



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:03 PM UTC

PDB ID : 2QCZ / pdb_00002qcz
Title : Structure of N-terminal domain of E. Coli YaeT
Authors : Kim, S.; Malinverni, J.C.; Sliz, P.; Silhavy, T.J.; Harrison, S.C.; Kahne, D.
Deposited on : 2007-06-20
Resolution : 2.70 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

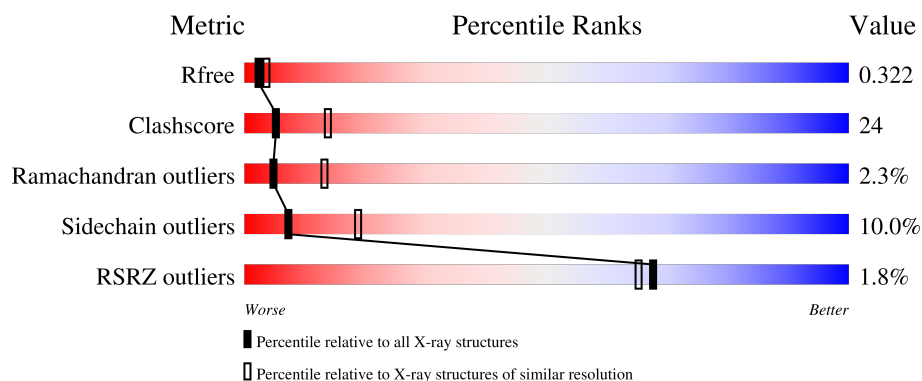
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	335	2% 54% 32% 6% 7%
1	B	335	2% 45% 41% 7% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4834 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 Outer membrane protein assembly factor yaeT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2417	1518	417	478	4			
1	B	310	Total	C	N	O	S	0	0	0
			2417	1518	417	478	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	cloning artifact	UNP P0A940
A	18	SER	-	cloning artifact	UNP P0A940
A	19	HIS	-	cloning artifact	UNP P0A940
A	20	MET	-	cloning artifact	UNP P0A940
B	17	GLY	-	cloning artifact	UNP P0A940
B	18	SER	-	cloning artifact	UNP P0A940
B	19	HIS	-	cloning artifact	UNP P0A940
B	20	MET	-	cloning artifact	UNP P0A940

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.72Å 94.05Å 109.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.70) 99.2 (50.00-2.71)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.329 0.258 , 0.322	Depositor DCC
R_{free} test set	989 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	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	4834	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5950e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.54	0/2449	1.04	10/3306 (0.3%)
1	B	0.47	0/2449	0.97	12/3306 (0.4%)
All	All	0.51	0/4898	1.00	22/6612 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	GLU	N-CA-C	7.48	119.22	111.14
1	B	72	PHE	N-CA-C	7.01	120.94	109.72
1	B	281	SER	N-CA-C	-6.99	103.67	111.28
1	B	130	ILE	N-CA-C	6.67	117.36	110.36
1	B	328	ILE	N-CA-C	6.60	116.96	108.12
1	A	73	GLU	N-CA-C	-6.57	105.41	113.50
1	A	256	VAL	N-CA-C	6.42	117.12	107.75
1	A	299	THR	N-CA-C	-6.33	104.46	111.36
1	B	88	VAL	N-CA-C	5.79	116.70	108.42
1	B	82	ASP	N-CA-C	-5.77	106.58	113.97
1	B	161	ASN	N-CA-C	-5.77	104.87	112.72
1	A	275	GLY	N-CA-C	5.59	118.86	111.70
1	A	54	VAL	N-CA-C	5.52	116.42	108.48
1	A	161	ASN	N-CA-C	-5.44	103.51	111.30
1	B	73	GLU	N-CA-C	-5.32	106.95	113.50
1	A	239	ASN	N-CA-C	5.29	117.00	108.32
1	A	259	ASN	N-CA-C	5.24	116.85	108.41
1	A	42	ALA	N-CA-C	-5.24	105.47	111.07
1	B	184	GLY	N-CA-C	-5.22	107.81	114.85
1	A	113	ASN	N-CA-C	-5.16	105.66	111.28
1	B	182	ILE	N-CA-C	5.06	115.77	108.48
1	B	275	GLY	N-CA-C	5.02	119.39	112.52

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	2417	0	2408	100	0
1	B	2417	0	2408	145	0
All	All	4834	0	4816	236	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 24.

