



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:58 PM UTC

PDB ID : 1TLQ / pdb_00001tlq
Title : Crystal structure of protein ypjQ from Bacillus subtilis, Pfam DUF64
Authors : Kniewel, R.; Rajashankar, K.R.; Solorzano, V.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-06-09
Resolution : 2.40 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

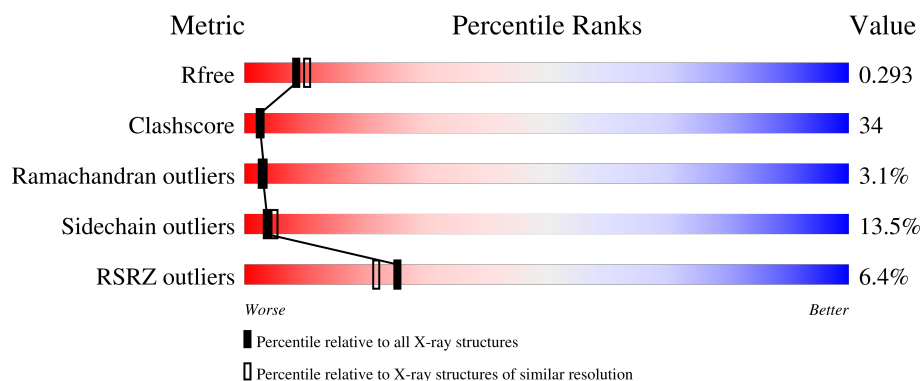
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	189	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1287 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 Hypothetical protein ypjQ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	Se	0	0	0
			1262	803	208	245	1	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP P54173
A	2	SER	-	cloning artifact	UNP P54173
A	3	LEU	-	cloning artifact	UNP P54173
A	8	MSE	MET	modified residue	UNP P54173
A	11	MSE	MET	modified residue	UNP P54173
A	18	MSE	MET	modified residue	UNP P54173
A	25	MSE	MET	modified residue	UNP P54173
A	50	MSE	MET	modified residue	UNP P54173
A	180	GLU	-	expression tag	UNP P54173
A	181	GLY	-	expression tag	UNP P54173
A	182	GLY	-	expression tag	UNP P54173
A	183	SER	-	expression tag	UNP P54173
A	184	HIS	-	expression tag	UNP P54173
A	185	HIS	-	expression tag	UNP P54173
A	186	HIS	-	expression tag	UNP P54173
A	187	HIS	-	expression tag	UNP P54173
A	188	HIS	-	expression tag	UNP P54173
A	189	HIS	-	expression tag	UNP P54173

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

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

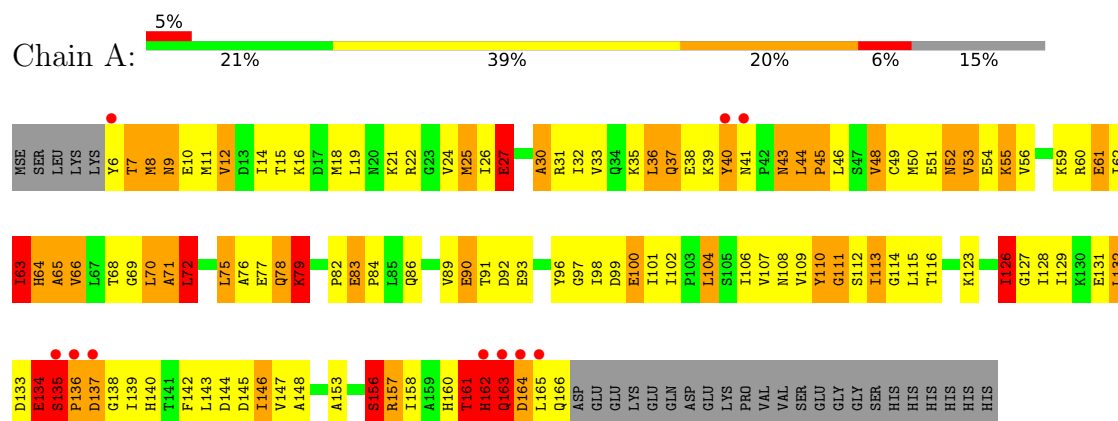
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	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: Hypothetical protein ypjQ



