



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:11 PM UTC

PDB ID : 6IXY / pdb_00006ixy
Title : X-ray structure of major pilin from *C. perfringens* SM101
Authors : Kamitori, S.; Tamai, E.
Deposited on : 2018-12-12
Resolution : 2.72 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

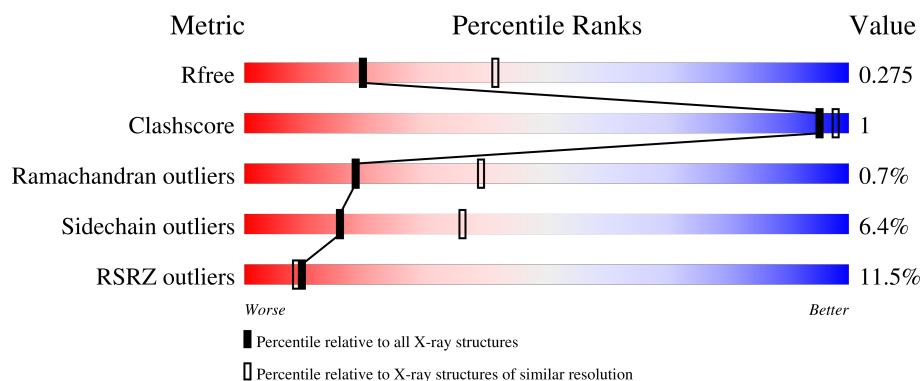
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	476	2% 84% 9% • 6%
1	B	476	13% 85% 9% • 5%
1	C	476	12% 86% 7% • 6%
1	D	476	16% 87% 8% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14021 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 pilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3458	2174	557	724	3			
1	B	454	Total	C	N	O	S	0	0	0
			3503	2204	563	733	3			
1	C	448	Total	C	N	O	S	0	0	0
			3458	2174	557	724	3			
1	D	454	Total	C	N	O	S	0	0	0
			3503	2204	563	733	3			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	expression tag	UNP Q0SWL8
A	14	ASN	-	expression tag	UNP Q0SWL8
A	15	HIS	-	expression tag	UNP Q0SWL8
A	16	LYS	-	expression tag	UNP Q0SWL8
A	17	VAL	-	expression tag	UNP Q0SWL8
A	18	HIS	-	expression tag	UNP Q0SWL8
A	19	HIS	-	expression tag	UNP Q0SWL8
A	20	HIS	-	expression tag	UNP Q0SWL8
A	21	HIS	-	expression tag	UNP Q0SWL8
A	22	HIS	-	expression tag	UNP Q0SWL8
A	23	HIS	-	expression tag	UNP Q0SWL8
A	24	ILE	-	expression tag	UNP Q0SWL8
A	25	GLU	-	expression tag	UNP Q0SWL8
A	26	GLY	-	expression tag	UNP Q0SWL8
A	27	ARG	-	expression tag	UNP Q0SWL8
A	28	HIS	-	expression tag	UNP Q0SWL8
A	29	MET	-	expression tag	UNP Q0SWL8
B	13	MET	-	expression tag	UNP Q0SWL8
B	14	ASN	-	expression tag	UNP Q0SWL8
B	15	HIS	-	expression tag	UNP Q0SWL8
B	16	LYS	-	expression tag	UNP Q0SWL8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	VAL	-	expression tag	UNP Q0SWL8
B	18	HIS	-	expression tag	UNP Q0SWL8
B	19	HIS	-	expression tag	UNP Q0SWL8
B	20	HIS	-	expression tag	UNP Q0SWL8
B	21	HIS	-	expression tag	UNP Q0SWL8
B	22	HIS	-	expression tag	UNP Q0SWL8
B	23	HIS	-	expression tag	UNP Q0SWL8
B	24	ILE	-	expression tag	UNP Q0SWL8
B	25	GLU	-	expression tag	UNP Q0SWL8
B	26	GLY	-	expression tag	UNP Q0SWL8
B	27	ARG	-	expression tag	UNP Q0SWL8
B	28	HIS	-	expression tag	UNP Q0SWL8
B	29	MET	-	expression tag	UNP Q0SWL8
C	13	MET	-	expression tag	UNP Q0SWL8
C	14	ASN	-	expression tag	UNP Q0SWL8
C	15	HIS	-	expression tag	UNP Q0SWL8
C	16	LYS	-	expression tag	UNP Q0SWL8
C	17	VAL	-	expression tag	UNP Q0SWL8
C	18	HIS	-	expression tag	UNP Q0SWL8
C	19	HIS	-	expression tag	UNP Q0SWL8
C	20	HIS	-	expression tag	UNP Q0SWL8
C	21	HIS	-	expression tag	UNP Q0SWL8
C	22	HIS	-	expression tag	UNP Q0SWL8
C	23	HIS	-	expression tag	UNP Q0SWL8
C	24	ILE	-	expression tag	UNP Q0SWL8
C	25	GLU	-	expression tag	UNP Q0SWL8
C	26	GLY	-	expression tag	UNP Q0SWL8
C	27	ARG	-	expression tag	UNP Q0SWL8
C	28	HIS	-	expression tag	UNP Q0SWL8
C	29	MET	-	expression tag	UNP Q0SWL8
D	13	MET	-	expression tag	UNP Q0SWL8
D	14	ASN	-	expression tag	UNP Q0SWL8
D	15	HIS	-	expression tag	UNP Q0SWL8
D	16	LYS	-	expression tag	UNP Q0SWL8
D	17	VAL	-	expression tag	UNP Q0SWL8
D	18	HIS	-	expression tag	UNP Q0SWL8
D	19	HIS	-	expression tag	UNP Q0SWL8
D	20	HIS	-	expression tag	UNP Q0SWL8
D	21	HIS	-	expression tag	UNP Q0SWL8
D	22	HIS	-	expression tag	UNP Q0SWL8
D	23	HIS	-	expression tag	UNP Q0SWL8
D	24	ILE	-	expression tag	UNP Q0SWL8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	GLU	-	expression tag	UNP Q0SWL8
D	26	GLY	-	expression tag	UNP Q0SWL8
D	27	ARG	-	expression tag	UNP Q0SWL8
D	28	HIS	-	expression tag	UNP Q0SWL8
D	29	MET	-	expression tag	UNP Q0SWL8