All (236) 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:120:ARG:HG3	1:B:123:GLU:HG3	1.39	1.05
1:A:158:LEU:HB3	1:A:159:PRO:HD2	1.33	1.03
1:B:158:LEU:HB3	1:B:159:PRO:HD2	1.42	1.01
1:B:114:LEU:HB3	1:B:119:VAL:HG13	1.44	0.99
1:B:54:VAL:HG13	1:B:58:ASP:HB2	1.55	0.89
1:A:173:VAL:HG21	1:A:252:LYS:NZ	1.92	0.85
1:B:180:ILE:HG12	1:B:256:VAL:HB	1.62	0.81
1:A:321:ARG:HG3	1:A:342:ASP:HB3	1.63	0.78
1:A:158:LEU:HB3	1:A:159:PRO:CD	2.14	0.76
1:B:159:PRO:HG2	1:B:162:ARG:NH1	2.01	0.76
1:A:55:ASN:HD21	1:A:57:GLU:HB2	1.50	0.75
1:B:138:GLU:HG3	1:B:151:VAL:HG12	1.68	0.75
1:B:232:ASP:HA	1:B:297:ASN:O	1.87	0.75
1:A:298:GLY:H	1:A:301:VAL:HG23	1.50	0.74
1:B:321:ARG:HG3	1:B:342:ASP:HB3	1.69	0.74
1:A:297:ASN:HB3	1:A:300:LYS:HB3	1.68	0.73
1:B:285:GLU:O	1:B:288:THR:HG22	1.87	0.73
1:A:69:THR:HG21	1:A:71:ASN:ND2	2.04	0.73
1:B:156:THR:HB	1:B:164:ASP:OD1	1.88	0.73
1:B:346:ARG:HD3	1:B:348:TYR:OH	1.89	0.73
1:A:198:GLN:HA	1:A:217:GLN:CD	2.14	0.73
1:A:173:VAL:HG21	1:A:252:LYS:HZ2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD22	1:B:251:LYS:HA	1.71	0.71
1:B:120:ARG:CG	1:B:123:GLU:HG3	2.19	0.71
1:B:159:PRO:HG2	1:B:162:ARG:HH12	1.54	0.71
1:A:232:ASP:OD1	1:A:299:THR:HG23	1.91	0.69
1:B:141:TYR:HE1	1:B:171:GLU:HG2	1.58	0.69
1:A:321:ARG:CG	1:A:342:ASP:HB3	2.22	0.68
1:A:232:ASP:HA	1:A:297:ASN:O	1.93	0.68
1:A:244:GLN:HG3	1:A:257:THR:HG23	1.74	0.68
1:B:114:LEU:HD22	1:B:119:VAL:HG11	1.74	0.68
1:A:162:ARG:HG3	1:A:162:ARG:HH11	1.58	0.67
1:B:24:PHE:H	1:B:53:THR:HG22	1.57	0.67
1:B:24:PHE:HB3	1:B:54:VAL:O	1.94	0.66
1:B:244:GLN:HB2	1:B:257:THR:HG23	1.77	0.66
1:B:54:VAL:HG13	1:B:58:ASP:CB	2.24	0.65
1:A:69:THR:CG2	1:A:71:ASN:ND2	2.61	0.64
1:B:177:ILE:HG21	1:B:180:ILE:HG13	1.80	0.63
1:B:197:PHE:HB3	1:B:222:ASP:OD1	1.98	0.63
1:A:173:VAL:HG21	1:A:252:LYS:HZ1	1.62	0.62
1:A:219:LEU:HD22	1:A:223:LEU:HD22	1.80	0.62
1:A:292:PRO:HG2	1:A:293:GLY:H	1.65	0.62
1:B:281:SER:O	1:B:285:GLU:HB2	2.00	0.61
1:B:106:LYS:NZ	1:B:106:LYS:HB3	2.15	0.61
1:A:138:GLU:CG	1:A:151:VAL:HG13	2.30	0.61
1:B:141:TYR:O	1:B:144:VAL:HG12	2.00	0.61
1:B:336:LYS:NZ	1:B:338:ARG:HH21	1.99	0.61