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.11Å 118.11Å 65.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.40) 99.5 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.34 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.295 0.237 , 0.293	Depositor DCC
R_{free} test set	529 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1287	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% 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: 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	2.55	70/1275 (5.5%)	2.03	47/1721 (2.7%)

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	1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	ASN	C-O	14.23	1.40	1.24
1	A	112	SER	CA-C	-11.45	1.38	1.52
1	A	11	MSE	SE-CE	-11.16	1.61	1.95
1	A	48	VAL	CA-C	9.85	1.65	1.52
1	A	148	ALA	C-O	-9.29	1.13	1.24
1	A	60	ARG	CA-C	8.94	1.64	1.52
1	A	77	GLU	C-O	-8.51	1.13	1.24
1	A	101	ILE	CA-CB	8.34	1.66	1.54
1	A	109	VAL	CA-CB	-8.26	1.43	1.54
1	A	30	ALA	CA-C	-8.25	1.41	1.52
1	A	62	ILE	CA-CB	8.22	1.64	1.54
1	A	98	ILE	CA-C	8.17	1.64	1.52
1	A	24	VAL	CA-CB	8.00	1.66	1.54
1	A	162	HIS	C-O	7.54	1.33	1.24
1	A	162	HIS	CA-C	7.30	1.62	1.52
1	A	50	MSE	SE-CE	-7.03	1.74	1.95
1	A	53	VAL	CA-CB	-7.02	1.45	1.54
1	A	64	HIS	CA-C	6.97	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CD-OE1	6.93	1.38	1.25
1	A	52	ASN	CA-C	6.70	1.61	1.52
1	A	25	MSE	CB-CG	6.70	1.72	1.52
1	A	68	THR	CA-CB	-6.59	1.42	1.53
1	A	96	TYR	C-O	-6.54	1.16	1.24
1	A	146	ILE	CA-CB	-6.50	1.46	1.54
1	A	14	ILE	CA-CB	-6.36	1.47	1.54
1	A	100	GLU	C-O	-6.36	1.15	1.24
1	A	71	ALA	CA-C	6.28	1.61	1.52
1	A	54	GLU	CA-C	-6.23	1.44	1.52
1	A	139	ILE	CG1-CD1	-6.16	1.27	1.51
1	A	126	ILE	CA-C	-6.15	1.45	1.52
1	A	45	PRO	C-O	6.14	1.30	1.23
1	A	27	GLU	CA-C	-6.09	1.44	1.52
1	A	102	ILE	N-CA	-6.09	1.39	1.46
1	A	22	ARG	NE-CZ	6.07	1.39	1.33
1	A	50	MSE	C-O	6.06	1.31	1.24
1	A	22	ARG	CZ-NH1	6.06	1.41	1.32
1	A	12	VAL	CA-CB	-6.04	1.47	1.54
1	A	111	GLY	C-O	-6.03	1.15	1.23
1	A	102	ILE	CA-C	5.99	1.59	1.52
1	A	90	GLU	CA-CB	-5.98	1.44	1.53
1	A	91	THR	CA-CB	5.96	1.64	1.53
1	A	96	TYR	CA-C	5.90	1.60	1.52
1	A	99	ASP	N-CA	-5.86	1.38	1.46
1	A	18	MSE	CA-CB	-5.83	1.44	1.53
1	A	59	LYS	N-CA	5.77	1.53	1.46
1	A	65	ALA	CA-C	-5.72	1.45	1.52
1	A	50	MSE	CG-SE	5.72	2.12	1.95
1	A	66	VAL	CA-C	5.71	1.60	1.52
1	A	96	TYR	N-CA	5.68	1.53	1.46
1	A	82	PRO	C-O	5.62	1.30	1.23
1	A	134	GLU	C-O	5.58	1.29	1.23
1	A	147	VAL	N-CA	-5.56	1.39	1.46
1	A	137	ASP	C-O	5.51	1.30	1.24
1	A	46	LEU	N-CA	-5.48	1.39	1.46
1	A	164	ASP	CA-C	5.35	1.60	1.52
1	A	163	GLN	N-CA	5.32	1.52	1.46
1	A	15	THR	CA-C	-5.30	1.46	1.52
1	A	106	ILE	N-CA	-5.29	1.40	1.46
