



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:33 PM UTC

PDB ID : 2XTL / pdb_00002xtl
Title : Structure of the major pilus backbone protein from Streptococcus Agalactiae
Authors : Rinauda, D.; Gourlay, L.J.; Soriano, M.; Grandi, G.; Bolognesi, M.
Deposited on : 2010-10-11
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
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

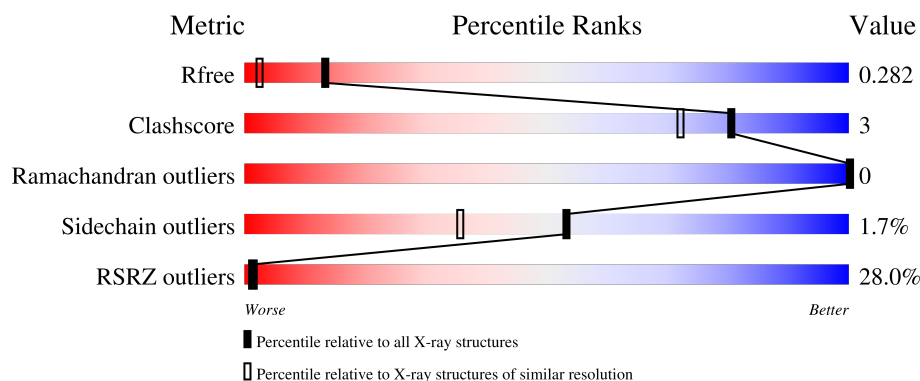
1 Overall quality at a glance

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	452	25% 94% 6%
1	B	452	31% 92% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7974 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 CELL WALL SURFACE ANCHOR FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	12	0
			3502	2198	580	723	1			
1	B	452	Total	C	N	O	S	0	21	0
			3574	2246	588	739	1			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	B	1	Total	K	0	0
			1	1		

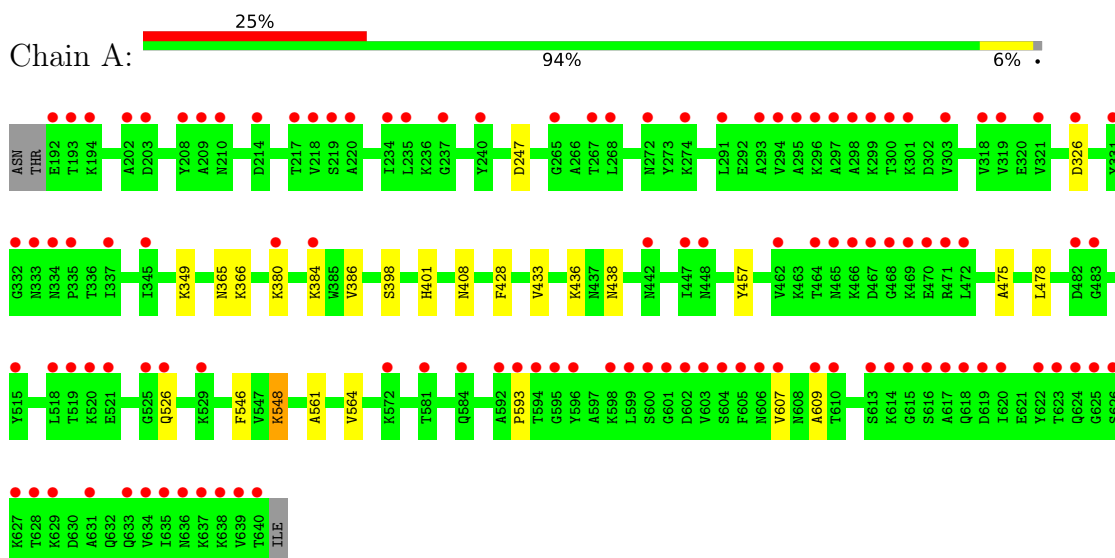
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	454	Total	O	0	0
			454	454		
3	B	441	Total	O	0	0
			441	441		

