Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:20 AM GMT

PDB ID	:	2QCZ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

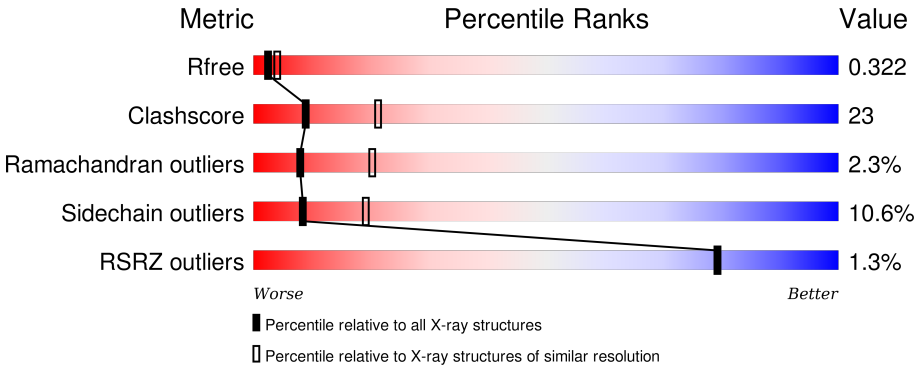
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	335	% 57% 30% 6% 7%
1	B	335	2% 48% 39% 5% 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:

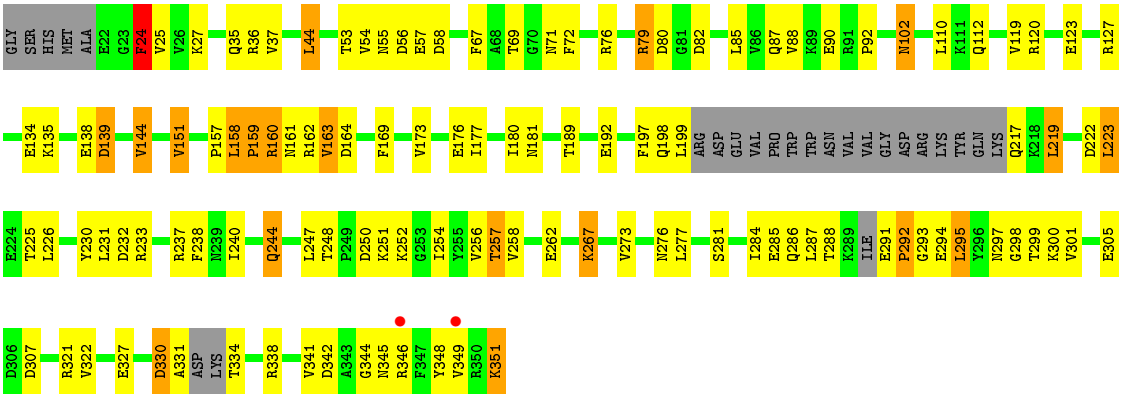
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	CLONING ARTIFACT	UNP P0A940
A	18	SER	-	CLONING ARTIFACT	UNP P0A940
A	19	HIS	-	CLONING ARTIFACT	UNP P0A940
A	20	MET	-	CLONING ARTIFACT	UNP P0A940
B	17	GLY	-	CLONING ARTIFACT	UNP P0A940
B	18	SER	-	CLONING ARTIFACT	UNP P0A940
B	19	HIS	-	CLONING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

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 errors 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.

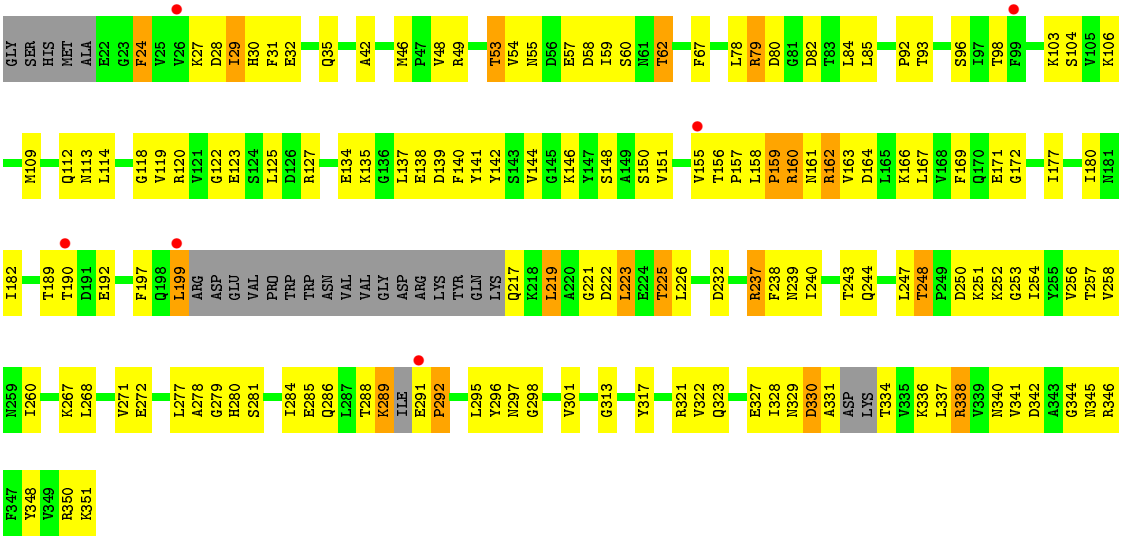
- Molecule 1: Outer membrane protein assembly factor yaeT

Chain A:



- Molecule 1: Outer membrane protein assembly factor yaeT

Chain B:



4 Data and refinement statistics (i)

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 47.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.70) 99.3 (47.21-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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%)	DCC
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 20363 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/2449	0.71	0/3306
1	B	0.40	0/2449	0.64	0/3306
All	All	0.42	0/4898	0.67	0/6612

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	2417	0	2408	98	0
1	B	2417	0	2408	135	0
All	All	4834	0	4816	225	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 23.

