



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:42 AM UTC

PDB ID : 5MU4 / pdb_00005mu4
Title : Tail Tubular Protein A of Klebsiella pneumoniae bacteriophage KP32
Authors : Pyra, A.; Brzozowska, E.; Pawlik, K.; Dauter, M.; Dauter, Z.; Gamian, A.
Deposited on : 2017-01-12
Resolution : 1.90 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

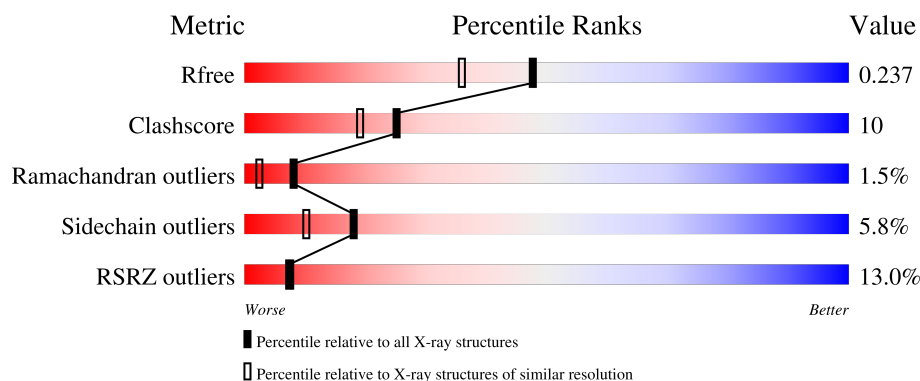
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	201	7% 83% 11% ...
1	B	201	3% 76% 12% 8%
1	C	201	19% 67% 15% 7% 8%
1	D	201	19% 76% 15% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6671 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 Tail tubular protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	3	0
			1553	966	268	309	10			
1	B	184	Total	C	N	O	S	0	0	0
			1428	889	244	286	9			
1	C	185	Total	C	N	O	S	0	1	0
			1447	899	248	291	9			
1	D	187	Total	C	N	O	S	0	0	1
			1452	903	249	290	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	SER	-	expression tag	UNP D1L2W4
A	-7	GLY	-	expression tag	UNP D1L2W4
A	-6	LEU	-	expression tag	UNP D1L2W4
A	-5	VAL	-	expression tag	UNP D1L2W4
A	-4	PRO	-	expression tag	UNP D1L2W4
A	-3	ARG	-	expression tag	UNP D1L2W4
A	-2	GLY	-	expression tag	UNP D1L2W4
A	-1	SER	-	expression tag	UNP D1L2W4
A	0	HIS	-	expression tag	UNP D1L2W4
B	-8	SER	-	expression tag	UNP D1L2W4
B	-7	GLY	-	expression tag	UNP D1L2W4
B	-6	LEU	-	expression tag	UNP D1L2W4
B	-5	VAL	-	expression tag	UNP D1L2W4
B	-4	PRO	-	expression tag	UNP D1L2W4
B	-3	ARG	-	expression tag	UNP D1L2W4
B	-2	GLY	-	expression tag	UNP D1L2W4
B	-1	SER	-	expression tag	UNP D1L2W4
B	0	HIS	-	expression tag	UNP D1L2W4
C	-8	SER	-	expression tag	UNP D1L2W4
C	-7	GLY	-	expression tag	UNP D1L2W4
C	-6	LEU	-	expression tag	UNP D1L2W4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	expression tag	UNP D1L2W4
C	-4	PRO	-	expression tag	UNP D1L2W4
C	-3	ARG	-	expression tag	UNP D1L2W4
C	-2	GLY	-	expression tag	UNP D1L2W4
C	-1	SER	-	expression tag	UNP D1L2W4
C	0	HIS	-	expression tag	UNP D1L2W4
D	-8	SER	-	expression tag	UNP D1L2W4
D	-7	GLY	-	expression tag	UNP D1L2W4
D	-6	LEU	-	expression tag	UNP D1L2W4
D	-5	VAL	-	expression tag	UNP D1L2W4
D	-4	PRO	-	expression tag	UNP D1L2W4
D	-3	ARG	-	expression tag	UNP D1L2W4
D	-2	GLY	-	expression tag	UNP D1L2W4
D	-1	SER	-	expression tag	UNP D1L2W4
D	0	HIS	-	expression tag	UNP D1L2W4

