



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 AM UTC

PDB ID : 3VGZ / pdb_00003vgz
Title : Crystal structure of E. coli YncE
Authors : Kagawa, W.; Sagawa, T.; Niki, H.; Kurumizaka, H.
Deposited on : 2011-08-23
Resolution : 1.70 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
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

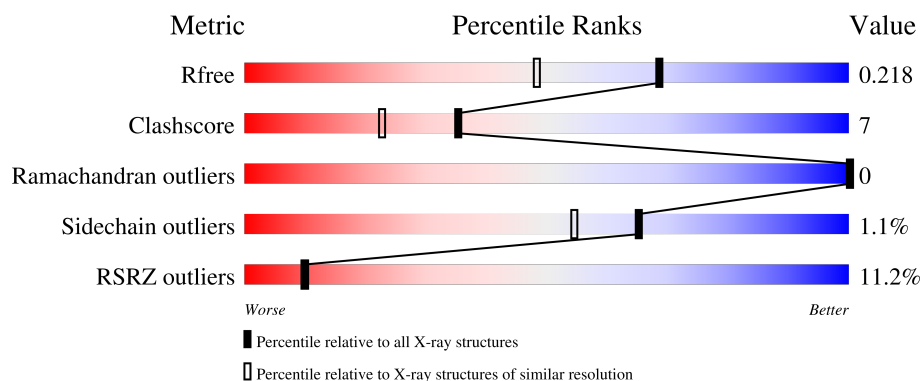
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	353	12% 73% 15% • 9%
1	B	353	8% 76% 13% • 9%
1	C	353	7% 79% 11% • 8%
1	D	353	14% 74% 15% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10221 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 Uncharacterized protein YncE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	Se	0	0	0
			2473	1547	437	486	3			
1	B	321	Total	C	N	O	Se	0	0	0
			2473	1547	437	486	3			
1	C	323	Total	C	N	O	Se	0	0	0
			2487	1555	439	490	3			
1	D	321	Total	C	N	O	Se	0	0	0
			2473	1547	437	486	3			

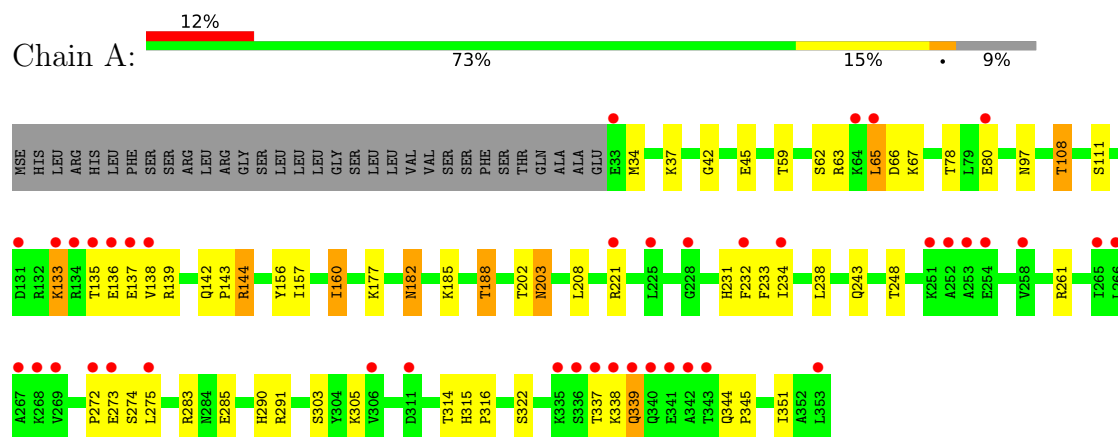
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		
2	B	91	Total	O	0	0
			91	91		
2	C	90	Total	O	0	0
			90	90		
2	D	60	Total	O	0	0
			60	60		