1:B:58:ASP:O	1:B:62:THR:HG22	2.00	0.61
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.67	0.60
1:B:182:ILE:HG12	1:B:258:VAL:HG13	1.83	0.60
1:A:135:LYS:HE3	1:A:139:ASP:OD1	2.02	0.60
1:A:346:ARG:HD3	1:A:348:TYR:OH	2.02	0.60
1:B:277:LEU:HD13	1:B:284:ILE:HD11	1.84	0.60
1:A:230:TYR:CE2	1:A:262:GLU:HG2	2.37	0.60
1:A:240:ILE:HG22	1:B:345:ASN:ND2	2.17	0.60
1:A:291:GLU:CB	1:A:294:GLU:HB2	2.32	0.59
1:A:134:GLU:O	1:A:138:GLU:HG3	2.02	0.59
1:A:25:VAL:HG12	1:A:53:THR:HG22	1.83	0.59
1:A:327:GLU:HG3	1:A:338:ARG:NH1	2.17	0.59
1:B:158:LEU:HB3	1:B:159:PRO:CD	2.24	0.59
1:A:144:VAL:HG13	1:A:144:VAL:O	2.02	0.59
1:A:159:PRO:HG2	1:A:162:ARG:HH12	1.67	0.59
1:B:159:PRO:CG	1:B:162:ARG:HH12	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLU:CD	1:B:292:PRO:HD2	2.28	0.58
1:A:138:GLU:HG2	1:A:151:VAL:HG13	1.84	0.58
1:B:277:LEU:HD12	1:B:281:SER:OG	2.02	0.58
1:B:271:VAL:HG22	1:B:337:LEU:HB2	1.85	0.58
1:B:122:GLY:O	1:B:123:GLU:HG2	2.03	0.58
1:A:322:VAL:HG22	1:A:341:VAL:HG22	1.86	0.58
1:B:248:THR:HB	1:B:253:GLY:O	2.03	0.58
1:A:55:ASN:ND2	1:A:57:GLU:HB2	2.18	0.58
1:B:289:LYS:NZ	1:B:289:LYS:HB3	2.19	0.57
1:B:118:GLY:O	1:B:120:ARG:HG2	2.03	0.57
1:B:59:ILE:O	1:B:62:THR:HG23	2.04	0.57
1:B:134:GLU:O	1:B:138:GLU:HG3	2.04	0.57
1:B:79:ARG:HG3	1:B:80:ASP:N	2.18	0.57
1:B:96:SER:OG	1:B:164:ASP:HB2	2.04	0.57
1:B:260:ILE:HD12	1:B:260:ILE:C	2.30	0.56
1:B:288:THR:HG23	1:B:289:LYS:HD2	1.87	0.56
1:A:76:ARG:HB3	1:A:87:GLN:HB2	1.88	0.56
1:A:102:ASN:ND2	1:A:102:ASN:H	2.03	0.56
1:B:29:ILE:HD11	1:B:31:PHE:CE1	2.40	0.56
1:B:155:VAL:HG13	1:B:163:VAL:HG21	1.87	0.56
1:A:24:PHE:HB3	1:A:54:VAL:O	2.05	0.56
1:B:141:TYR:CE1	1:B:171:GLU:HG2	2.39	0.56
1:B:158:LEU:HB2	1:B:162:ARG:HB2	1.87	0.55
1:B:250:ASP:O	1:B:252:LYS:HG3	2.06	0.55
1:B:327:GLU:HB2	1:B:336:LYS:HB3	1.89	0.55
1:A:247:LEU:HD12	1:B:351:LYS:HB3	1.88	0.55
1:A:325:MET:HE1	1:B:338:ARG:HB3	1.89	0.55
1:B:182:ILE:HG12	1:B:258:VAL:CG1	2.36	0.55
1:B:237:ARG:NH2	1:B:328:ILE:HB	2.21	0.54
1:A:36:ARG:HB3	1:A:90:GLU:OE1	2.08	0.54
1:A:291:GLU:HB2	1:A:294:GLU:HB2	1.90	0.54
1:B:29:ILE:CD1	1:B:46:MET:HE1	2.38	0.54