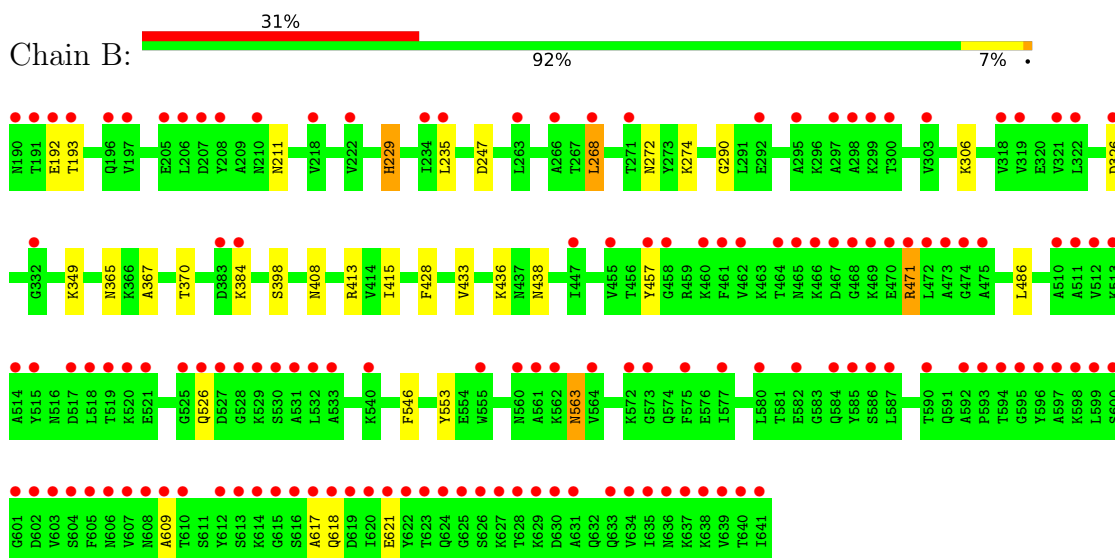
3 Residue-property plots

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: CELL WALL SURFACE ANCHOR FAMILY PROTEIN



• Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.86Å 104.68Å 159.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 40.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.75) 100.0 (40.00-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.216 0.252 , 0.282	Depositor DCC
R_{free} test set	5403 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7974	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% 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: K

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	0.43	0/3588	0.62	0/4850
1	B	0.42	0/3687	0.62	0/4979
All	All	0.42	0/7275	0.62	0/9829

There are no bond length outliers.

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	3502	0	3509	17	0
1	B	3574	0	3602	22	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	454	0	0	0	0
3	B	441	0	0	3	0
All	All	7974	0	7111	37	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 3.

