3	1.59	0.44
1:A:611:LYS:HE3	1:A:707:ASN:CG	2.37	0.43
1:A:752:VAL:HG22	1:A:776:ILE:HD12	2.00	0.43
1:A:145:ASN:HA	1:A:172:TYR:HA	1.99	0.43
1:A:67:SER:O	1:A:68:LYS:HG3	2.18	0.43
1:A:85:ASP:HB2	1:A:248:SER:HA	2.01	0.43
1:A:737:ARG:O	1:A:785:SER:HB2	2.19	0.43
1:A:574:LEU:HB3	1:A:586:ILE:HG21	2.00	0.42
1:A:722:VAL:HG21	1:A:725:ASN:HD22	1.84	0.42
1:A:184:THR:N	1:A:228:LEU:HD21	2.34	0.42
1:A:93:GLN:HA	1:A:104:SER:HA	2.01	0.42
1:A:125:THR:HG21	1:A:351:THR:HB	2.00	0.42
1:A:457:ALA:HB2	1:A:465:LEU:HD23	2.02	0.42
1:A:807:GLU:H	1:A:807:GLU:HG2	1.80	0.42
1:A:47:LYS:HA	1:A:62:SER:O	2.19	0.41
1:A:95:VAL:HG22	1:A:308:ARG:HD3	2.01	0.41
1:A:78:LEU:HD23	1:A:241:LYS:CB	2.50	0.41
1:A:519:ILE:HD13	1:A:582:PHE:HE2	1.84	0.41
1:A:354:ILE:HA	1:A:479:ILE:HG12	2.02	0.41
1:A:737:ARG:HG3	3:A:903:IOD:I	2.91	0.41
1:A:688:VAL:HG13	1:A:707:ASN:OD1	2.20	0.41
1:A:523:GLN:HE22	1:A:554:LYS:HG3	1.84	0.41
1:A:613:LEU:HD23	1:A:613:LEU:HA	1.87	0.41
1:A:759:LEU:HD12	1:A:759:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ILE:HD12	1:A:776:ILE:HG21	2.02	0.41
1:A:306:LYS:HG2	1:A:316:ILE:HD12	2.02	0.40
1:A:503:VAL:HA	1:A:504:PRO:HD3	1.87	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	780/793 (98%)	737 (94%)	43 (6%)	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	622/697 (89%)	591 (95%)	31 (5%)	24 58

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	MET
1	A	170	THR
1	A	183	ASN

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Mol	Chain	Res	Type
1	A	394	ILE
1	A	426	ASP
1	A	451	LYS
1	A	513	THR
1	A	548	THR
1	A	549	ASN
1	A	560	THR
1	A	584	LYS
1	A	587	LYS
1	A	606	SER
1	A	611	LYS
1	A	613	LEU
1	A	617	ASN
1	A	619	LEU
1	A	621	LYS
1	A	631	SER
1	A	645	THR
1	A	647	VAL
1	A	662	ARG
1	A	709	LYS
1	A	723	PHE
1	A	725	ASN
1	A	752	VAL
1	A	755	LYS
1	A	757	THR
1	A	776	ILE
1	A	791	GLU
1	A	792	GLU

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	360	HIS
1	A	523	GLN
1	A	684	ASN
1	A	725	ASN
1	A	753	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