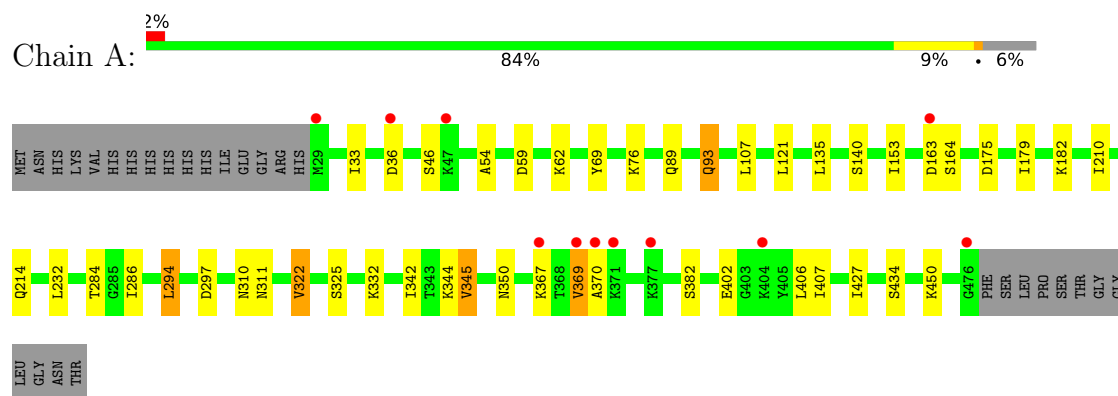
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	27	Total	O	0	0
			27	27		
2	C	23	Total	O	0	0
			23	23		
2	D	17	Total	O	0	0
			17	17		