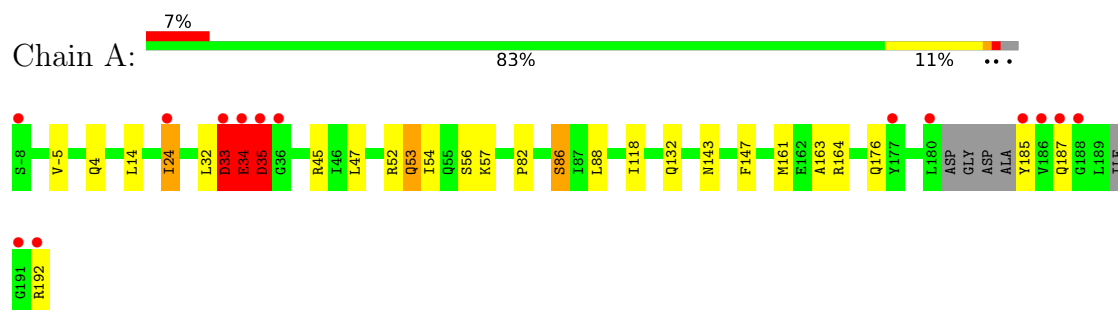
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	236	Total O 236 236	0	0
2	B	241	Total O 241 241	0	0
2	C	150	Total O 150 150	0	0
2	D	164	Total O 164 164	0	0

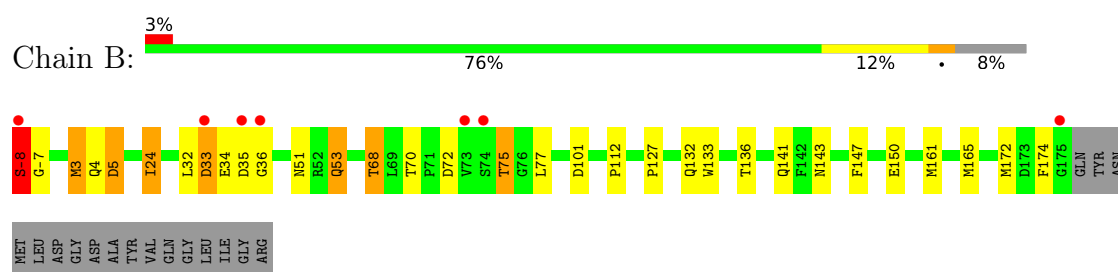
3 Residue-property plots [i](#)

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.