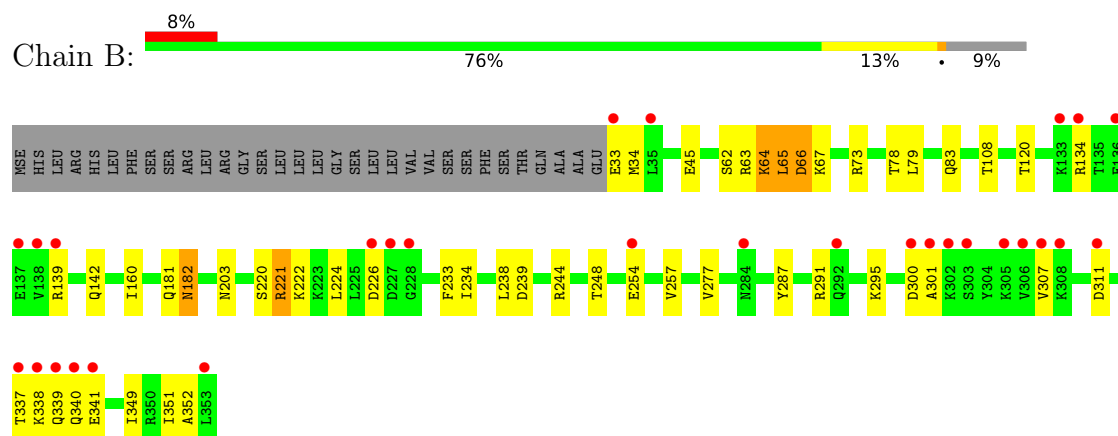
3 Residue-property plots [i](#)

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.

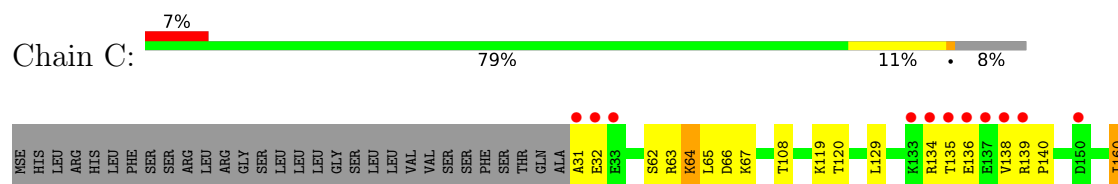
• Molecule 1: Uncharacterized protein YncE