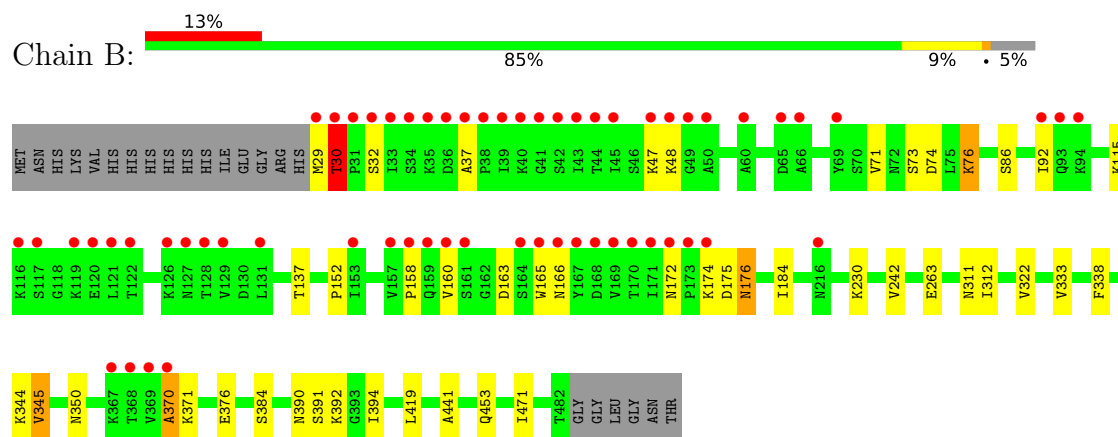
3 Residue-property plots [i](#)

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.

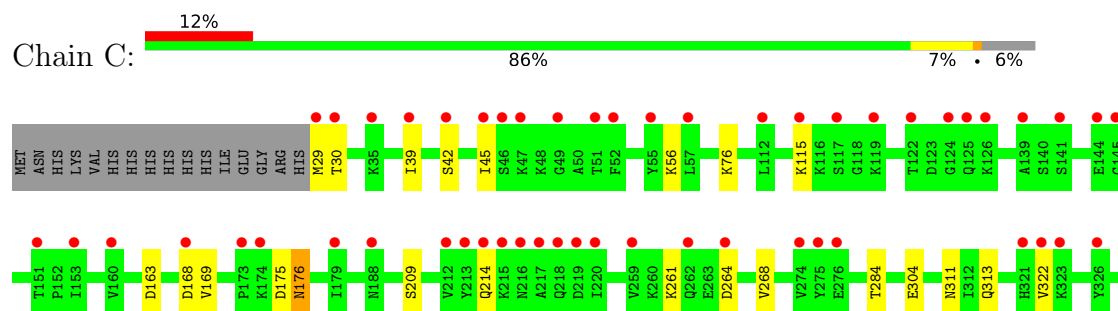
• Molecule 1: pilin

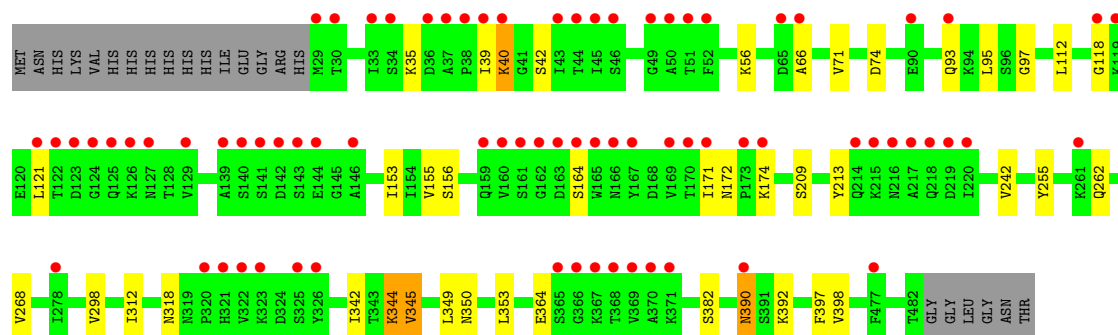


• Molecule 1: pilin



• Molecule 1: pilin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.14Å 111.83Å 118.59Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	48.71 – 2.72 48.71 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.71-2.72) 99.2 (48.71-2.72)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.227 , 0.276 0.231 , 0.275	Depositor DCC
R_{free} test set	3502 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14021	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