1	A	114	GLY	CA-C	5.26	1.57	1.52
1	A	110	TYR	CE1-CZ	5.25	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLY	C-O	-5.22	1.16	1.23
1	A	6	TYR	N-CA	5.21	1.56	1.46
1	A	60	ARG	CZ-NH1	5.19	1.40	1.32
1	A	79	LYS	CA-CB	-5.19	1.44	1.53
1	A	75	LEU	N-CA	-5.14	1.39	1.46
1	A	56	VAL	CA-CB	5.10	1.60	1.54
1	A	156	SER	CA-CB	5.06	1.61	1.53
1	A	158	ILE	N-CA	-5.04	1.39	1.46
1	A	63	ILE	CA-CB	5.02	1.60	1.54
1	A	102	ILE	C-O	5.01	1.28	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	LEU	N-CA-C	-9.38	101.13	111.36
1	A	44	LEU	CB-CA-C	8.80	120.27	110.15
1	A	25	MSE	CG-SE-CE	-8.73	79.72	98.92
1	A	65	ALA	N-CA-C	-8.45	101.09	111.40
1	A	76	ALA	N-CA-C	-8.41	101.34	111.69
1	A	12	VAL	N-CA-C	8.33	119.11	110.62
1	A	41	ASN	CB-CA-C	-7.67	101.64	111.15
1	A	8	MSE	CG-SE-CE	-7.56	82.29	98.92
1	A	83	GLU	N-CA-C	-7.48	99.02	110.32
1	A	50	MSE	CA-C-O	7.43	128.29	120.42
1	A	68	THR	N-CA-C	-7.24	102.79	111.69
1	A	116	THR	N-CA-CB	-7.17	99.55	110.16
1	A	113	ILE	CA-C-N	-7.15	112.15	119.94
1	A	113	ILE	C-N-CA	-7.15	112.15	119.94
1	A	157	ARG	CG-CD-NE	-7.15	96.28	112.00
1	A	145	ASP	N-CA-C	-7.08	103.62	112.90
1	A	18	MSE	CG-SE-CE	-7.08	83.35	98.92
1	A	112	SER	N-CA-C	6.98	118.97	111.36
1	A	134	GLU	N-CA-C	6.81	118.87	109.54
1	A	40	TYR	CA-C-N	6.42	128.34	122.37
1	A	40	TYR	C-N-CA	6.42	128.34	122.37
1	A	163	GLN	N-CA-C	6.36	121.17	113.41
1	A	51	GLU	N-CA-C	-6.28	104.54	111.82
1	A	90	GLU	CB-CA-C	-6.14	100.60	110.79
1	A	146	ILE	CB-CG1-CD1	-6.04	101.11	113.80
1	A	144	ASP	CB-CA-C	-6.00	101.21	110.81
1	A	60	ARG	NE-CZ-NH2	-5.97	113.82	119.20
1	A	11	MSE	CB-CG-SE	-5.90	94.99	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH2	-5.89	113.89	119.20
1	A	89	VAL	N-CA-C	5.89	116.06	110.53
1	A	43	ASN	CA-C-N	-5.78	112.06	122.28
1	A	43	ASN	C-N-CA	-5.78	112.06	122.28
1	A	19	LEU	N-CA-C	5.62	117.41	111.28
1	A	22	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	A	161	THR	N-CA-C	-5.39	99.31	110.80
1	A	50	MSE	N-CA-C	5.39	117.24	111.36
1	A	25	MSE	CB-CG-SE	-5.39	96.53	112.70
1	A	102	ILE	O-C-N	5.36	123.85	120.42
1	A	41	ASN	N-CA-C	-5.32	101.10	108.76
1	A	55	LYS	N-CA-C	-5.32	105.57	111.36
1	A	108	ASN	O-C-N	5.27	127.50	122.07
1	A	104	LEU	N-CA-C	-5.27	106.36	112.89
1	A	113	ILE	N-CA-C	-5.21	104.53	111.05
1	A	127	GLY	CA-C-O	-5.21	115.81	122.01
1	A	157	ARG	NE-CZ-NH2	-5.17	114.54	119.20
1	A	7	THR	OG1-CB-CG2	-5.07	99.15	109.30
1	A	116	THR	CA-CB-CG2	5.05	119.08	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	GLN	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	1262	0	1289	86	0
2	A	1	0	0	0	0
3	A	24	0	0	8	0
All	All	1287	0	1289	86	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 34.