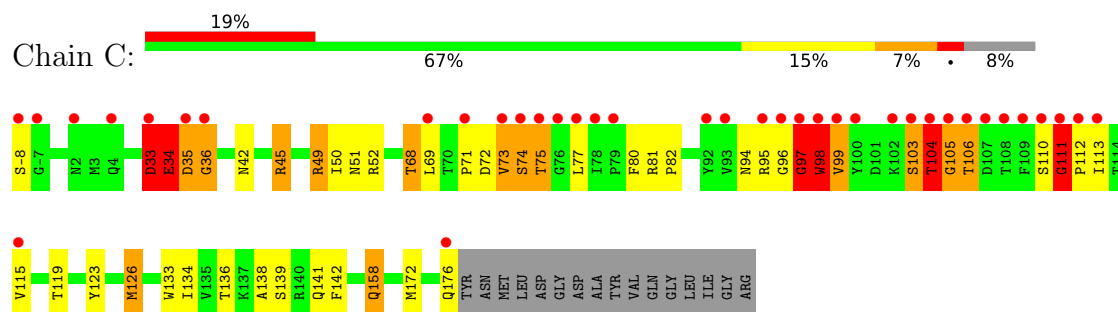
• Molecule 1: Tail tubular protein A



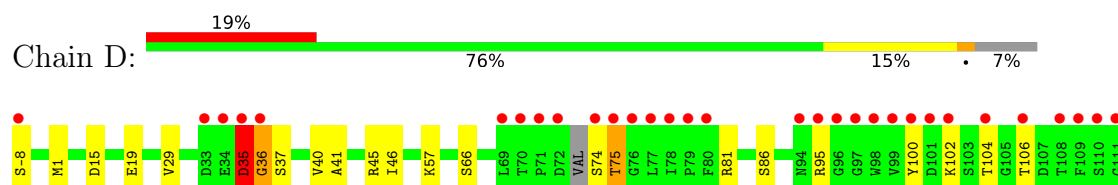
• Molecule 1: Tail tubular protein A

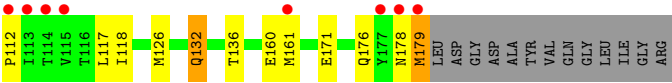


• Molecule 1: Tail tubular protein A



• Molecule 1: Tail tubular protein A





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	138.32Å 138.32Å 102.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.95 – 1.90 29.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.95-1.90) 95.0 (29.95-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.183 , 0.230 0.192 , 0.237	Depositor DCC
R_{free} test set	1650 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6671	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 i

5.1 Standard geometry i

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	1.46	5/1583 (0.3%)	1.25	4/2139 (0.2%)
1	B	1.54	7/1456 (0.5%)	1.27	2/1973 (0.1%)
1	C	1.34	7/1475 (0.5%)	1.24	9/1999 (0.5%)
1	D	1.23	1/1480 (0.1%)	1.16	5/2004 (0.2%)
All	All	1.40	20/5994 (0.3%)	1.23	20/8115 (0.2%)

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	3
1	B	0	2
1	C	0	6
1	D	0	2
All	All	0	13

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	ASP	C-O	6.37	1.31	1.23
1	A	56	SER	C-O	-6.33	1.15	1.24
1	B	51	ASN	C-O	6.23	1.31	1.24
1	B	127	PRO	C-O	6.04	1.30	1.23
1	A	86	SER	CB-OG	-5.71	1.30	1.42
1	C	142	PHE	C-O	5.50	1.30	1.24
1	C	123	TYR	CA-CB	5.43	1.62	1.53
1	C	139	SER	C-O	5.42	1.30	1.24
1	D	126	MET	C-O	-5.38	1.19	1.24
1	C	51	ASN	C-O	5.21	1.30	1.24
1	C	42	ASN	CA-C	5.18	1.59	1.52
1	C	133	TRP	CA-C	5.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	TRP	C-O	5.17	1.30	1.24
1	A	47	LEU	CA-CB	-5.16	1.45	1.53
1	A	53	GLN	C-O	-5.16	1.18	1.24
1	B	141	GLN	CA-C	5.09	1.59	1.52
1	C	136	THR	N-CA	-5.08	1.40	1.46
1	A	-5	VAL	N-CA	5.04	1.51	1.46
1	B	53	GLN	N-CA	-5.01	1.40	1.46
1	B	33	ASP	CA-C	-5.00	1.46	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ASP	N-CA-C	8.55	123.43	112.92
1	D	37	SER	N-CA-C	-8.42	94.79	108.52
1	C	111	GLY	C-N-CD	-8.19	102.58	120.60
1	C	34	GLU	N-CA-C	-7.89	98.78	110.46
1	C	113	ILE	N-CA-C	7.65	118.92	107.75
1	D	36	GLY	N-CA-C	-6.91	96.82	113.18
1	B	32	LEU	CA-C-N	-6.53	113.91	123.05
1	B	32	LEU	C-N-CA	-6.53	113.91	123.05
1	A	45	ARG	N-CA-C	5.96	117.86	111.36
1	C	36	GLY	N-CA-C	-5.88	96.24	113.30
1	C	97	GLY	CA-C-N	5.72	129.93	120.94
1	C	97	GLY	C-N-CA	5.72	129.93	120.94
1	A	35	ASP	N-CA-CB	5.72	120.16	110.49
1	D	41	ALA	N-CA-C	5.61	117.39	111.28
1	C	98	TRP	N-CA-CB	-5.36	102.45	110.17
1	A	52	ARG	N-CA-C	5.20	116.95	111.28
1	D	46	ILE	O-C-N	5.12	126.83	121.87
1	C	45	ARG	N-CA-C	5.09	116.91	111.36
1	D	45	ARG	N-CA-C	5.08	116.90	111.36
1	C	98	TRP	CB-CA-C	5.01	118.77	109.54

