Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:00 am BST

PDB ID	:	3VGZ
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 following versions of software and data (see references ⓘ) were used in the production of this report:

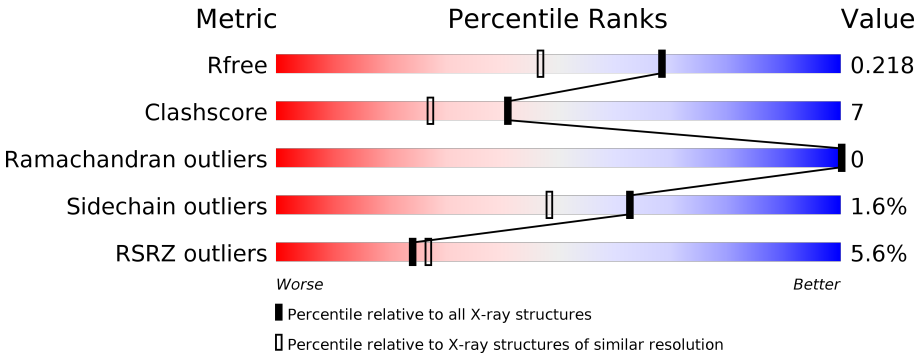
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 on 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 <=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	6% 76% 14% • 9%
1	B	353	3% 79% 11% • 9%
1	C	353	5% 82% 9% • 8%
1	D	353	6% 76% 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.

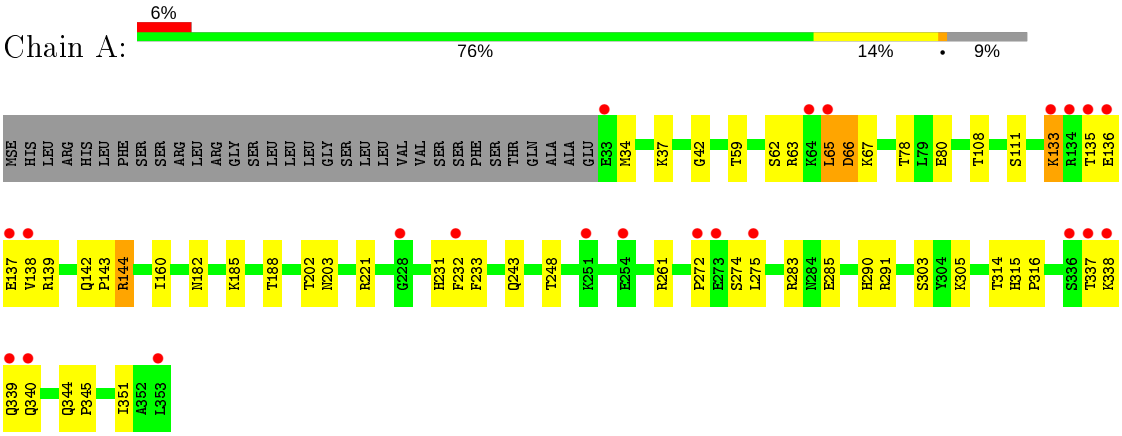
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		
2	B	91	Total	O	0	0
			91	91		
2	C	90	Total	O	0	0
			90	90		
2	D	60	Total	O	0	0
			60	60		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

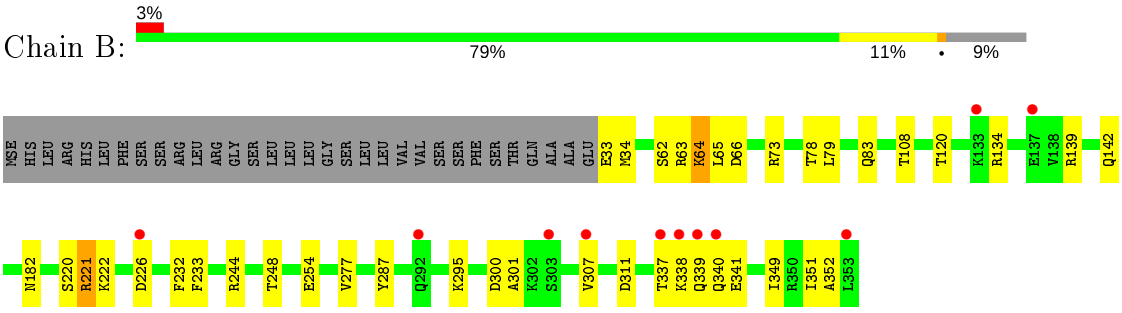
- Molecule 1: Uncharacterized protein YncE