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	0.51	0/3510	0.65	0/4745
1	B	0.52	0/3557	0.63	0/4810
1	C	0.52	0/3510	0.65	0/4745
1	D	0.52	0/3557	0.66	0/4810
All	All	0.52	0/14134	0.65	0/19110

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
1	C	0	4
1	D	0	6
All	All	0	17

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	SER	Peptide
1	A	179	ILE	Peptide
1	B	29	MET	Peptide
1	B	30	THR	Peptide
1	B	37	ALA	Peptide
1	B	370	ALA	Peptide
1	B	394	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	C	175	ASP	Peptide
1	C	264	ASP	Peptide
1	C	368	THR	Peptide
1	C	389	THR	Peptide
1	D	118	GLY	Peptide
1	D	164	SER	Peptide
1	D	344	LYS	Peptide
1	D	364	GLU	Peptide
1	D	397	PHE	Peptide
1	D	66	ALA	Peptide

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	3458	0	3415	13	0
1	B	3503	0	3459	11	0
1	C	3458	0	3415	5	0
1	D	3503	0	3458	5	0
2	A	32	0	0	0	0
2	B	27	0	0	0	0
2	C	23	0	0	0	0
2	D	17	0	0	0	0
All	All	14021	0	13747	34	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 1.

All (34) 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:137:THR:HG22	1:B:152:PRO:HB3	1.87	0.56
1:C:304:GLU:HG2	1:C:438:THR:HB	1.90	0.54
1:C:176:ASN:C	1:C:176:ASN:HD22	2.18	0.51
1:B:419:LEU:HD11	1:B:471:ILE:CG2	2.41	0.51
1:A:54:ALA:HB2	1:A:121:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HE3	1:B:176:ASN:HD21	1.77	0.49
1:A:33:ILE:HG21	1:A:62:LYS:HD2	1.96	0.48
1:B:390:ASN:HB3	1:B:392:LYS:H	1.79	0.47
1:A:322:VAL:HG22	1:A:325:SER:HB2	1.96	0.47
1:A:107:LEU:HD23	1:A:135:LEU:HD23	1.96	0.47
1:B:184:ILE:HG13	1:B:333:VAL:HG21	1.97	0.47
1:B:338:PHE:CE1	1:B:441:ALA:HB2	2.50	0.47
1:A:402:GLU:HB2	1:A:427:ILE:O	2.15	0.46
1:A:89:GLN:O	1:A:93:GLN:NE2	2.48	0.46
1:B:73:SER:HA	1:B:76:LYS:CD	2.47	0.45
1:B:158:PRO:HB2	1:B:165:TRP:HB2	1.99	0.45
1:C:390:ASN:HB2	1:C:394:ILE:O	2.17	0.45
1:A:342:ILE:HD12	1:A:407:ILE:HG21	2.00	0.43
1:C:369:VAL:HG21	1:C:405:TYR:HE1	1.83	0.43
1:A:59:ASP:O	1:A:69:TYR:HA	2.19	0.43
1:D:353:LEU:HD13	1:D:392:LYS:HA	1.99	0.43
1:D:39:ILE:HG23	1:D:40:LYS:HG3	2.01	0.42
1:C:313:GLN:HG3	1:C:330:THR:HG22	2.02	0.42
1:B:174:LYS:CE	1:B:176:ASN:HD21	2.32	0.42
1:A:367:LYS:HB3	1:A:369:VAL:HG23	2.02	0.42
1:A:232:LEU:HD23	1:A:294:LEU:HD12	2.02	0.41
1:A:182:LYS:HE2	1:A:310:ASN:HB3	1.88	0.41
1:A:210:ILE:HD11	1:A:286:ILE:HG12	2.01	0.41
1:D:345:VAL:HG13	1:D:350:ASN:HA	2.02	0.41
1:B:345:VAL:HG13	1:B:350:ASN:HA	2.02	0.41
1:D:390:ASN:HD22	1:D:390:ASN:HA	1.60	0.41
1:A:345:VAL:HG13	1:A:350:ASN:HA	2.03	0.40
1:B:176:ASN:HD22	1:B:176:ASN:HA	1.64	0.40
1:D:242:VAL:HG11	1:D:255:TYR:CE2	2.56	0.40