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	LEU	Peptide
1	A	33	ASP	Peptide
1	A	34	GLU	Peptide
1	B	-8	SER	Peptide
1	B	36	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	-8	SER	Peptide
1	C	111	GLY	Peptide
1	C	34	GLU	Peptide
1	C	35	ASP	Peptide
1	C	97	GLY	Peptide
1	C	98	TRP	Peptide
1	D	35	ASP	Peptide
1	D	36	GLY	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	1553	0	1475	35	0
1	B	1428	0	1356	26	0
1	C	1447	0	1371	40	0
1	D	1452	0	1374	14	0
2	A	236	0	0	13	1
2	B	241	0	0	10	1
2	C	150	0	0	10	0
2	D	164	0	0	1	0
All	All	6671	0	5576	111	1

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 10.

All (111) 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:C:126:MET:SD	2:C:326:HOH:O	1.97	1.22
1:C:126:MET:CE	2:C:326:HOH:O	2.01	1.06
1:A:192[B]:ARG:HG2	1:A:192[B]:ARG:O	1.53	1.00
1:A:192[B]:ARG:HH11	1:A:192[B]:ARG:HG3	1.27	0.95
1:A:34:GLU:C	2:A:201:HOH:O	2.11	0.94
1:C:119:THR:HG22	2:C:286:HOH:O	1.69	0.90
1:A:35:ASP:N	2:A:201:HOH:O	2.06	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192[B]:ARG:HH11	1:A:192[B]:ARG:CG	1.87	0.87
1:C:33:ASP:CG	1:C:33:ASP:O	2.23	0.82
1:C:94:ASN:OD1	1:C:97:GLY:HA2	1.81	0.80
1:C:126:MET:HE3	2:C:326:HOH:O	1.73	0.80
1:C:34:GLU:HB3	1:C:36:GLY:N	1.98	0.78
1:C:94:ASN:OD1	1:C:97:GLY:CA	2.34	0.76
1:B:33:ASP:HB2	2:B:367:HOH:O	1.84	0.75
1:C:71:PRO:HD3	1:C:111:GLY:O	1.86	0.75
1:B:75:THR:HG21	2:B:408:HOH:O	1.87	0.74
1:C:119:THR:CG2	2:C:286:HOH:O	2.31	0.73
1:A:34:GLU:CA	2:A:201:HOH:O	2.37	0.72
1:A:132:GLN:HG3	2:A:394:HOH:O	1.91	0.69
1:A:176:GLN:O	1:A:192[B]:ARG:NH1	2.26	0.69
1:A:187:GLN:NE2	2:A:202:HOH:O	2.19	0.68
1:B:24:ILE:HD11	1:B:143:ASN:HB2	1.76	0.68
1:A:192[B]:ARG:CG	1:A:192[B]:ARG:NH1	2.49	0.67
1:D:160:GLU:OE2	2:D:201:HOH:O	2.13	0.66
1:C:73:VAL:O	1:C:74:SER:HB3	1.94	0.66
1:C:34:GLU:HB3	1:C:35:ASP:C	2.21	0.66