Chain A:



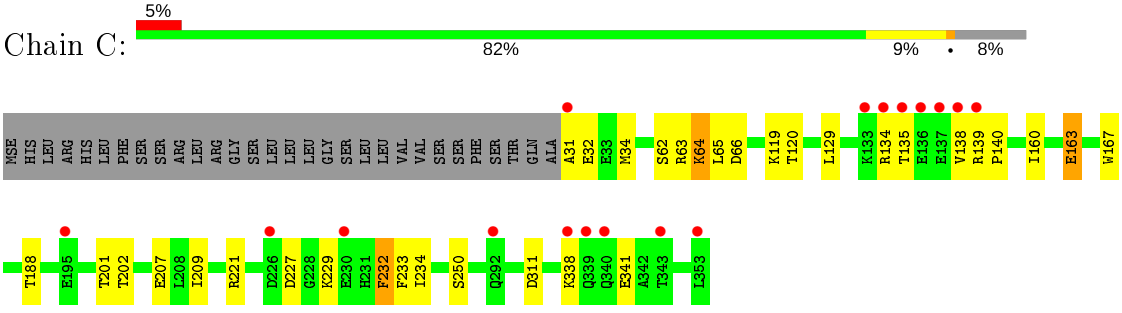
- Molecule 1: Uncharacterized protein YncE

Chain B:



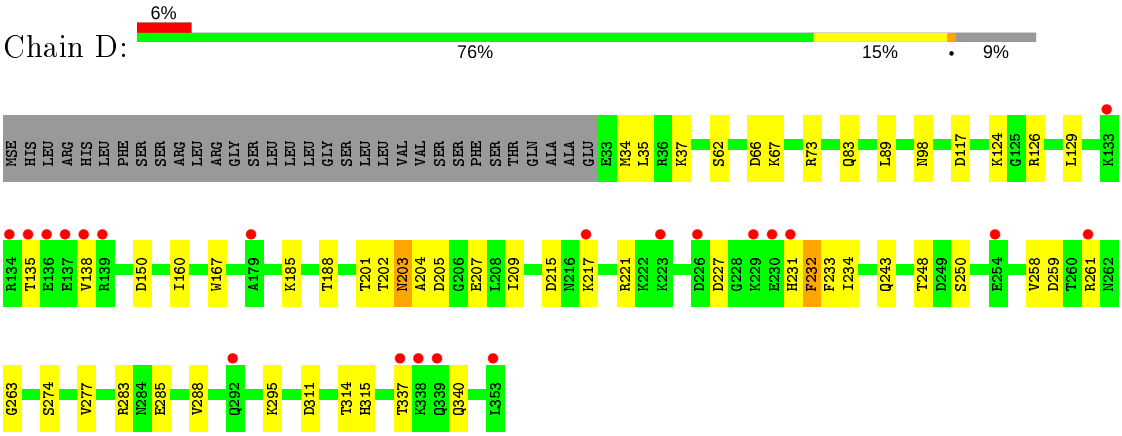
- Molecule 1: Uncharacterized protein YncE

Chain C:



- Molecule 1: Uncharacterized protein YncE

Chain D:


6%
76%
15%
9%
MSE HIS LEU ARG HIS LEU PHE SER SER ARG LEU ARG GLY SER LEU LEU LEU GLY SER LEU LEU VAL VAL SER SER PHE SER THR GLN ALA ALA GLU E33 M34 L35 R36 K37 S62 D66 K67 R73 Q83 L89 N98 D117 K124 G125 R126 L129 K133
R134 T135 E136 E137 V138 R139 D150 I160 W167 A179 K185 T188 T201 T202 N203 A204 D205 G206 E207 L208 I209 D215 N216 K217 R221 K222 K223 D226 D227 G228 K229 E230 H231 F232 F233 I234 Q243 T248 D249 S250 E254 V258 D259 T260 R261 N262
G263 S274 V277 R283 N284 E285 V288 Q292 K295 D311 T314 H315 T337 K338 Q339 Q340 L353