1:B:336:LYS:HZ3	1:B:338:ARG:HH21	1.55	0.53
1:A:247:LEU:HB2	1:B:351:LYS:HA	1.89	0.53
1:A:120:ARG:HG3	1:A:123:GLU:CG	2.39	0.53
1:B:296:TYR:CE2	1:B:301:VAL:HG21	2.43	0.53
1:B:267:LYS:HA	1:B:295:LEU:HA	1.91	0.53
1:B:98:THR:O	1:B:166:LYS:HA	2.09	0.53
1:B:135:LYS:HE3	1:B:139:ASP:OD1	2.08	0.53
1:A:250:ASP:O	1:A:252:LYS:HG3	2.09	0.52
1:A:138:GLU:HG2	1:A:151:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:HB3	1:A:222:ASP:OD1	2.10	0.52
1:A:345:ASN:ND2	1:B:240:ILE:HG22	2.25	0.52
1:B:27:LYS:HB2	1:B:82:ASP:HB3	1.91	0.51
1:B:144:VAL:HG13	1:B:146:LYS:HG2	1.90	0.51
1:B:162:ARG:HG3	1:B:162:ARG:HH11	1.76	0.51
1:A:110:LEU:HD13	1:A:169:PHE:CZ	2.46	0.51
1:B:29:ILE:HD12	1:B:46:MET:HE1	1.92	0.51
1:B:138:GLU:CG	1:B:151:VAL:HG12	2.38	0.51
1:B:238:PHE:O	1:B:239:ASN:HB2	2.09	0.51
1:B:48:VAL:O	1:B:49:ARG:HG3	2.11	0.51
1:B:27:LYS:O	1:B:28:ASP:HB2	2.11	0.51
1:B:103:LYS:H	1:B:171:GLU:CD	2.17	0.51
1:B:336:LYS:NZ	1:B:338:ARG:NH2	2.59	0.51
1:B:137:LEU:HD13	1:B:169:PHE:HZ	1.75	0.50
1:A:162:ARG:HH11	1:A:162:ARG:CG	2.21	0.50
1:B:29:ILE:HD11	1:B:31:PHE:CZ	2.47	0.50
1:B:221:GLY:O	1:B:225:THR:HG23	2.11	0.50
1:A:120:ARG:HG3	1:A:123:GLU:HG2	1.94	0.49
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.24	0.49
1:A:351:LYS:HB2	1:A:351:LYS:NZ	2.27	0.49
1:B:141:TYR:HB3	1:B:146:LYS:HB2	1.94	0.49
1:A:291:GLU:CD	1:A:292:PRO:HD2	2.37	0.49
1:A:102:ASN:H	1:A:102:ASN:HD22	1.59	0.49
1:B:138:GLU:OE2	1:B:150:SER:HA	2.13	0.49
1:A:112:GLN:HE22	1:B:112:GLN:HE22	1.61	0.49
1:B:32:GLU:HG3	1:B:85:LEU:HD11	1.94	0.49
1:B:237:ARG:CZ	1:B:328:ILE:HG21	2.43	0.48
1:A:37:VAL:HG23	1:A:90:GLU:CD	2.39	0.48
1:B:137:LEU:HD11	1:B:167:LEU:HD13	1.94	0.48
1:B:155:VAL:CG1	1:B:163:VAL:HG21	2.44	0.48
1:A:345:ASN:HD21	1:B:243:THR:HG23	1.78	0.48
1:B:55:ASN:OD1	1:B:57:GLU:HB2	2.14	0.48
1:A:231:LEU:O	1:A:297:ASN:O	2.32	0.48
1:B:277:LEU:O	1:B:279:GLY:N	2.47	0.48
1:A:277:LEU:HD13	1:A:284:ILE:CD1	2.43	0.47
1:B:346:ARG:HB3	1:B:348:TYR:HE1	1.79	0.47
1:B:258:VAL:HG22	1:B:260:ILE:HG23	1.96	0.47
1:B:291:GLU:OE1	1:B:292:PRO:HD2	2.15	0.47
1:A:287:LEU:HD13	1:A:307:ASP:HB3	1.96	0.47
1:A:291:GLU:HA	1:A:291:GLU:OE1	2.15	0.47