All (37) 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:349:LYS:H	1:B:408:ASN:HD21	1.28	0.80
1:A:349:LYS:H	1:A:408:ASN:HD21	1.27	0.79
1:A:401:HIS:HD2	1:B:367:ALA:H	1.31	0.78
1:B:436:LYS:HE3	1:B:438:ASN:HD21	1.58	0.68
1:A:401:HIS:CD2	1:B:367:ALA:H	2.13	0.67
1:B:563:ASN:HD22	1:B:563:ASN:H	1.41	0.67
1:A:561:ALA:HB3	1:A:564[B]:VAL:HG23	1.77	0.66
1:B:370[B]:THR:HG22	3:B:2229:HOH:O	1.99	0.63
1:A:561:ALA:HB3	1:A:564[A]:VAL:HG13	1.80	0.62
1:B:365:ASN:HD22	1:B:398:SER:H	1.46	0.60
1:B:384[A]:LYS:NZ	3:B:2246:HOH:O	2.36	0.58
1:A:247:ASP:HA	1:A:326:ASP:O	2.03	0.57
1:A:436:LYS:HE2	1:A:438:ASN:HD21	1.70	0.55
1:A:384:LYS:HE3	1:A:386:VAL:HG22	1.89	0.54
1:A:365:ASN:HD22	1:A:398:SER:H	1.56	0.53
1:B:247:ASP:HA	1:B:326:ASP:O	2.09	0.52
1:B:268:LEU:HD22	1:B:272:ASN:CG	2.36	0.50
1:B:365:ASN:ND2	1:B:398:SER:H	2.09	0.50
1:B:193:THR:HB	1:B:235:LEU:HD12	1.95	0.49
1:A:478:LEU:HD22	1:A:564[B]:VAL:HG11	1.95	0.49
1:B:563:ASN:HD22	1:B:563:ASN:N	2.11	0.49
1:A:457:TYR:CE1	1:A:609:ALA:HA	2.49	0.48
1:B:413:ARG:CZ	1:B:415:ILE:HD11	2.43	0.48
1:B:617:ALA:O	1:B:618:GLN:HB2	2.16	0.46
1:B:272:ASN:HD22	1:B:290:GLY:HA2	1.81	0.46
1:A:428:PHE:CD2	1:A:433:VAL:HG22	2.51	0.46
1:B:229:HIS:HD2	1:B:306:LYS:NZ	2.14	0.45
1:B:486:LEU:HD11	1:B:553:TYR:CG	2.52	0.45
1:A:561:ALA:HB3	1:A:564[B]:VAL:CG2	2.46	0.45
1:A:457:TYR:HB2	1:A:607:VAL:CG1	2.48	0.42
1:A:365:ASN:ND2	1:A:398:SER:H	2.17	0.42
1:B:457:TYR:CE1	1:B:609:ALA:HA	2.54	0.42
1:A:548:LYS:N	1:A:548:LYS:HD3	2.35	0.42
1:B:428:PHE:CD2	1:B:433:VAL:HG22	2.55	0.41
1:A:475:ALA:HB2	1:A:593:PRO:HG3	2.03	0.41
1:B:274[B]:LYS:NZ	3:B:2081:HOH:O	2.47	0.41
1:B:471:ARG:NH2	1:B:621:GLU:O	2.54	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	459/452 (102%)	456 (99%)	3 (1%)	0	100	100
1	B	471/452 (104%)	465 (99%)	6 (1%)	0	100	100
All	All	930/904 (103%)	921 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	388/379 (102%)	383 (99%)	5 (1%)	61	46
1	B	400/379 (106%)	391 (98%)	9 (2%)	44	24
All	All	788/758 (104%)	774 (98%)	14 (2%)	53	33

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	366	LYS
1	A	380	LYS
1	A	526	GLN
1	A	546	PHE
1	A	548	LYS
1	B	192	GLU
1	B	211	ASN
1	B	229	HIS

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Mol	Chain	Res	Type
1	B	268	LEU
1	B	471	ARG
1	B	526[A]	GLN
1	B	526[B]	GLN
1	B	546	PHE
1	B	563	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	280	GLN
1	A	365	ASN
1	A	401	HIS
1	A	408	ASN
1	A	430	ASN
1	A	438	ASN
1	A	442	ASN
1	A	584	GLN
1	A	606	ASN
1	B	196	GLN
1	B	229	HIS
1	B	272	ASN
1	B	280	GLN
1	B	334	ASN
1	B	365	ASN
1	B	408	ASN
1	B	438	ASN
1	B	563	ASN
1	B	606	ASN
1	B	624	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [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

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, 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	449/452 (99%)	1.34	114 (25%)	1 2	13, 30, 53, 78	18 (4%)
1	B	452/452 (100%)	1.45	138 (30%)	1 1	12, 30, 56, 80	29 (6%)
All	All	901/904 (99%)	1.39	252 (27%)	1 1	12, 30, 54, 80	47 (5%)