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	446/476 (94%)	436 (98%)	9 (2%)	1 (0%)	43	66
1	B	452/476 (95%)	434 (96%)	14 (3%)	4 (1%)	14	33
1	C	446/476 (94%)	422 (95%)	22 (5%)	2 (0%)	30	52
1	D	452/476 (95%)	419 (93%)	28 (6%)	5 (1%)	11	27
All	All	1796/1904 (94%)	1711 (95%)	73 (4%)	12 (1%)	18	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	LYS
1	C	369	VAL
1	A	370	ALA
1	D	172	ASN
1	B	30	THR
1	D	174	LYS
1	D	318	ASN
1	B	370	ALA
1	D	35	LYS
1	C	45	ILE
1	D	97	GLY
1	B	160	VAL

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	390/414 (94%)	368 (94%)	22 (6%)	19	42
1	B	396/414 (96%)	369 (93%)	27 (7%)	14	33
1	C	390/414 (94%)	364 (93%)	26 (7%)	15	34
1	D	396/414 (96%)	370 (93%)	26 (7%)	15	35
All	All	1572/1656 (95%)	1471 (94%)	101 (6%)	16	36

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	46	SER
1	A	76	LYS
1	A	93	GLN
1	A	153	ILE
1	A	163	ASP
1	A	164	SER
1	A	175	ASP
1	A	214	GLN
1	A	284	THR
1	A	294	LEU
1	A	297	ASP
1	A	311	ASN
1	A	322	VAL
1	A	332	LYS
1	A	344	LYS
1	A	345	VAL
1	A	369	VAL
1	A	382	SER
1	A	406	LEU
1	A	434	SER
1	A	450	LYS
1	B	30	THR
1	B	32	SER
1	B	47	LYS
1	B	48	LYS
1	B	71	VAL
1	B	74	ASP
1	B	76	LYS
1	B	86	SER
1	B	92	ILE
1	B	163	ASP
1	B	166	ASN
1	B	172	ASN
1	B	175	ASP
1	B	176	ASN
1	B	230	LYS
1	B	242	VAL
1	B	263	GLU
1	B	311	ASN
1	B	312	ILE
1	B	322	VAL
1	B	344	LYS

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Mol	Chain	Res	Type
1	B	345	VAL
1	B	371	LYS
1	B	376	GLU
1	B	384	SER
1	B	391	SER
1	B	453	GLN
1	C	29	MET
1	C	30	THR
1	C	39	ILE
1	C	42	SER
1	C	56	LYS
1	C	76	LYS
1	C	115	LYS
1	C	163	ASP
1	C	168	ASP
1	C	169	VAL
1	C	176	ASN
1	C	209	SER
1	C	214	GLN
1	C	261	LYS
1	C	268	VAL
1	C	284	THR
1	C	311	ASN
1	C	322	VAL
1	C	344	LYS
1	C	345	VAL
1	C	348	GLU
1	C	384	SER
1	C	390	ASN
1	C	401	LYS
1	C	434	SER
1	C	474	HIS
1	D	40	LYS
1	D	42	SER
1	D	56	LYS
1	D	71	VAL
1	D	74	ASP
1	D	93	GLN
1	D	95	LEU
1	D	112	LEU
1	D	121	LEU
1	D	153	ILE

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Mol	Chain	Res	Type
1	D	155	VAL
1	D	156	SER
1	D	171	ILE
1	D	209	SER
1	D	213	TYR
1	D	262	GLN
1	D	268	VAL
1	D	298	VAL
1	D	312	ILE
1	D	342	ILE
1	D	344	LYS
1	D	345	VAL
1	D	349	LEU
1	D	382	SER
1	D	390	ASN
1	D	398	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	93	GLN
1	A	108	HIS
1	A	183	ASN
1	A	216	ASN
1	A	350	ASN
1	A	430	ASN
1	A	474	HIS
1	B	93	GLN
1	B	176	ASN
1	B	214	GLN
1	B	390	ASN
1	B	430	ASN
1	B	470	GLN
1	C	166	ASN
1	C	176	ASN
1	C	214	GLN
1	C	319	ASN
1	C	321	HIS
1	C	390	ASN
1	C	430	ASN
1	C	470	GLN