1:B:199:LEU:HD13	1:B:199:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HA	1:A:256:VAL:O	2.14	0.47
1:A:327:GLU:HG3	1:A:338:ARG:HH11	1.80	0.47
1:B:244:GLN:HB2	1:B:257:THR:CG2	2.42	0.47
1:A:69:THR:HG21	1:A:71:ASN:HD21	1.74	0.47
1:A:92:PRO:HG2	1:A:127:ARG:NH2	2.29	0.47
1:A:247:LEU:HD23	1:A:254:ILE:HG22	1.97	0.47
1:A:267:LYS:HA	1:A:295:LEU:HD12	1.97	0.47
1:B:92:PRO:HG2	1:B:127:ARG:NH1	2.30	0.47
1:B:189:THR:OG1	1:B:192:GLU:HB2	2.15	0.47
1:B:250:ASP:OD1	1:B:252:LYS:HB2	2.14	0.47
1:A:138:GLU:HG3	1:A:151:VAL:HG13	1.97	0.47
1:B:298:GLY:H	1:B:301:VAL:HG23	1.79	0.47
1:A:180:ILE:HG13	1:A:256:VAL:HB	1.97	0.47
1:B:106:LYS:HB3	1:B:106:LYS:HZ3	1.80	0.47
1:A:237:ARG:NH1	1:A:330:ASP:OD1	2.47	0.46
1:B:267:LYS:O	1:B:334:THR:HA	2.15	0.46
1:A:226:LEU:CD1	1:A:238:PHE:HZ	2.28	0.46
1:B:219:LEU:HD22	1:B:223:LEU:HD22	1.97	0.46
1:B:331:ALA:O	1:B:334:THR:HG23	2.15	0.46
1:A:247:LEU:HD13	1:A:251:LYS:HG2	1.97	0.46
1:B:148:SER:HB2	1:B:172:GLY:HA3	1.97	0.46
1:B:162:ARG:HH11	1:B:162:ARG:CG	2.29	0.46
1:B:323:GLN:HE21	1:B:340:ASN:HD22	1.64	0.46
1:A:189:THR:O	1:A:192:GLU:N	2.47	0.46
1:B:330:ASP:OD1	1:B:330:ASP:N	2.48	0.46
1:A:291:GLU:HB3	1:A:294:GLU:HB2	1.97	0.46
1:B:268:LEU:HD11	1:B:337:LEU:HD12	1.98	0.46
1:A:330:ASP:O	1:A:331:ALA:HB2	2.14	0.45
1:B:92:PRO:HG2	1:B:127:ARG:CZ	2.46	0.45
1:A:277:LEU:HD13	1:A:284:ILE:HD11	1.97	0.45
1:B:313:GLY:HA2	1:B:317:TYR:O	2.17	0.45
1:A:219:LEU:HD22	1:A:223:LEU:CD2	2.45	0.45
1:B:268:LEU:HD11	1:B:337:LEU:CD1	2.46	0.45
1:A:173:VAL:CG2	1:A:252:LYS:HZ1	2.30	0.45
1:B:155:VAL:HG13	1:B:163:VAL:CG2	2.47	0.45
1:A:157:PRO:HA	1:A:163:VAL:HG23	1.97	0.45
1:B:120:ARG:O	1:B:123:GLU:HB2	2.16	0.45
1:B:122:GLY:C	1:B:123:GLU:HG2	2.42	0.45
1:B:170:GLN:O	1:B:171:GLU:C	2.59	0.45
1:A:297:ASN:HB3	1:A:300:LYS:CB	2.42	0.44
1:B:322:VAL:HG22	1:B:341:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ARG:HD3	1:B:348:TYR:HH	1.81	0.44
1:B:238:PHE:CG	1:B:239:ASN:N	2.85	0.44
1:A:281:SER:HB3	1:A:285:GLU:OE2	2.17	0.44
1:A:284:ILE:O	1:A:288:THR:HG23	2.18	0.44
1:A:349:VAL:HG21	1:B:142:TYR:OH	2.17	0.44