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	641	ILE	7.0
1	B	192	GLU	7.0
1	B	598	LYS	6.0
1	A	617	ALA	5.9
1	A	639	VAL	5.7
1	B	640	THR	5.6
1	A	337	ILE	5.3
1	B	625	GLY	5.3
1	B	526[A]	GLN	5.3
1	A	442	ASN	5.2
1	B	193	THR	4.9
1	B	639	VAL	4.9
1	B	634	VAL	4.8
1	B	620	ILE	4.7
1	A	640	THR	4.7
1	B	594	THR	4.6
1	B	617	ALA	4.6
1	A	629	LYS	4.3
1	B	599	LEU	4.3
1	B	635	ILE	4.3
1	A	635	ILE	4.2
1	A	616	SER	4.2
1	A	469	LYS	4.1
1	B	191	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	620	ILE	4.1
1	B	618	GLN	4.0
1	A	468	GLY	4.0
1	A	618	GLN	4.0
1	B	628	THR	3.9
1	A	625	GLY	3.9
1	A	627	LYS	3.9
1	B	469	LYS	3.9
1	B	616	SER	3.9
1	B	462	VAL	3.8
1	A	192	GLU	3.8
1	B	520	LYS	3.8
1	B	597	ALA	3.8
1	B	190	ASN	3.8
1	A	193	THR	3.7
1	A	521	GLU	3.7
1	A	624	GLN	3.7
1	B	326	ASP	3.6
1	A	520	LYS	3.6
1	A	299	LYS	3.5
1	B	603	VAL	3.5
1	B	234	ILE	3.5
1	B	596	TYR	3.4
1	B	218	VAL	3.4
1	B	464	THR	3.4
1	B	468	GLY	3.4
1	B	467	ASP	3.3
1	A	604[A]	SER	3.3
1	A	626	SER	3.3
1	B	627	LYS	3.3
1	A	333	ASN	3.3
1	B	300	THR	3.3
1	B	629	LYS	3.3
1	B	609	ALA	3.3
1	A	594	THR	3.3
1	B	623	THR	3.3
1	A	210[A]	ASN	3.2
1	B	601	GLY	3.2
1	B	626	SER	3.2
1	B	235	LEU	3.2
1	A	628	THR	3.2
1	B	610	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	622	TYR	3.1
1	A	638	LYS	3.1
1	B	519	THR	3.1
1	B	604[A]	SER	3.1
1	A	384	LYS	3.1
1	A	610	THR	3.1
1	A	607	VAL	3.1
1	B	607	VAL	3.1
1	A	614	LYS	3.1
1	B	518	LEU	3.1
1	A	298	ALA	3.1
1	B	605	PHE	3.0
1	A	526	GLN	3.0
1	A	274	LYS	3.0
1	A	598	LYS	3.0
1	B	631	ALA	3.0
1	A	326	ASP	3.0
1	B	473	ALA	3.0
1	B	533	ALA	3.0
1	B	592	ALA	3.0
1	B	633	GLN	3.0
1	A	447	ILE	3.0
1	B	637	LYS	3.0
1	A	334	ASN	3.0
1	B	602	ASP	2.9
1	B	530[A]	SER	2.9
1	A	599	LEU	2.9
1	B	472	LEU	2.9
1	A	300	THR	2.9
1	B	525	GLY	2.9
1	B	615	GLY	2.9
1	A	294	VAL	2.9
1	B	319	VAL	2.9
1	B	515	TYR	2.9
1	B	572	LYS	2.9
1	A	634	VAL	2.8
1	B	528	GLY	2.8
1	B	619	ASP	2.8
1	B	593	PRO	2.8
1	B	461	PHE	2.8
1	B	383[A]	ASP	2.8
1	A	319	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	603	VAL	2.8
1	A	601	GLY	2.8
1	B	606	ASN	2.7
1	B	624	GLN	2.7
1	A	472	LEU	2.7
1	A	596	TYR	2.7
1	B	595	GLY	2.7
1	A	584	GLN	2.7
1	B	303	VAL	2.7
1	B	600	SER	2.7
1	A	214	ASP	2.7
1	A	462	VAL	2.7
1	B	318	VAL	2.7
1	A	332	GLY	2.7
1	B	510	ALA	2.7
1	B	613	SER	2.6
1	A	482	ASP	2.6
1	A	619	ASP	2.6
1	B	299	LYS	2.6
1	B	268	LEU	2.6
1	B	531	ALA	2.6
1	A	217	THR	2.6