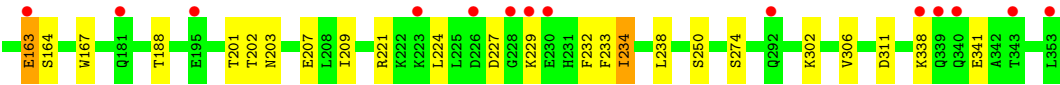


• Molecule 1: Uncharacterized protein YncE

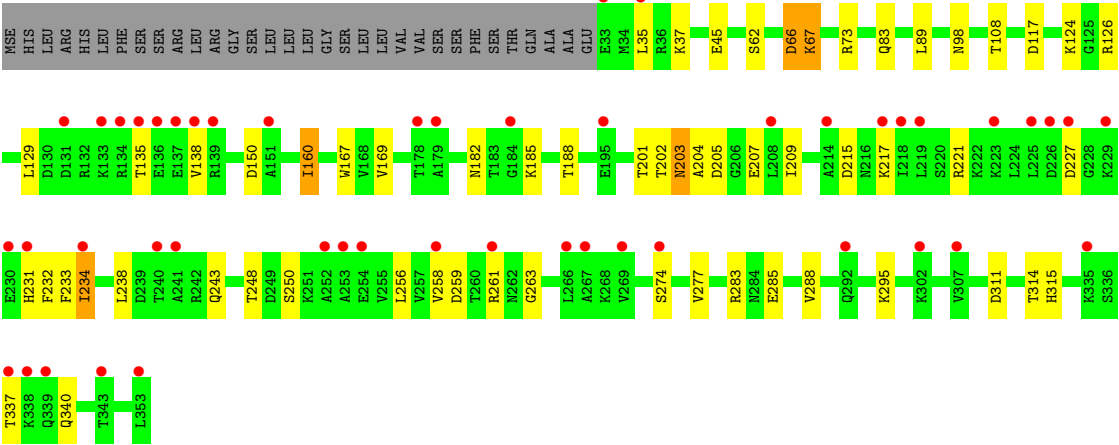


• Molecule 1: Uncharacterized protein YncE





● Molecule 1: Uncharacterized protein YncE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.17Å 139.31Å 173.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.70) 95.7 (50.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.70Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.220 , 0.244 0.221 , 0.218	Depositor DCC
R_{free} test set	7574 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.6	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	0.94	EDS
Total number of atoms	10221	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	0.35	0/2503	0.92	13/3385 (0.4%)
1	B	0.36	0/2503	0.93	13/3385 (0.4%)
1	C	0.35	0/2517	0.93	12/3404 (0.4%)
1	D	0.33	0/2503	0.88	9/3385 (0.3%)
All	All	0.35	0/10026	0.92	47/13559 (0.3%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ASN	N-CA-C	7.78	118.53	108.34
1	A	339	GLN	N-CA-C	-7.30	106.30	114.62
1	C	234	ILE	N-CA-C	7.11	117.21	110.53
1	B	160	ILE	N-CA-C	6.88	119.63	108.97
1	D	234	ILE	N-CA-C	6.85	117.64	110.72
1	C	136	GLU	N-CA-C	-6.58	104.98	114.12
1	B	67	LYS	N-CA-C	-6.42	98.73	109.07
1	C	203	ASN	N-CA-C	6.33	117.78	108.86
1	B	181	GLN	N-CA-C	6.32	119.08	110.55
1	A	160	ILE	N-CA-C	6.24	118.64	108.97
1	B	234	ILE	N-CA-C	6.12	118.74	111.09
1	A	234	ILE	N-CA-C	6.02	116.66	110.82
1	B	238	LEU	N-CA-C	5.92	119.70	110.17
1	D	238	LEU	N-CA-C	5.91	119.68	110.17
1	D	182	ASN	N-CA-C	5.89	119.52	111.39
1	D	66	ASP	N-CA-C	5.87	119.39	109.76