4 Data and refinement statistics (i)

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 90.56 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.70) 95.6 (90.56-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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)	0.36 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.31	0/2503	0.66	0/3385
1	B	0.31	0/2503	0.67	0/3385
1	C	0.31	0/2517	0.67	0/3404
1	D	0.29	0/2503	0.65	0/3385
All	All	0.31	0/10026	0.66	0/13559

There are no bond length outliers.

There are no bond angle outliers.

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	46	0
1	B	2473	0	2524	36	0
1	C	2487	0	2535	30	0
1	D	2473	0	2524	35	0
2	A	74	0	0	0	0
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	142	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 (142) 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:HA	1:B:340:GLN:HE21	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: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: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
1:D:203:ASN:HD22	1:D:203:ASN:C	2.04	0.61
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:C:64:LYS:HD2	1:C:341:GLU:CD	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:232:PHE:CD1	1:C:234:ILE:HD13	2.39	0.56
1:B:220:SER:HB2	1:C:31:ALA:HA	1.85	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:340:GLN:HA	1:B:340:GLN:NE2	2.20	0.55
1:B:34:MSE:HG2	1:B:351:ILE:HG12	1.88	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: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: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
1:A:144:ARG:HH11	1:A:144:ARG:HG2	1.77	0.50
1:D:35:LEU:HD21	1:D:37:LYS:HG2	1.94	0.50
1:A:274:SER:C	1:A:275:LEU:HD12	2.32	0.49
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:GLU:OE1	1:C:163:GLU:N	2.48	0.47
1:C:63:ARG:HH12	1:C:338:LYS:CE	2.24	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:A:337:THR:C	1:A:339:GLN:H	2.18	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:N	1:A:133:LYS:HD2	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: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:78:THR:O	1:B:79:LEU:HB2	2.16	0.45
1:C:163:GLU:CD	1:C:163:GLU:H	2.19	0.45
1:A:67:LYS:HE3	1:B:120:THR:O	2.18	0.44
1:B:233:PHE:HA	1:B:248:THR:O	2.17	0.44
1:B:34:MSE:HE3	1:B:351:ILE:HD11	1.98	0.44
1:A:231:HIS:C	1:A:232:PHE:HD1	2.20	0.44
1:D:274:SER:HB3	1:D:288:VAL:CG1	2.47	0.44
1:C:163:GLU:O	1:C:163:GLU:CG	2.65	0.44
1:C:62:SER:OG	1:C:64:LYS:HD3	2.18	0.44
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:O	1:B:226:ASP:OD1	2.36	0.43
1:B:340:GLN:CA	1:B:340:GLN:NE2	2.81	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:B:64:LYS:HB3	1:B:64:LYS:HE3	1.79	0.42
1:B:134:ARG:CZ	1:B:139:ARG:HH11	2.32	0.42
1:A:63:ARG:HH12	1:A:338:LYS:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:HIS:HA	1:A:316:PRO:HD2	1.97	0.41
1:A:42:GLY:O	1:A:59:THR:HA	2.20	0.41
1:B:300:ASP:HB2	1:B:307:VAL:CG1	2.50	0.41
1:D:73:ARG:HB3	1:D:83:GLN:HB3	2.01	0.41
1:B:340:GLN:O	1:B:340:GLN:HG3	2.21	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:D:232:PHE:C	1:D:232:PHE:CD1	2.94	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:A:37:LYS:HZ1	1:A:80:GLU:HG2	1.84	0.40
1:D:203:ASN:ND2	1:D:205:ASP:H	2.18	0.40
1:B:108:THR:O	1:B:142:GLN:CD	2.60	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