All (86) 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:7:THR:CG2	1:A:10:GLU:HG3	1.65	1.24
1:A:78:GLN:HG2	3:A:212:HOH:O	1.39	1.22
1:A:7:THR:HG22	1:A:10:GLU:CG	1.75	1.16
1:A:7:THR:HG22	1:A:10:GLU:HG3	1.10	1.08
1:A:113:ILE:HG22	1:A:156:SER:HB2	1.43	0.97
1:A:12:VAL:O	1:A:16:LYS:HG3	1.73	0.86
1:A:162:HIS:HA	1:A:165:LEU:HG	1.60	0.84
1:A:131:GLU:O	1:A:134:GLU:HB3	1.77	0.83
1:A:136:PRO:C	1:A:138:GLY:H	1.87	0.81
1:A:162:HIS:O	1:A:165:LEU:HB2	1.82	0.80
1:A:7:THR:HG23	1:A:10:GLU:H	1.45	0.79
1:A:12:VAL:HG22	1:A:63:ILE:HD11	1.64	0.79
1:A:134:GLU:HG3	3:A:203:HOH:O	1.85	0.76
1:A:79:LYS:HE2	3:A:206:HOH:O	1.86	0.76
1:A:78:GLN:CG	3:A:212:HOH:O	2.10	0.75
1:A:113:ILE:CG2	1:A:156:SER:HB2	2.16	0.75
1:A:79:LYS:N	1:A:79:LYS:HD3	2.03	0.74
1:A:8:MSE:O	1:A:12:VAL:HG23	1.90	0.72
1:A:71:ALA:O	1:A:75:LEU:HG	1.90	0.72
1:A:79:LYS:N	1:A:79:LYS:CD	2.54	0.70
1:A:134:GLU:OE1	1:A:134:GLU:C	2.35	0.69
1:A:136:PRO:C	1:A:138:GLY:N	2.53	0.67
1:A:104:LEU:HA	1:A:107:VAL:HG22	1.77	0.66
1:A:83:GLU:OE2	1:A:83:GLU:HA	1.96	0.65
1:A:70:LEU:HD11	1:A:143:LEU:HD13	1.79	0.64
1:A:157:ARG:HD2	3:A:202:HOH:O	1.98	0.64
1:A:7:THR:CG2	1:A:10:GLU:CG	2.50	0.62
1:A:7:THR:HG22	1:A:10:GLU:CD	2.24	0.61
1:A:40:TYR:HD1	1:A:40:TYR:O	1.84	0.60
1:A:126:ILE:O	1:A:129:ILE:HB	2.04	0.58
1:A:161:THR:HG22	1:A:162:HIS:N	2.20	0.57
1:A:40:TYR:C	1:A:40:TYR:CD1	2.85	0.55
1:A:86:GLN:NE2	1:A:90:GLU:HG3	2.20	0.55
1:A:40:TYR:HD1	1:A:40:TYR:C	2.14	0.55
1:A:135:SER:CB	1:A:136:PRO:CD	2.85	0.55
1:A:134:GLU:OE1	1:A:134:GLU:N	2.40	0.54
1:A:132:LEU:O	1:A:140:HIS:NE2	2.41	0.54
1:A:134:GLU:OE1	1:A:134:GLU:CA	2.55	0.54
1:A:32:ILE:HG23	1:A:126:ILE:HD11	1.91	0.53
1:A:104:LEU:HA	1:A:107:VAL:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:OE2	1:A:84:PRO:HA	2.09	0.53
1:A:161:THR:O	1:A:163:GLN:N	2.42	0.53
1:A:79:LYS:CE	3:A:206:HOH:O	2.53	0.52
1:A:134:GLU:O	1:A:134:GLU:CG	2.54	0.52
1:A:36:LEU:C	1:A:37:GLN:HE21	2.17	0.51
1:A:97:GLY:HA2	1:A:100:GLU:OE1	2.10	0.51
1:A:135:SER:HB3	1:A:136:PRO:HD3	1.92	0.51
1:A:86:GLN:O	1:A:90:GLU:HB2	2.10	0.50
1:A:30:ALA:HB1	1:A:49:CYS:HB2	1.94	0.48
1:A:9:ASN:HD22	1:A:9:ASN:H	1.62	0.48
1:A:12:VAL:HG22	1:A:63:ILE:CD1	2.40	0.48
1:A:134:GLU:OE1	1:A:135:SER:O	2.31	0.47
1:A:52:ASN:OD1	1:A:157:ARG:NH2	2.39	0.47
1:A:79:LYS:CD	1:A:79:LYS:H	2.27	0.47
1:A:128:ILE:O	1:A:132:LEU:HB2	2.15	0.47
1:A:86:GLN:HE21	1:A:90:GLU:HG3	1.79	0.47