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, 95^{th} 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	782/793 (98%)	1.00	135 (17%) 1 1	11, 89, 178, 238	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	ALA	7.7
1	A	155	ASN	7.0
1	A	209	SER	6.5
1	A	212	THR	6.4
1	A	162	PRO	5.9
1	A	206	GLY	5.6
1	A	473	VAL	5.6
1	A	197	THR	5.6
1	A	67	SER	5.6
1	A	205	ALA	5.4
1	A	71	THR	5.4
1	A	238	SER	5.2
1	A	194	ALA	5.2
1	A	343	LEU	5.2
1	A	252	ALA	5.1
1	A	159	LEU	4.9
1	A	346	SER	4.6
1	A	140	GLY	4.6
1	A	459	GLY	4.6
1	A	163	TYR	4.4
1	A	335	PHE	4.3
1	A	68	LYS	4.3
1	A	351	THR	4.3
1	A	193	ARG	4.3
1	A	207	GLY	4.2
1	A	148	VAL	4.2
1	A	333	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	344	ARG	4.1
1	A	166	TYR	4.1
1	A	266	TYR	4.1
1	A	226	LEU	3.9
1	A	117	ASN	3.9
1	A	307	PHE	3.8
1	A	312	ASN	3.8
1	A	153	ASP	3.8
1	A	147	LYS	3.8
1	A	309	TYR	3.8
1	A	350	ILE	3.8
1	A	239	ASN	3.7
1	A	146	LYS	3.7
1	A	92	ASN	3.7
1	A	145	ASN	3.7
1	A	334	ILE	3.7
1	A	186	LEU	3.6
1	A	139	PHE	3.6
1	A	69	LEU	3.6
1	A	332	ASN	3.5
1	A	247	LEU	3.5
1	A	224	ALA	3.5
1	A	233	MET	3.5
1	A	310	SER	3.4
1	A	208	ASN	3.4
1	A	138	GLY	3.4
1	A	90	MET	3.4
1	A	375	LEU	3.4
1	A	416	ALA	3.3
1	A	86	LEU	3.3
1	A	203	SER	3.3
1	A	126	ILE	3.3
1	A	352	ASP	3.3
1	A	345	ASP	3.2
1	A	682	SER	3.2
1	A	364	ILE	3.2
1	A	302	PHE	3.2
1	A	102	THR	3.2
1	A	116	THR	3.2
1	A	283	ARG	3.1
1	A	161	ARG	3.1
1	A	100	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	165	PRO	3.0
1	A	189	SER	3.0
1	A	88	GLY	3.0
1	A	257	ASP	3.0
1	A	251	PHE	2.9
1	A	44	THR	2.9
1	A	236	ALA	2.9
1	A	692	ASN	2.9
1	A	398	ASN	2.9
1	A	157	TRP	2.9
1	A	173	TYR	2.8
1	A	160	PHE	2.8
1	A	235	SER	2.8
1	A	216	ILE	2.8
1	A	340	GLU	2.7
1	A	253	ASN	2.7
1	A	98	PHE	2.6
1	A	112	THR	2.6
1	A	254	MET	2.6
1	A	295	LEU	2.6
1	A	248	SER	2.6
1	A	280	PHE	2.6
1	A	93	GLN	2.6
1	A	460	SER	2.6
1	A	255	VAL	2.6
1	A	111	ASN	2.6
1	A	192	ALA	2.6
1	A	210	ILE	2.5
1	A	196	LYS	2.5
1	A	450	LYS	2.5
1	A	347	PHE	2.5
1	A	303	TYR	2.5
1	A	304	SER	2.5
1	A	97	SER	2.5
1	A	75	THR	2.5
1	A	306	LYS	2.5
1	A	41	PRO	2.4
1	A	95	VAL	2.4
1	A	83	VAL	2.4
1	A	315	SER	2.4
1	A	114	ARG	2.4
1	A	202	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	338	ASN	2.4
1	A	105	ARG	2.3
1	A	143	ILE	2.3
1	A	96	GLN	2.3
1	A	244	VAL	2.3
1	A	150	GLN	2.3
1	A	337	ALA	2.2
1	A	291	LEU	2.2
1	A	792	GLU	2.2
1	A	199	VAL	2.2
1	A	164	TRP	2.2
1	A	215	GLY	2.2
1	A	478	GLY	2.2
1	A	237	ARG	2.1
1	A	411	LEU	2.1
1	A	245	ILE	2.1
1	A	472	SER	2.1
1	A	132	ASN	2.1
1	A	214	SER	2.1
1	A	349	ASP	2.1
1	A	232	LEU	2.1
1	A	123	ILE	2.1
1	A	324	ARG	2.0
1	A	486	THR	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 monosaccharides 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, 95^{th} 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	MG	A	901	1/1	0.77	0.12	104,104,104,104	0
3	IOD	A	913	1/1	0.81	0.29	97,97,97,97	1
3	IOD	A	909	1/1	0.87	0.18	93,93,93,93	1
3	IOD	A	911	1/1	0.89	0.17	60,60,60,60	1
3	IOD	A	905	1/1	0.89	0.11	66,66,66,66	1
4	CA	A	917	1/1	0.91	0.08	104,104,104,104	0
3	IOD	A	916	1/1	0.93	0.13	79,79,79,79	1
3	IOD	A	912	1/1	0.94	0.07	94,94,94,94	1
3	IOD	A	903	1/1	0.96	0.14	66,66,66,66	1
3	IOD	A	914	1/1	0.96	0.06	77,77,77,77	1
3	IOD	A	904	1/1	0.96	0.11	57,57,57,57	1
3	IOD	A	902	1/1	0.96	0.13	64,64,64,64	1
3	IOD	A	908	1/1	0.98	0.11	54,54,54,54	1
3	IOD	A	906	1/1	0.98	0.10	61,61,61,61	1
3	IOD	A	910	1/1	0.98	0.06	67,67,67,67	1
3	IOD	A	907	1/1	0.99	0.05	83,83,83,83	0
3	IOD	A	915	1/1	0.99	0.07	55,55,55,55	1

6.5 Other polymers (i)

There are no such residues in this entry.