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%)	264 (98%)	5 (2%)	57	41
1	B	269/293 (92%)	265 (98%)	4 (2%)	65	51
1	C	270/293 (92%)	265 (98%)	5 (2%)	57	41
1	D	269/293 (92%)	266 (99%)	3 (1%)	73	63
All	All	1077/1172 (92%)	1060 (98%)	17 (2%)	62	48

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	66	ASP
1	A	133	LYS
1	A	144	ARG
1	A	340	GLN
1	B	64	LYS
1	B	221	ARG
1	B	232	PHE
1	B	341	GLU
1	C	34	MSE
1	C	64	LYS
1	C	65	LEU
1	C	163	GLU
1	C	232	PHE
1	D	34	MSE
1	D	203	ASN
1	D	232	PHE

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

Mol	Chain	Res	Type
1	A	61	GLN
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	182	ASN
1	B	315	HIS
1	B	317	ASN
1	B	340	GLN
1	C	51	GLN
1	C	61	GLN
1	C	315	HIS
1	C	317	ASN
1	C	340	GLN
1	D	50	GLN
1	D	61	GLN
1	D	142	GLN
1	D	203	ASN
1	D	231	HIS
1	D	264	ASN
1	D	315	HIS
1	D	317	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} 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%)	0.45	22 (6%)	16	19	12, 24, 48, 63	0
1	B	318/353 (90%)	0.28	11 (3%)	44	49	13, 23, 42, 57	0
1	C	320/353 (90%)	0.23	17 (5%)	26	29	13, 22, 42, 60	0
1	D	318/353 (90%)	0.55	21 (6%)	18	20	13, 28, 46, 62	0
All	All	1274/1412 (90%)	0.38	71 (5%)	24	27	12, 24, 45, 63	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	GLU	7.8
1	A	134	ARG	6.9
1	D	338	LYS	6.5
1	A	340	GLN	6.5
1	B	338	LYS	6.3
1	A	137	GLU	6.1
1	A	337	THR	5.5
1	D	139	ARG	5.5
1	B	339	GLN	5.2
1	C	230	GLU	5.2
1	A	339	GLN	5.1
1	D	137	GLU	5.0
1	D	136	GLU	4.9
1	A	338	LYS	4.7
1	D	339	GLN	4.6
1	C	31	ALA	4.6
1	C	137	GLU	4.5
1	A	273	GLU	4.0
1	B	292	GLN	3.9
1	C	339	GLN	3.9
1	B	340	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	230	GLU	3.9
1	D	223	LYS	3.8
1	A	232	PHE	3.8
1	D	134	ARG	3.7
1	A	336	SER	3.7
1	C	138	VAL	3.6
1	C	136	GLU	3.5
1	D	226	ASP	3.5
1	B	137	GLU	3.4
1	C	135	THR	3.4
1	A	135	THR	3.4
1	C	134	ARG	3.3
1	B	307	VAL	3.3
1	A	251	LYS	3.2
1	B	226	ASP	3.1
1	B	353	LEU	3.1
1	D	217	LYS	3.0
1	A	138	VAL	3.0
1	C	226	ASP	3.0
1	D	135	THR	3.0
1	B	337	THR	2.9
1	C	139	ARG	2.8
1	B	303	SER	2.8
1	C	338	LYS	2.8
1	D	353	LEU	2.8
1	C	195	GLU	2.7
1	A	65	LEU	2.6
1	A	272	PRO	2.6
1	C	133	LYS	2.5
1	D	292	GLN	2.5
1	A	228	GLY	2.5
1	A	254	GLU	2.5
1	D	261	ARG	2.4
1	D	231	HIS	2.4
1	D	138	VAL	2.3
1	D	337	THR	2.3
1	A	133	LYS	2.3
1	A	64	LYS	2.3
1	D	254	GLU	2.3
1	A	275	LEU	2.3
1	D	229	LYS	2.3
1	C	292	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	343	THR	2.2
1	D	133	LYS	2.2
1	A	33	GLU	2.2
1	D	179	ALA	2.2
1	C	340	GLN	2.1
1	A	353	LEU	2.1
1	B	133	LYS	2.1
1	C	353	LEU	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 carbohydrates 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.