1:A:161:THR:O	1:A:164:ASP:N	2.49	0.46
1:A:110:TYR:CD1	1:A:153:ALA:HB1	2.51	0.45
1:A:45:PRO:O	1:A:48:VAL:HB	2.16	0.45
1:A:32:ILE:O	1:A:33:VAL:C	2.57	0.45
1:A:113:ILE:HD12	1:A:160:HIS:CE1	2.52	0.45
1:A:72:LEU:HB3	1:A:142:PHE:CE1	2.53	0.44
1:A:7:THR:O	1:A:10:GLU:HB2	2.17	0.44
1:A:9:ASN:H	1:A:9:ASN:ND2	2.16	0.44
1:A:16:LYS:HE3	1:A:26:ILE:HD11	1.99	0.44
1:A:135:SER:CB	1:A:136:PRO:HD3	2.47	0.44
1:A:25:MSE:C	1:A:27:GLU:N	2.75	0.44
1:A:131:GLU:C	1:A:133:ASP:N	2.74	0.43
1:A:35:LYS:O	1:A:35:LYS:HG3	2.14	0.43
1:A:38:GLU:O	1:A:39:LYS:C	2.61	0.43
1:A:69:GLY:HA3	1:A:146:ILE:HD11	2.01	0.43
1:A:134:GLU:CG	3:A:203:HOH:O	2.55	0.43
1:A:43:ASN:O	1:A:45:PRO:HD3	2.18	0.43
1:A:61:GLU:HG3	3:A:205:HOH:O	2.18	0.43
1:A:66:VAL:CG1	1:A:70:LEU:HD22	2.49	0.43
1:A:66:VAL:HG12	1:A:70:LEU:HD22	2.00	0.42
1:A:111:GLY:O	1:A:115:LEU:HD13	2.20	0.42
1:A:79:LYS:HZ2	1:A:79:LYS:HG2	1.59	0.42
1:A:44:LEU:HA	1:A:45:PRO:HD3	1.64	0.41
1:A:30:ALA:HB1	1:A:49:CYS:CB	2.51	0.41
1:A:92:ASP:O	1:A:93:GLU:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:CG	1:A:39:LYS:N	2.84	0.41
1:A:70:LEU:CD1	1:A:143:LEU:HD13	2.48	0.40
1:A:44:LEU:HD12	1:A:45:PRO:HD2	2.02	0.40
1:A:27:GLU:HB2	1:A:31:ARG:NH2	2.37	0.40
1:A:64:HIS:O	1:A:65:ALA:C	2.63	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	159/189 (84%)	141 (89%)	13 (8%)	5 (3%)	3 3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	53	VAL
1	A	135	SER
1	A	137	ASP
1	A	136	PRO

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	141/161 (88%)	122 (86%)	19 (14%)	4 5

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	21	LYS
1	A	27	GLU
1	A	36	LEU
1	A	37	GLN
1	A	55	LYS
1	A	63	ILE
1	A	70	LEU
1	A	72	LEU
1	A	78	GLN
1	A	79	LYS
1	A	123	LYS
1	A	126	ILE
1	A	132	LEU
1	A	134	GLU
1	A	135	SER
1	A	156	SER
1	A	161	THR
1	A	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	20	ASN
1	A	34	GLN
1	A	37	GLN
1	A	87	HIS
1	A	108	ASN
1	A	117	ASN

5.3.3 RNA ⓘ

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	156/189 (82%)	0.12	10 (6%)	25 22	24, 40, 80, 87	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	TYR	4.0
1	A	165	LEU	3.6
1	A	163	GLN	3.0
1	A	137	ASP	2.8
1	A	135	SER	2.7
1	A	162	HIS	2.6
1	A	6	TYR	2.4
1	A	136	PRO	2.3
1	A	41	ASN	2.2
1	A	164	ASP	2.2

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	CA	A	190	1/1	1.00	0.01	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.