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Mol	Chain	Res	Type
1	D	93	GLN
1	D	127	ASN
1	D	172	ASN
1	D	214	GLN
1	D	216	ASN
1	D	262	GLN
1	D	390	ASN
1	D	430	ASN
1	D	453	GLN
1	D	464	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

There are no ligands in this entry.

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	448/476 (94%)	0.07	11 (2%) 58 55	21, 32, 59, 86	0
1	B	454/476 (95%)	0.59	61 (13%) 7 6	21, 37, 99, 99	0
1	C	448/476 (94%)	0.63	59 (13%) 7 6	18, 45, 86, 99	0
1	D	454/476 (95%)	0.84	76 (16%) 4 4	23, 46, 98, 99	0
All	All	1804/1904 (94%)	0.53	207 (11%) 9 8	18, 39, 94, 99	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	ALA	8.2
1	B	369	VAL	7.4
1	B	167	TYR	7.2
1	D	122	THR	6.5
1	D	121	LEU	6.2
1	D	369	VAL	6.1
1	A	369	VAL	5.7
1	B	368	THR	5.4
1	B	38	PRO	5.2
1	D	366	GLY	5.1
1	B	169	VAL	5.0
1	D	29	MET	4.9
1	D	39	ILE	4.9
1	B	33	ILE	4.8
1	D	37	ALA	4.6
1	B	171	ILE	4.6
1	B	39	ILE	4.4
1	B	165	TRP	4.4
1	B	161	SER	4.4
1	B	367	LYS	4.4
1	B	174	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	171	ILE	4.3
1	C	139	ALA	4.3
1	D	38	PRO	4.2
1	D	30	THR	4.2
1	D	162	GLY	4.1
1	D	371	LYS	4.0
1	B	35	LYS	4.0
1	B	40	LYS	4.0
1	D	126	LYS	4.0
1	B	160	VAL	4.0
1	D	139	ALA	3.9
1	D	174	LYS	3.9
1	D	166	ASN	3.9
1	B	29	MET	3.9
1	C	188	ASN	3.8
1	C	369	VAL	3.8
1	D	173	PRO	3.8
1	D	367	LYS	3.7
1	D	165	TRP	3.7
1	B	41	GLY	3.6
1	B	370	ALA	3.6
1	C	145	GLY	3.6
1	C	212	VAL	3.6
1	D	368	THR	3.6
1	B	131	LEU	3.6
1	C	217	ALA	3.6
1	D	143	SER	3.6
1	D	167	TYR	3.5
1	D	164	SER	3.5
1	A	370	ALA	3.5
1	A	367	LYS	3.4
1	D	215	LYS	3.4
1	B	34	SER	3.3
1	D	46	SER	3.3
1	B	36	ASP	3.3
1	D	123	ASP	3.3
1	B	45	ILE	3.3
1	C	122	THR	3.3
1	D	370	ALA	3.3
1	C	52	PHE	3.3
1	C	322	VAL	3.2
1	B	30	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	218	GLN	3.2
1	C	112	LEU	3.2
1	B	31	PRO	3.2
1	B	42	SER	3.2
1	B	50	ALA	3.2
1	C	42	SER	3.2
1	B	43	ILE	3.2
1	C	366	GLY	3.2
1	B	48	LYS	3.1
1	C	367	LYS	3.1
1	C	39	ILE	3.1
1	D	50	ALA	3.1
1	B	65	ASP	3.1
1	C	144	GLU	3.1
1	B	173	PRO	3.1
1	B	122	THR	3.1
1	C	46	SER	3.1
1	C	45	ILE	3.1
1	D	33	ILE	3.1
1	C	321	HIS	3.0
1	D	43	ILE	3.0
1	B	126	LYS	3.0
1	D	325	SER	3.0