1:B:3:MET:O	2:B:201:HOH:O	2.15	0.65
1:B:161:MET:O	1:B:165:MET:HG3	1.97	0.64
1:C:105:GLY:HA3	1:C:106:THR:HB	1.79	0.64
1:A:192[B]:ARG:O	1:A:192[B]:ARG:CG	2.36	0.64
1:B:132:GLN:O	1:B:136:THR:HG23	1.98	0.64
1:A:24:ILE:HD11	1:A:143:ASN:HD22	1.62	0.63
1:C:104:THR:HG23	1:C:106:THR:HG22	1.83	0.61
1:A:88:LEU:HD11	1:A:118:ILE:HD11	1.82	0.61
1:B:53:GLN:NE2	2:B:207:HOH:O	2.36	0.59
1:B:68:THR:CG2	2:B:316:HOH:O	2.50	0.59
1:D:178:ASN:O	1:D:179:MET:HB2	2.01	0.58
1:B:5:ASP:HB2	2:B:210:HOH:O	2.02	0.58
1:C:73:VAL:O	1:C:74:SER:CB	2.52	0.58
1:C:104:THR:HG23	1:C:106:THR:CG2	2.34	0.58
1:C:172:MET:HE3	1:D:57:LYS:HD3	1.86	0.58
1:D:1:MET:HE3	1:D:81:ARG:NH2	2.19	0.57
1:D:15:ASP:O	1:D:19:GLU:HG3	2.05	0.56
1:C:34:GLU:CB	1:C:35:ASP:C	2.79	0.56
1:B:34:GLU:CB	1:B:35:ASP:HA	2.36	0.56
1:D:132:GLN:O	1:D:136:THR:HG23	2.07	0.55
1:C:96:GLY:HA3	1:C:98:TRP:CE3	2.41	0.55
1:D:74:SER:O	1:D:75:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:H	1:A:35:ASP:CB	2.20	0.54
1:C:68:THR:HG23	2:C:299:HOH:O	2.08	0.53
1:A:57:LYS:HD3	1:B:172:MET:HE3	1.91	0.53
1:B:35:ASP:HB3	2:B:231:HOH:O	2.08	0.53
1:A:34:GLU:H	1:A:35:ASP:HB3	1.73	0.52
1:C:105:GLY:N	1:C:106:THR:HG22	2.25	0.52
1:B:174:PHE:C	2:B:238:HOH:O	2.52	0.51
1:D:95:ARG:HG3	1:D:100:TYR:CD1	2.44	0.51
1:C:68:THR:CG2	2:C:299:HOH:O	2.58	0.51
1:A:132:GLN:HG2	1:A:163:ALA:HB2	1.93	0.50
1:A:34:GLU:CB	2:A:201:HOH:O	2.59	0.50
1:B:35:ASP:CB	2:B:231:HOH:O	2.59	0.50
1:C:103:SER:C	1:C:104:THR:HG22	2.36	0.50
1:D:104:THR:OG1	1:D:106:THR:HG22	2.12	0.50
1:D:35:ASP:OD1	1:D:35:ASP:N	2.45	0.50
1:B:132:GLN:HG2	2:B:315:HOH:O	2.11	0.49
1:D:1:MET:O	1:D:81:ARG:NH1	2.45	0.49
1:A:132:GLN:CG	2:A:394:HOH:O	2.54	0.49
1:B:24:ILE:HG12	1:B:147:PHE:CD1	2.48	0.49
1:B:72:ASP:HB3	1:B:75:THR:HG22	1.95	0.49
1:C:98:TRP:CD2	1:C:98:TRP:N	2.80	0.48
1:A:34:GLU:N	1:A:35:ASP:OD1	2.46	0.48