1	A	45	GLU	N-CA-C	5.78	118.36	110.55
1	C	108	THR	N-CA-C	5.77	118.03	111.11
1	A	97	ASN	N-CA-C	-5.71	99.22	108.41
1	B	224	LEU	N-CA-C	5.65	117.44	111.28
1	B	45	GLU	N-CA-C	5.62	118.14	110.55
1	C	160	ILE	N-CA-C	5.59	117.95	109.12
1	C	67	LYS	N-CA-C	-5.54	100.16	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LYS	N-CA-C	-5.53	105.33	112.68
1	D	160	ILE	N-CA-C	5.49	117.48	108.97
1	A	182	ASN	N-CA-C	5.49	119.20	111.52
1	A	238	LEU	N-CA-C	5.40	118.87	110.17
1	D	45	GLU	N-CA-C	5.37	117.46	110.53
1	A	188	THR	N-CA-C	5.36	116.92	111.14
1	C	164	SER	N-CA-C	5.36	117.44	110.53
1	A	322	SER	N-CA-C	-5.34	103.47	110.53
1	D	108	THR	N-CA-C	5.33	117.50	111.11
1	C	238	LEU	N-CA-C	5.32	118.73	110.17
1	B	182	ASN	N-CA-C	5.29	118.62	111.17
1	A	208	LEU	N-CA-C	-5.28	99.91	108.52
1	C	306	VAL	N-CA-C	-5.24	100.78	108.54
1	A	108	THR	N-CA-C	5.23	117.72	111.71
1	B	257	VAL	N-CA-C	-5.22	100.81	108.11
1	D	67	LYS	N-CA-C	-5.22	100.67	109.07
1	C	274	SER	N-CA-C	5.17	117.73	109.81
1	C	302	LYS	N-CA-C	-5.16	106.67	113.12
1	C	224	LEU	N-CA-C	5.13	116.88	111.28
1	B	291	ARG	N-CA-C	5.09	117.23	111.02
1	B	239	ASP	N-CA-C	-5.07	98.08	107.71
1	B	66	ASP	N-CA-C	5.06	117.74	109.59
1	D	169	VAL	N-CA-C	5.05	115.86	108.53
1	A	203	ASN	N-CA-C	5.01	116.29	109.18

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	2473	0	2524	48	0
1	B	2473	0	2524	36	0
1	C	2487	0	2535	32	0
1	D	2473	0	2524	37	0
2	A	74	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	91	0	0	2	0
2	C	90	0	0	1	0
2	D	60	0	0	0	0
All	All	10221	0	10107	148	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 7.