1:A:177:ILE:HD13	1:A:180:ILE:HD12	1.99	0.44
1:A:55:ASN:O	1:A:58:ASP:N	2.48	0.44
1:A:112:GLN:HE22	1:B:112:GLN:NE2	2.15	0.44
1:B:42:ALA:O	1:B:46:MET:HG3	2.18	0.44
1:B:54:VAL:HA	1:B:58:ASP:OD1	2.17	0.44
1:A:160:ARG:HB3	1:A:161:ASN:H	1.53	0.44
1:A:244:GLN:H	1:A:244:GLN:HG2	1.56	0.44
1:A:92:PRO:HG2	1:A:127:ARG:CZ	2.48	0.44
1:A:92:PRO:HA	1:A:161:ASN:O	2.17	0.43
1:A:162:ARG:CG	1:A:162:ARG:NH1	2.81	0.43
1:B:336:LYS:HZ3	1:B:338:ARG:NH2	2.17	0.43
1:B:137:LEU:HD13	1:B:169:PHE:CZ	2.52	0.43
1:B:106:LYS:HB2	1:B:109:MET:HG2	2.01	0.43
1:B:160:ARG:HB3	1:B:161:ASN:H	1.59	0.43
1:A:305:GLU:HG2	1:A:322:VAL:HG12	2.00	0.43
1:B:24:PHE:CZ	1:B:79:ARG:HD3	2.54	0.43
1:B:104:SER:N	1:B:171:GLU:OE1	2.52	0.43
1:B:28:ASP:CG	1:B:29:ILE:N	2.77	0.42
1:B:248:THR:HG22	1:B:251:LYS:N	2.34	0.42
1:B:329:ASN:HD21	1:B:331:ALA:HB3	1.83	0.42
1:B:288:THR:CG2	1:B:289:LYS:HD2	2.49	0.42
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.93	0.42
1:A:285:GLU:HA	1:A:288:THR:HG23	2.01	0.42
1:B:93:THR:O	1:B:163:VAL:N	2.48	0.42
1:B:247:LEU:HA	1:B:254:ILE:HG22	2.01	0.42
1:A:273:VAL:HG21	1:A:284:ILE:HD12	2.00	0.42
1:A:313:GLY:C	1:A:315:TYR:H	2.28	0.42
1:B:350:ARG:HG3	1:B:350:ARG:HH11	1.85	0.41
1:B:298:GLY:N	1:B:301:VAL:HG23	2.34	0.41
1:A:181:ASN:O	1:A:257:THR:HA	2.20	0.41
1:B:157:PRO:O	1:B:158:LEU:HD23	2.21	0.41
1:B:289:LYS:HB3	1:B:289:LYS:HZ3	1.86	0.41
1:A:228:SER:O	1:A:229:TYR:C	2.62	0.41
1:B:103:LYS:C	1:B:105:VAL:H	2.27	0.41
1:B:237:ARG:CZ	1:B:328:ILE:CG2	2.99	0.41
1:B:280:HIS:O	1:B:284:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:SER:O	1:B:282:ALA:C	2.64	0.41
1:B:84:LEU:HD12	1:B:84:LEU:HA	1.90	0.41
1:B:113:ASN:ND2	1:B:140:PHE:CD2	2.89	0.41
1:B:295:LEU:O	1:B:296:TYR:C	2.63	0.41
1:B:24:PHE:H	1:B:53:THR:CG2	2.30	0.40
1:A:267:LYS:HB2	1:A:334:THR:HG22	2.03	0.40
1:A:24:PHE:HE2	1:A:82:ASP:HA	1.86	0.40
1:B:114:LEU:HB3	1:B:119:VAL:CG1	2.31	0.40
1:B:247:LEU:HD13	1:B:251:LYS:HG2	2.02	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	302/335 (90%)	278 (92%)	17 (6%)	7 (2%)	5	13
1	B	302/335 (90%)	270 (89%)	25 (8%)	7 (2%)	5	13
All	All	604/670 (90%)	548 (91%)	42 (7%)	14 (2%)	5	13