1:A:161:MET:HE1	1:A:164:ARG:HH12	1.78	0.48
1:B:24:ILE:HD11	1:B:143:ASN:CB	2.43	0.48
1:C:80:PHE:HB3	1:C:97:GLY:HA3	1.96	0.47
1:B:34:GLU:HB2	1:B:35:ASP:HA	1.95	0.47
1:D:86:SER:HB3	1:D:118:ILE:HD12	1.95	0.47
1:A:24:ILE:HG12	1:A:147:PHE:CD2	2.50	0.47
1:A:132:GLN:CD	2:A:250:HOH:O	2.57	0.47
1:A:82:PRO:O	2:A:203:HOH:O	2.20	0.47
1:A:24:ILE:HD11	1:A:143:ASN:ND2	2.28	0.47
1:B:75:THR:HG23	1:B:77:LEU:HG	1.97	0.47
1:A:53:GLN:NE2	2:A:213:HOH:O	2.47	0.46
1:A:54:ILE:HA	1:B:172:MET:HE2	1.98	0.46
1:C:49:ARG:NH1	1:C:141:GLN:OE1	2.48	0.46
1:C:50:ILE:HD13	1:C:138:ALA:HA	1.98	0.46
1:C:34:GLU:HB3	1:C:36:GLY:H	1.76	0.46
1:A:54:ILE:HA	1:B:172:MET:CE	2.46	0.46
1:C:158[A]:GLN:C	1:C:158[A]:GLN:NE2	2.73	0.46
1:A:187:GLN:CD	2:A:202:HOH:O	2.54	0.45
1:C:81:ARG:HB3	1:C:82:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:H	1:A:35:ASP:CG	2.25	0.45
1:C:34:GLU:CB	2:C:288:HOH:O	2.64	0.45
1:C:105:GLY:HA3	1:C:106:THR:CB	2.46	0.44
1:C:50:ILE:CD1	1:C:138:ALA:HA	2.47	0.44
1:D:171:GLU:OE2	1:D:176:GLN:HG2	2.17	0.44
1:B:70:THR:HG23	1:B:112:PRO:HG3	1.99	0.44
1:C:33:ASP:O	1:C:33:ASP:OD1	2.35	0.44
1:C:34:GLU:HG3	1:C:35:ASP:O	2.17	0.44
1:A:161:MET:CE	1:A:164:ARG:HH12	2.31	0.44
1:C:72:ASP:O	1:C:73:VAL:HG22	2.18	0.44
1:B:-8:SER:OG	1:B:-7:GLY:HA3	2.18	0.43
1:A:86:SER:HB3	1:A:118:ILE:HD12	2.00	0.43
1:A:185:TYR:N	1:A:187:GLN:NE2	2.67	0.42
1:C:75:THR:HB	1:C:77:LEU:HG	2.00	0.42
1:A:192[B]:ARG:HB2	2:A:282:HOH:O	2.19	0.42
1:C:52:ARG:NH1	2:C:201:HOH:O	2.14	0.42
1:B:72:ASP:OD1	1:B:72:ASP:C	2.63	0.41
1:D:29:VAL:HG11	1:D:40:VAL:HG21	2.01	0.41
1:A:164:ARG:NH2	2:A:220:HOH:O	2.53	0.41
1:B:34:GLU:N	1:B:35:ASP:HA	2.34	0.41
1:C:126:MET:HE1	1:C:134:ILE:CD1	2.51	0.41
1:C:45:ARG:NH1	2:C:214:HOH:O	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:419:HOH:O	2:B:318:HOH:O[2_655]	2.15	0.05