All (148) 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:D:234:ILE:HD11	1:D:250:SER:HB3	1.06	1.03
1:D:117:ASP:HB2	1:D:124:LYS:HE3	1.41	0.99
1:D:234:ILE:CD1	1:D:250:SER:HB3	2.01	0.88
1:B:64:LYS:HD2	1:B:65:LEU:HD22	1.59	0.84
1:A:111:SER:H	1:A:142:GLN:HE22	1.24	0.82
1:A:135:THR:HB	1:A:138:VAL:HG12	1.63	0.80
1:B:337:THR:HG22	1:B:339:GLN:H	1.49	0.76
1:D:117:ASP:CB	1:D:124:LYS:HE3	2.16	0.76
1:D:234:ILE:HD11	1:D:250:SER:CB	2.02	0.75
1:A:303:SER:HB2	1:A:305:LYS:HE2	1.69	0.74
1:C:63:ARG:HH12	1:C:338:LYS:HE2	1.53	0.74
1:D:215:ASP:OD1	1:D:217:LYS:HG2	1.88	0.72
1:B:340:GLN:HE21	1:B:340:GLN:HA	1.55	0.71
1:A:135:THR:HG22	1:A:137:GLU:H	1.56	0.70
1:B:34:MSE:HE2	1:B:349:ILE:HG21	1.72	0.70
1:B:64:LYS:HD2	1:B:65:LEU:CD2	2.23	0.69
1:A:133:LYS:HD3	1:A:138:VAL:HG11	1.76	0.68
1:A:111:SER:N	1:A:142:GLN:HE22	1.91	0.68
1:C:64:LYS:HD2	1:C:341:GLU:OE2	1.95	0.66
1:D:201:THR:HG22	1:D:209:ILE:HB	1.78	0.66
1:D:203:ASN:HD22	1:D:203:ASN:C	2.04	0.66
1:A:65:LEU:HG	1:A:66:ASP:OD1	1.96	0.66
1:B:64:LYS:CD	1:B:65:LEU:HD22	2.25	0.66
1:A:135:THR:HB	1:A:138:VAL:CG1	2.26	0.65
1:A:314:THR:HG22	1:A:315:HIS:CD2	2.31	0.64
1:B:139:ARG:NH2	1:B:142:GLN:HE21	1.94	0.64
1:C:64:LYS:HD2	1:C:341:GLU:CD	2.24	0.63
1:B:244:ARG:HH22	1:B:301:ALA:HB1	1.64	0.62
1:B:222:LYS:HB2	1:C:31:ALA:N	2.14	0.62
1:D:337:THR:OG1	1:D:340:GLN:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:THR:OG1	1:A:339:GLN:HG2	2.00	0.61
1:D:62:SER:HB3	1:D:66:ASP:OD1	2.02	0.60
1:D:243:GLN:OE1	1:D:261:ARG:HD3	2.02	0.59
1:D:160:ILE:HG21	1:D:188:THR:HG22	1.84	0.59
1:B:254:GLU:HG2	2:B:372:HOH:O	2.02	0.59
2:B:377:HOH:O	1:C:32:GLU:HB2	2.01	0.58
1:B:139:ARG:HH22	1:B:142:GLN:HE21	1.49	0.58
1:A:272:PRO:HG2	1:A:290:HIS:CE1	2.38	0.58
1:C:232:PHE:CE1	1:C:234:ILE:HD13	2.38	0.58
1:D:129:LEU:HD13	1:D:167:TRP:CE3	2.38	0.57
1:A:37:LYS:NZ	1:A:80:GLU:HG2	2.19	0.57
1:C:129:LEU:HD13	1:C:167:TRP:CE3	2.40	0.57
1:B:220:SER:HB2	1:C:31:ALA:HA	1.85	0.56
1:C:232:PHE:CD1	1:C:234:ILE:HD13	2.39	0.56
1:C:63:ARG:NH1	1:C:338:LYS:HE2	2.20	0.56
1:A:135:THR:HG22	1:A:136:GLU:N	2.20	0.56
1:A:62:SER:OG	1:A:65:LEU:HD23	2.07	0.56
1:B:34:MSE:HG2	1:B:351:ILE:HG12	1.88	0.55
1:B:340:GLN:HA	1:B:340:GLN:NE2	2.20	0.55
1:D:295:LYS:HD3	1:D:311:ASP:HA	1.88	0.55
1:C:135:THR:OG1	1:C:138:VAL:HG12	2.06	0.55
1:A:274:SER:C	1:A:275:LEU:HD12	2.32	0.55