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ARG
1	B	24	PHE
1	B	35	GLN
1	B	292	PRO
1	A	344	GLY
1	B	160	ARG
1	B	344	GLY
1	A	292	PRO
1	B	159	PRO

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Mol	Chain	Res	Type
1	B	278	ALA
1	A	24	PHE
1	A	159	PRO
1	A	35	GLN
1	A	158	LEU

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	264/288 (92%)	232 (88%)	32 (12%)	5	12
1	B	264/288 (92%)	243 (92%)	21 (8%)	11	28
All	All	528/576 (92%)	475 (90%)	53 (10%)	7	19

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	PHE
1	A	36	ARG
1	A	39	VAL
1	A	44	LEU
1	A	67	PHE
1	A	79	ARG
1	A	85	LEU
1	A	88	VAL
1	A	115	GLU
1	A	119	VAL
1	A	125	LEU
1	A	139	ASP
1	A	144	VAL
1	A	151	VAL
1	A	163	VAL
1	A	164	ASP
1	A	176	GLU
1	A	199	LEU

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Mol	Chain	Res	Type
1	A	219	LEU
1	A	223	LEU
1	A	225	THR
1	A	233	ARG
1	A	244	GLN
1	A	248	THR
1	A	257	THR
1	A	258	VAL
1	A	267	LYS
1	A	276	ASN
1	A	286	GLN
1	A	295	LEU
1	A	304	MET
1	A	351	LYS
1	B	29	ILE
1	B	53	THR
1	B	60	SER
1	B	62	THR
1	B	79	ARG
1	B	119	VAL
1	B	125	LEU
1	B	162	ARG
1	B	190	THR
1	B	199	LEU
1	B	217	GLN
1	B	219	LEU
1	B	223	LEU
1	B	225	THR
1	B	226	LEU
1	B	248	THR
1	B	258	VAL
1	B	272	GLU
1	B	286	GLN
1	B	289	LYS
1	B	311	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	71	ASN
1	A	87	GLN

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	112	GLN
1	A	113	ASN
1	A	179	GLN
1	A	217	GLN
1	A	239	ASN
1	A	276	ASN
1	A	323	GLN
1	B	30	HIS
1	B	61	ASN
1	B	102	ASN
1	B	113	ASN
1	B	170	GLN
1	B	179	GLN
1	B	217	GLN
1	B	239	ASN
1	B	244	GLN
1	B	259	ASN
1	B	276	ASN
1	B	286	GLN
1	B	329	ASN
1	B	340	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 [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	310/335 (92%)	0.03	3 (0%) 79 78	33, 53, 79, 100	0
1	B	310/335 (92%)	0.37	8 (2%) 57 54	41, 70, 95, 108	0
All	All	620/670 (92%)	0.20	11 (1%) 67 65	33, 62, 89, 108	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	ALA	5.0
1	B	331	ALA	4.8
1	B	199	LEU	3.4
1	B	319	TYR	2.8
1	B	291	GLU	2.6
1	A	319	TYR	2.3
1	A	199	LEU	2.3
1	B	278	ALA	2.2
1	B	190	THR	2.1
1	B	226	LEU	2.1
1	B	230	TYR	2.1

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.