1	B	153	ILE	3.0
1	B	44	THR	3.0
1	B	66	ALA	3.0
1	C	365	SER	2.9
1	C	264	ASP	2.9
1	A	476	GLY	2.9
1	B	121	LEU	2.9
1	C	364	GLU	2.9
1	D	119	LYS	2.9
1	B	92	ILE	2.9
1	D	45	ILE	2.9
1	B	170	THR	2.9
1	B	49	GLY	2.9
1	B	93	GLN	2.9
1	D	141	SER	2.9
1	D	118	GLY	2.9
1	C	174	LYS	2.9
1	C	173	PRO	2.8
1	B	164	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	127	ASN	2.8
1	C	220	ILE	2.8
1	C	323	LYS	2.8
1	D	477	PHE	2.8
1	D	159	GLN	2.7
1	B	120	GLU	2.7
1	C	219	ASP	2.7
1	D	326	TYR	2.7
1	C	215	LYS	2.7
1	D	34	SER	2.7
1	D	51	THR	2.7
1	B	166	ASN	2.7
1	C	57	LEU	2.6
1	D	90	GLU	2.6
1	B	172	ASN	2.6
1	D	160	VAL	2.6
1	C	29	MET	2.6
1	D	93	GLN	2.6
1	A	404	LYS	2.6
1	C	47	LYS	2.6
1	D	169	VAL	2.6
1	C	141	SER	2.5
1	D	163	ASP	2.5
1	B	47	LYS	2.5
1	C	213	TYR	2.5
1	A	377	LYS	2.5
1	B	158	PRO	2.5
1	D	125	GLN	2.5
1	B	128	THR	2.5
1	A	371	LYS	2.5
1	C	115	LYS	2.5
1	D	142	ASP	2.5
1	D	217	ALA	2.5
1	C	151	THR	2.5
1	D	40	LYS	2.5
1	C	474	HIS	2.5
1	B	216	ASN	2.4
1	D	216	ASN	2.4
1	B	168	ASP	2.4
1	D	66	ALA	2.4
1	C	51	THR	2.4
1	D	44	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	153	ILE	2.4
1	D	161	SER	2.4
1	C	126	LYS	2.4
1	C	160	VAL	2.4
1	D	322	VAL	2.4
1	A	47	LYS	2.4
1	D	261	LYS	2.4
1	C	262	GLN	2.3
1	D	49	GLY	2.3
1	D	278	ILE	2.3
1	C	216	ASN	2.3
1	D	36	ASP	2.3
1	C	55	TYR	2.3
1	A	36	ASP	2.3
1	D	129	VAL	2.3
1	C	179	ILE	2.3
1	D	321	HIS	2.3
1	C	35	LYS	2.3
1	C	326	TYR	2.3
1	D	219	ASP	2.3
1	C	214	GLN	2.3
1	B	119	LYS	2.2
1	C	368	THR	2.2
1	D	144	GLU	2.2
1	D	320	PRO	2.2
1	D	140	SER	2.2
1	C	124	GLY	2.2
1	D	124	GLY	2.2
1	C	259	VAL	2.2
1	D	170	THR	2.2
1	B	117	SER	2.2
1	A	163	ASP	2.2
1	D	323	LYS	2.2
1	B	60	ALA	2.2
1	C	276	GLU	2.2
1	C	275	TYR	2.2
1	D	390	ASN	2.2
1	B	94	LYS	2.2
1	C	119	LYS	2.2
1	B	32	SER	2.2
1	C	125	GLN	2.1
1	D	65	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	117	SER	2.1
1	D	52	PHE	2.1
1	B	129	VAL	2.1
1	D	214	GLN	2.1
1	C	168	ASP	2.1
1	D	365	SER	2.1
1	B	116	LYS	2.1
1	C	30	THR	2.1
1	D	127	ASN	2.1
1	B	69	TYR	2.1
1	B	157	VAL	2.1
1	C	274	VAL	2.1
1	D	146	ALA	2.0
1	D	220	ILE	2.0
1	A	29	MET	2.0
1	B	159	GLN	2.0
1	D	218	GLN	2.0
1	C	49	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.