1:D:314:THR:HG22	1:D:315:HIS:CD2	2.42	0.55
1:A:135:THR:CG2	1:A:136:GLU:N	2.69	0.55
1:D:135:THR:OG1	1:D:138:VAL:HG12	2.07	0.54
1:A:78:THR:OG1	1:A:80:GLU:HG3	2.08	0.54
1:A:108:THR:O	1:A:142:GLN:NE2	2.41	0.54
1:D:201:THR:CG2	1:D:209:ILE:HB	2.37	0.54
1:A:142:GLN:HE21	1:A:143:PRO:HD2	1.73	0.54
1:C:134:ARG:HG2	1:C:140:PRO:HD2	1.89	0.53
1:A:182:ASN:O	1:A:221:ARG:NH2	2.41	0.53
1:D:283:ARG:O	1:D:285:GLU:HG3	2.09	0.52
1:D:202:THR:HB	1:D:233:PHE:HB2	1.91	0.52
1:C:234:ILE:HG13	1:C:250:SER:HB3	1.91	0.52
1:A:275:LEU:HD12	1:A:275:LEU:N	2.25	0.51
1:C:207:GLU:OE2	1:C:221:ARG:HD3	2.09	0.51
1:A:337:THR:C	1:A:339:GLN:H	2.18	0.51
1:A:34:MSE:HG2	1:A:351:ILE:HG12	1.92	0.50
1:C:120:THR:O	1:D:67:LYS:HE3	2.11	0.50
1:D:227:ASP:OD1	1:D:231:HIS:HE1	1.94	0.50
1:D:185:LYS:HD2	1:D:204:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.77	0.50
1:D:35:LEU:HD21	1:D:37:LYS:HG2	1.94	0.50
1:A:344:GLN:HG3	1:A:345:PRO:HD2	1.94	0.49
1:B:337:THR:HB	1:B:340:GLN:HB3	1.93	0.49
1:C:163:GLU:H	1:C:163:GLU:CD	2.19	0.49
1:D:203:ASN:ND2	1:D:207:GLU:H	2.11	0.49
1:B:182:ASN:O	1:B:221:ARG:NH2	2.46	0.49
1:A:231:HIS:C	1:A:232:PHE:HD1	2.20	0.49
1:B:33:GLU:HG2	1:B:352:ALA:HB3	1.94	0.49
1:B:62:SER:HB3	1:B:66:ASP:OD2	2.13	0.49
1:C:62:SER:HB3	1:C:66:ASP:OD1	2.12	0.48
1:A:160:ILE:HG21	1:A:188:THR:HG22	1.96	0.47
1:C:160:ILE:HG21	1:C:188:THR:HG22	1.96	0.47
1:A:133:LYS:CD	1:A:138:VAL:HG11	2.42	0.47
1:C:119:LYS:HD2	2:C:425:HOH:O	2.14	0.47
1:D:98:ASN:HB2	1:D:150:ASP:OD2	2.15	0.47
1:C:63:ARG:HH12	1:C:338:LYS:CE	2.24	0.47
1:C:163:GLU:N	1:C:163:GLU:OE1	2.48	0.47
1:A:202:THR:HB	1:A:233:PHE:HB2	1.97	0.46
1:D:89:LEU:HD12	1:D:126:ARG:HD3	1.97	0.46
1:A:243:GLN:OE1	1:A:261:ARG:HD3	2.15	0.46
1:C:139:ARG:HG3	1:C:139:ARG:HH11	1.79	0.46
1:D:209:ILE:HD12	1:D:221:ARG:HB3	1.98	0.46
1:D:203:ASN:HD21	1:D:207:GLU:H	1.63	0.46
1:A:133:LYS:HD2	1:A:133:LYS:N	2.31	0.45
1:A:133:LYS:O	1:A:138:VAL:HG13	2.16	0.45
1:C:134:ARG:HG2	1:C:140:PRO:CD	2.45	0.45
1:C:201:THR:CG2	1:C:209:ILE:HB	2.45	0.45
1:C:201:THR:HG22	1:C:209:ILE:HB	1.98	0.45
1:B:182:ASN:HD22	1:C:311:ASP:HB2	1.81	0.45
1:D:232:PHE:C	1:D:232:PHE:CD1	2.94	0.45
1:B:63:ARG:HH12	1:B:338:LYS:HE2	1.80	0.45
1:B:295:LYS:HD3	1:B:311:ASP:HA	1.98	0.45
1:B:108:THR:O	1:B:142:GLN:CD	2.60	0.45
1:B:78:THR:O	1:B:79:LEU:HB2	2.16	0.45