1	A	483	GLY	2.6
1	B	521	GLU	2.6
1	A	235	LEU	2.6
1	A	518	LEU	2.6
1	A	240	TYR	2.6
1	A	600	SER	2.6
1	A	637	LYS	2.6
1	B	210[A]	ASN	2.6
1	B	266	ALA	2.6
1	B	475	ALA	2.6
1	A	519	THR	2.5
1	B	636	ASN	2.5
1	B	205	GLU	2.5
1	A	592	ALA	2.5
1	B	561	ALA	2.5
1	B	562	LYS	2.5
1	A	219	SER	2.5
1	B	586	SER	2.5
1	B	292[A]	GLU	2.5
1	A	291	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	295	ALA	2.5
1	A	297	ALA	2.5
1	B	297	ALA	2.5
1	A	633	GLN	2.5
1	B	575	PHE	2.5
1	B	585	TYR	2.5
1	A	615	GLY	2.5
1	B	321	VAL	2.5
1	B	455	VAL	2.5
1	B	466	LYS	2.5
1	B	608	ASN	2.4
1	B	587	LEU	2.4
1	B	614	LYS	2.4
1	B	582[A]	GLU	2.4
1	A	209	ALA	2.4
1	B	612	TYR	2.4
1	B	207	ASP	2.4
1	A	194	LYS	2.4
1	B	638	LYS	2.4
1	A	471	ARG	2.4
1	A	593	PRO	2.4
1	A	609	ALA	2.4
1	A	321	VAL	2.4
1	A	470	GLU	2.4
1	B	573	GLY	2.4
1	A	331	TYR	2.4
1	B	197	VAL	2.4
1	B	560	ASN	2.3
1	A	272	ASN	2.3
1	B	465	ASN	2.3
1	A	525	GLY	2.3
1	B	474	GLY	2.3
1	A	466	LYS	2.3
1	B	540	LYS	2.3
1	B	511	ALA	2.3
1	B	206	LEU	2.3
1	B	584	GLN	2.3
1	A	465	ASN	2.3
1	A	303	VAL	2.3
1	A	605	PHE	2.3
1	A	622	TYR	2.3
1	B	457	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	2.3
1	B	621	GLU	2.2
1	A	293	ALA	2.2
1	B	298	ALA	2.2
1	A	606	ASN	2.2
1	B	263	LEU	2.2
1	B	527	ASP	2.2
1	B	208	TYR	2.2
1	B	564	VAL	2.2
1	A	631	ALA	2.2
1	A	613	SER	2.2
1	A	602	ASP	2.2
1	B	322	LEU	2.2
1	A	595	GLY	2.2
1	B	196	GLN	2.2
1	B	470	GLU	2.2
1	A	208	TYR	2.2
1	B	471	ARG	2.2
1	A	464	THR	2.2
1	A	636	ASN	2.2
1	A	380	LYS	2.2
1	B	512	VAL	2.2
1	B	513	LYS	2.2
1	A	467	ASP	2.2
1	A	265	GLY	2.2
1	B	532	LEU	2.2
1	B	580	LEU	2.2
1	A	448	ASN	2.2
1	A	572	LYS	2.2
1	A	267	THR	2.2
1	A	218	VAL	2.1
1	A	318	VAL	2.1
1	B	458	GLY	2.1
1	B	555	TRP	2.1
1	B	271	THR	2.1
1	B	517	ASP	2.1
1	B	590	THR	2.1
1	B	630	ASP	2.1
1	A	345	ILE	2.1
1	B	447	ILE	2.1
1	B	577	ILE	2.1
1	A	220	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	514	ALA	2.1
1	B	332	GLY	2.1
1	A	581	THR	2.1
1	A	202	ALA	2.1
1	B	222	VAL	2.1
1	A	335	PRO	2.1
1	B	384[A]	LYS	2.1
1	B	460	LYS	2.1
1	A	234	ILE	2.1
1	A	203	ASP	2.0
1	A	268	LEU	2.0
1	A	623	THR	2.0
1	A	515	TYR	2.0
1	B	295	ALA	2.0
1	A	296	LYS	2.0
1	A	301	LYS	2.0
1	A	529	LYS	2.0
1	B	529	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
2	K	A	1642	1/1	0.95	0.09	31,31,31,31	0
2	K	A	1641	1/1	0.99	0.09	22,22,22,22	0
2	K	B	1642	1/1	0.99	0.08	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.