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	192/201 (96%)	186 (97%)	4 (2%)	2 (1%)	12	5
1	B	182/201 (90%)	177 (97%)	5 (3%)	0	100	100
1	C	184/201 (92%)	165 (90%)	11 (6%)	8 (4%)	2	0
1	D	183/201 (91%)	174 (95%)	8 (4%)	1 (0%)	24	16
All	All	741/804 (92%)	702 (95%)	28 (4%)	11 (2%)	8	2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	C	73	VAL
1	C	74	SER
1	C	99	VAL
1	C	104	THR
1	C	112	PRO
1	A	35	ASP
1	C	33	ASP
1	C	103	SER
1	C	105	GLY
1	D	112	PRO

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	165/165 (100%)	161 (98%)	4 (2%)	43	38
1	B	152/165 (92%)	144 (95%)	8 (5%)	20	12
1	C	154/165 (93%)	138 (90%)	16 (10%)	7	2
1	D	154/165 (93%)	145 (94%)	9 (6%)	18	10
All	All	625/660 (95%)	588 (94%)	37 (6%)	18	10

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	14	LEU
1	A	24	ILE
1	A	33	ASP
1	B	-8	SER
1	B	3	MET
1	B	4	GLN
1	B	5	ASP
1	B	24	ILE
1	B	68	THR
1	B	75	THR
1	B	150	GLU
1	C	33	ASP
1	C	34	GLU
1	C	49	ARG
1	C	68	THR
1	C	69	LEU
1	C	75	THR
1	C	95	ARG
1	C	99	VAL
1	C	104	THR
1	C	106	THR
1	C	110	SER
1	C	115	VAL
1	C	126	MET
1	C	158[A]	GLN
1	C	158[B]	GLN
1	C	176	GLN
1	D	-8	SER
1	D	35	ASP
1	D	66	SER
1	D	75	THR
1	D	102	LYS
1	D	117	LEU
1	D	132	GLN
1	D	161	MET
1	D	179	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	143	ASN
1	B	53	GLN
1	B	132	GLN
1	B	158	GLN
1	C	176	GLN
1	D	178	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	196/201 (97%)	0.20	14 (7%) 22 23	8, 20, 45, 97	3 (1%)
1	B	184/201 (91%)	0.03	7 (3%) 44 47	10, 17, 41, 79	0
1	C	185/201 (92%)	0.85	38 (20%) 2 2	11, 26, 82, 93	1 (0%)
1	D	187/201 (93%)	0.86	39 (20%) 2 2	11, 27, 81, 95	0
All	All	752/804 (93%)	0.48	98 (13%) 7 7	8, 22, 75, 97	4 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	PRO	6.4
1	A	180	LEU	5.8
1	C	77	LEU	5.7
1	C	-8	SER	5.5
1	C	100	TYR	5.1
1	D	111	GLY	5.0
1	C	98	TRP	4.9
1	D	177	TYR	4.9
1	C	99	VAL	4.9
1	C	73	VAL	4.8
1	D	109	PHE	4.7
1	D	98	TRP	4.6
1	D	179	MET	4.6
1	D	71	PRO	4.6
1	D	36	GLY	4.5
1	D	35	ASP	4.4
1	A	33	ASP	4.3
1	C	109	PHE	4.3
1	D	75	THR	4.2
1	D	110	SER	4.1
1	D	77	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	76	GLY	4.0
1	B	-8	SER	4.0
1	D	112	PRO	3.9
1	D	100	TYR	3.8
1	D	-8	SER	3.8
1	D	76	GLY	3.7
1	C	108	THR	3.7
1	D	74	SER	3.6
1	B	73	VAL	3.6
1	D	108	THR	3.6
1	C	111	GLY	3.5
1	A	36	GLY	3.5
1	A	192[A]	ARG	3.5
1	D	95	ARG	3.5
1	C	107	ASP	3.5
1	C	96	GLY	3.4
1	D	99	VAL	3.4
1	B	36	GLY	3.4
1	A	35	ASP	3.4
1	B	74	SER	3.4
1	C	95	ARG	3.4
1	C	33	ASP	3.3
1	D	104	THR	3.3
1	C	75	THR	3.3
1	C	35	ASP	3.2
1	D	113	ILE	3.1
1	C	2	ASN	3.1
1	C	97	GLY	3.1
1	D	96	GLY	3.1
1	D	69	LEU	3.1
1	A	24	ILE	3.1
1	C	74	SER	3.1
1	D	78	ILE	3.0
1	D	70	THR	2.9
1	C	176	GLN	2.9
1	C	104	THR	2.9
1	D	106	THR	2.9
1	C	78	ILE	2.9
1	C	36	GLY	2.9
1	D	80	PHE	2.8
1	A	34	GLU	2.8
1	C	113	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	185	TYR	2.8
1	B	175	GLY	2.8
1	C	102	LYS	2.7
1	C	93	VAL	2.7
1	C	4	GLN	2.7
1	A	188	GLY	2.6
1	D	178	ASN	2.6
1	D	33	ASP	2.6
1	A	177	TYR	2.6
1	C	105	GLY	2.5
1	D	94	ASN	2.5
1	C	69	LEU	2.5
1	D	79	PRO	2.5
1	D	72	ASP	2.5
1	A	-8	SER	2.5
1	B	33	ASP	2.5
1	C	110	SER	2.4
1	D	161	MET	2.4
1	C	106	THR	2.4
1	D	97	GLY	2.3
1	D	115	VAL	2.3
1	D	114	THR	2.3
1	A	191	GLY	2.2
1	D	102	LYS	2.2
1	A	186	VAL	2.2
1	C	92	TYR	2.2
1	C	79	PRO	2.1
1	C	-7	GLY	2.1
1	D	34	GLU	2.1
1	B	35	ASP	2.1
1	A	187	GLN	2.0
1	C	115	VAL	2.0
1	D	101	ASP	2.0
1	C	103	SER	2.0
1	C	71	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.