1:A:67:LYS:HE3	1:B:120:THR:O	2.18	0.44
1:B:34:MSE:HE3	1:B:351:ILE:HD11	1.98	0.44
1:B:233:PHE:HA	1:B:248:THR:O	2.17	0.44
1:D:274:SER:HB3	1:D:288:VAL:CG1	2.47	0.44
1:D:232:PHE:C	1:D:232:PHE:HD1	2.25	0.44
1:C:62:SER:OG	1:C:64:LYS:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.83	0.43
1:A:233:PHE:HA	1:A:248:THR:O	2.19	0.43
1:B:226:ASP:OD1	1:B:226:ASP:O	2.36	0.43
1:C:163:GLU:CG	1:C:163:GLU:O	2.65	0.43
1:D:248:THR:HG23	1:D:277:VAL:HB	2.00	0.43
1:A:185:LYS:O	1:A:203:ASN:HB2	2.19	0.43
1:A:142:GLN:HE21	1:A:142:GLN:HA	1.83	0.43
1:C:227:ASP:OD1	1:C:229:LYS:HB2	2.19	0.43
1:B:73:ARG:HB3	1:B:83:GLN:HB3	2.01	0.42
1:C:163:GLU:CD	1:C:163:GLU:N	2.78	0.42
1:B:64:LYS:HE3	1:B:64:LYS:HB3	1.79	0.42
1:B:134:ARG:CZ	1:B:139:ARG:HH11	2.32	0.42
1:A:156:TYR:C	1:A:157:ILE:HG13	2.44	0.42
1:A:63:ARG:HH12	1:A:338:LYS:HD3	1.85	0.42
1:A:272:PRO:O	1:A:273:GLU:C	2.62	0.42
1:A:63:ARG:NH1	1:A:338:LYS:HD3	2.34	0.42
1:D:258:VAL:CG1	1:D:263:GLY:HA2	2.50	0.42
1:B:300:ASP:HB2	1:B:307:VAL:HG11	2.01	0.41
1:A:42:GLY:O	1:A:59:THR:HA	2.20	0.41
1:A:315:HIS:HA	1:A:316:PRO:HD2	1.97	0.41
1:B:300:ASP:HB2	1:B:307:VAL:CG1	2.50	0.41
1:A:37:LYS:HZ1	1:A:80:GLU:HG2	1.84	0.41
1:D:73:ARG:HB3	1:D:83:GLN:HB3	2.01	0.41
1:B:340:GLN:NE2	1:B:340:GLN:CA	2.81	0.41
1:A:142:GLN:NE2	1:A:142:GLN:HA	2.36	0.41
1:C:202:THR:HB	1:C:233:PHE:HB2	2.02	0.41
1:A:283:ARG:O	1:A:285:GLU:HG3	2.21	0.41
1:B:34:MSE:CE	1:B:349:ILE:HG21	2.46	0.41
1:B:340:GLN:O	1:B:340:GLN:HG3	2.21	0.41
1:D:203:ASN:C	1:D:203:ASN:ND2	2.74	0.41
1:A:133:LYS:CD	1:A:133:LYS:H	2.34	0.40
1:A:275:LEU:HD22	1:A:291:ARG:HB2	2.03	0.40
1:D:258:VAL:HG12	1:D:259:ASP:N	2.36	0.40
1:C:227:ASP:C	1:C:229:LYS:H	2.30	0.40
1:D:203:ASN:ND2	1:D:205:ASP:H	2.18	0.40
1:B:277:VAL:HA	1:B:287:TYR:O	2.21	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	319/353 (90%)	301 (94%)	18 (6%)	0	100	100
1	B	319/353 (90%)	304 (95%)	15 (5%)	0	100	100
1	C	321/353 (91%)	306 (95%)	15 (5%)	0	100	100
1	D	319/353 (90%)	303 (95%)	16 (5%)	0	100	100
All	All	1278/1412 (90%)	1214 (95%)	64 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	269/293 (92%)	266 (99%)	3 (1%)	65	54
1	B	269/293 (92%)	265 (98%)	4 (2%)	57	43
1	C	270/293 (92%)	267 (99%)	3 (1%)	65	54
1	D	269/293 (92%)	267 (99%)	2 (1%)	76	69
All	All	1077/1172 (92%)	1065 (99%)	12 (1%)	65	54

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	133	LYS

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Mol	Chain	Res	Type
1	A	144	ARG
1	B	64	LYS
1	B	65	LEU
1	B	221	ARG
1	B	341	GLU
1	C	64	LYS
1	C	65	LEU
1	C	163	GLU
1	D	203	ASN
1	D	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	264	ASN
1	A	315	HIS
1	A	317	ASN
1	A	339	GLN
1	A	344	GLN
1	B	61	GLN
1	B	101	GLN
1	B	182	ASN
1	B	216	ASN
1	B	235	ASN
1	B	340	GLN
1	C	51	GLN
1	C	107	ASN
1	C	216	ASN
1	C	235	ASN
1	C	315	HIS
1	C	317	ASN
1	C	340	GLN
1	C	344	GLN
1	D	50	GLN
1	D	142	GLN
1	D	203	ASN
1	D	231	HIS
1	D	235	ASN
1	D	264	ASN
1	D	315	HIS
1	D	317	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	318/353 (90%)	0.70	41 (12%) 7 7	12, 24, 48, 63	0
1	B	318/353 (90%)	0.57	29 (9%) 15 15	13, 23, 42, 57	0
1	C	320/353 (90%)	0.48	25 (7%) 19 20	13, 22, 42, 60	0
1	D	318/353 (90%)	0.93	48 (15%) 5 5	13, 28, 46, 62	0
All	All	1274/1412 (90%)	0.67	143 (11%) 10 10	12, 24, 45, 63	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	ALA	6.7
1	A	137	GLU	6.1
1	A	136	GLU	5.7
1	A	134	ARG	5.5
1	C	138	VAL	4.9
1	B	307	VAL	4.6
1	A	138	VAL	4.5
1	A	340	GLN	4.5
1	A	135	THR	4.4
1	A	337	THR	4.4
1	C	137	GLU	4.3
1	D	338	LYS	4.2
1	A	133	LYS	4.2
1	D	138	VAL	4.1
1	B	292	GLN	3.9
1	D	343	THR	3.9
1	A	232	PHE	3.9
1	C	195	GLU	3.8
1	B	302	LYS	3.8
1	D	137	GLU	3.8
1	B	339	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	303	SER	3.8
1	A	254	GLU	3.6
1	D	339	GLN	3.6
1	C	135	THR	3.6
1	B	353	LEU	3.5
1	A	272	PRO	3.4
1	B	133	LYS	3.4
1	C	133	LYS	3.4
1	C	226	ASP	3.4
1	D	226	ASP	3.4
1	C	343	THR	3.4
1	C	136	GLU	3.4
1	B	338	LYS	3.4
1	A	33	GLU	3.4
1	D	223	LYS	3.3
1	B	137	GLU	3.3
1	B	226	ASP	3.3
1	B	337	THR	3.3
1	B	305	LYS	3.3
1	D	230	GLU	3.3
1	A	336	SER	3.3
1	D	217	LYS	3.3
1	C	230	GLU	3.2
1	A	228	GLY	3.2
1	B	340	GLN	3.1
1	A	266	LEU	3.1
1	A	275	LEU	3.1
1	D	35	LEU	3.1
1	A	273	GLU	3.1
1	C	32	GLU	3.1
1	B	306	VAL	3.1
1	A	338	LYS	3.1
1	B	301	ALA	3.1
1	A	339	GLN	3.1
1	D	219	LEU	3.0
1	D	353	LEU	3.0
1	A	342	ALA	3.0
1	D	337	THR	2.9
1	A	225	LEU	2.9
1	B	136	GLU	2.9
1	D	133	LYS	2.9
1	D	139	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	2.8
1	D	253	ALA	2.7
1	B	254	GLU	2.7
1	B	284	ASN	2.7
1	D	218	ILE	2.7
1	A	341	GLU	2.7
1	B	308	LYS	2.7
1	C	134	ARG	2.7
1	D	134	ARG	2.7
1	D	225	LEU	2.7
1	A	268	LYS	2.6
1	A	269	VAL	2.6
1	C	228	GLY	2.6
1	A	65	LEU	2.6
1	C	163	GLU	2.6
1	D	231	HIS	2.6
1	C	353	LEU	2.6
1	D	229	LYS	2.6
1	D	234	ILE	2.6
1	B	33	GLU	2.6
1	B	228	GLY	2.5
1	C	139	ARG	2.5
1	D	136	GLU	2.5
1	D	254	GLU	2.5
1	C	339	GLN	2.5
1	A	343	THR	2.5
1	D	135	THR	2.5
1	A	353	LEU	2.4
1	D	266	LEU	2.4
1	B	139	ARG	2.4
1	A	252	ALA	2.4
1	D	179	ALA	2.4
1	C	181	GLN	2.4
1	A	64	LYS	2.4
1	D	195	GLU	2.4
1	C	292	GLN	2.4
1	A	265	ILE	2.4
1	D	258	VAL	2.4
1	D	261	ARG	2.4
1	D	241	ALA	2.4
1	A	251	LYS	2.4
1	C	229	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	138	VAL	2.4
1	A	267	ALA	2.3
1	B	35	LEU	2.3
1	D	292	GLN	2.3
1	D	274	SER	2.3
1	D	335	LYS	2.3
1	A	234	ILE	2.3
1	D	33	GLU	2.2
1	D	252	ALA	2.2
1	B	134	ARG	2.2
1	A	335	LYS	2.2
1	C	340	GLN	2.2
1	C	223	LYS	2.2
1	D	208	LEU	2.2
1	D	184	GLY	2.2
1	A	306	VAL	2.2
1	C	338	LYS	2.2
1	A	311	ASP	2.2
1	B	227	ASP	2.2
1	D	267	ALA	2.2
1	B	341	GLU	2.2
1	A	80	GLU	2.1
1	D	302	LYS	2.1
1	C	33	GLU	2.1
1	C	150	ASP	2.1
1	D	240	THR	2.1
1	D	151	ALA	2.1
1	A	258	VAL	2.1
1	D	307	VAL	2.1
1	A	131	ASP	2.1
1	D	227	ASP	2.1
1	D	178	THR	2.1
1	A	253	ALA	2.0
1	D	214	ALA	2.0
1	B	300	ASP	2.0
1	B	311	ASP	2.0
1	D	131	ASP	2.0
1	D	269	VAL	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.