All (225) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:321:ARG:HG3	1:B:342:ASP:HB3	1.69	0.74
1:A:298:GLY:H	1:A:301:VAL:HG23	1.50	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:346:ARG:HD3	1:B:348:TYR:OH	1.89	0.73
1:B:156:THR:HB	1:B:164:ASP:OD1	1.88	0.73
1:A:173:VAL:HG21	1:A:252:LYS:HZ2	1.53	0.72
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:A:198:GLN:HA	1:A:217:GLN:CD	2.14	0.68
1:B:114:LEU:HD22	1:B:119:VAL:HG11	1.74	0.68
1:A:162:ARG:HH11	1:A:162:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LYS:HB3	1:B:106:LYS:NZ	2.15	0.61
1:B:141:TYR:O	1:B:144:VAL:HG12	2.00	0.61
1:A:138:GLU:CG	1:A:151:VAL:HG13	2.30	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: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
1:A:144:VAL:O	1:A:144:VAL:HG13	2.02	0.59
1:B:277:LEU:HD12	1:B:281:SER:OG	2.02	0.58
1:A:138:GLU:HG2	1:A:151:VAL:HG13	1.84	0.58
1:B:271:VAL:HG22	1:B:337:LEU:HB2	1.85	0.58
1:B:79:ARG:HG3	1:B:80:ASP:N	2.18	0.58
1:B:122:GLY:O	1:B:123:GLU:HG2	2.03	0.58
1:B:248:THR:HB	1:B:253:GLY:O	2.03	0.58
1:A:322:VAL:HG22	1:A:341:VAL:HG22	1.86	0.58
1:A:55:ASN:ND2	1:A:57:GLU:HB2	2.18	0.58
1:B:289:LYS:HB3	1:B:289:LYS:NZ	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:96:SER:OG	1:B:164:ASP:HB2	2.04	0.57
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:B:141:TYR:CE1	1:B:171:GLU:HG2	2.39	0.56
1:A:24:PHE:HB3	1:A:54:VAL:O	2.05	0.56
1:B:158:LEU:HB2	1:B:162:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:GLU:HB2	1:B:336:LYS:HB3	1.89	0.55
1:B:250:ASP:O	1:B:252:LYS:HG3	2.06	0.55
1:A:247:LEU:HD12	1:B:351:LYS:HB3	1.88	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:B:291:GLU:CD	1:B:292:PRO:HD2	2.28	0.54
1:A:291:GLU:HB2	1:A:294:GLU:HB2	1.90	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:135:LYS:HE3	1:B:139:ASP:OD1	2.08	0.53
1:B:98:THR:O	1:B:166:LYS:HA	2.09	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
1:B:260:ILE:C	1:B:260:ILE:HD12	2.30	0.52
1:A:345:ASN:ND2	1:B:240:ILE:HG22	2.25	0.52
1:A:197:PHE:HB3	1:A:222:ASP:OD1	2.10	0.52
1:B:27:LYS:HB2	1:B:82:ASP:HB3	1.91	0.51
1:B:162:ARG:HH11	1:B:162:ARG:HG3	1.76	0.51
1:B:144:VAL:HG13	1:B:146:LYS:HG2	1.90	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:A:110:LEU:HD13	1:A:169:PHE:CZ	2.46	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: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:321:ARG:NH1	1:A:321:ARG:HG2	2.24	0.49
1:A:120:ARG:HG3	1:A:123:GLU:HG2	1.94	0.49
1:A:351:LYS:NZ	1:A:351:LYS:HB2	2.27	0.49
1:B:141:TYR:HB3	1:B:146:LYS:HB2	1.94	0.49
1:B:138:GLU:OE2	1:B:150:SER:HA	2.13	0.49
1:A:102:ASN:HD22	1:A:102:ASN:H	1.59	0.49
1:B:32:GLU:HG3	1:B:85:LEU:HD11	1.94	0.49
1:A:112:GLN:HE22	1:B:112:GLN:HE22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ARG:CZ	1:B:328:ILE:HG21	2.43	0.48
1:B:155:VAL:CG1	1:B:163:VAL:HG21	2.44	0.48
1:B:137:LEU:HD11	1:B:167:LEU:HD13	1.94	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:B:346:ARG:HB3	1:B:348:TYR:HE1	1.79	0.47
1:A:277:LEU:HD13	1:A:284:ILE:CD1	2.43	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:291:GLU:OE1	1:A:291:GLU:HA	2.15	0.47
1:A:287:LEU:HD13	1:A:307:ASP:HB3	1.96	0.47
1:B:199:LEU:HD13	1:B:199:LEU:O	2.13	0.47
1:A:180:ILE:HA	1:A:256:VAL:O	2.14	0.47
1:B:244:GLN:HB2	1:B:257:THR:CG2	2.42	0.47
1:A:327:GLU:HG3	1:A:338:ARG:HH11	1.80	0.47
1:A:69:THR:HG21	1:A:71:ASN:HD21	1.74	0.47
1:B:250:ASP:OD1	1:B:252:LYS:HB2	2.14	0.47
1:A:247:LEU:HD23	1:A:254:ILE:HG22	1.97	0.47
1:A:92:PRO:HG2	1:A:127:ARG:NH2	2.29	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: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:267:LYS:O	1:B:334:THR:HA	2.15	0.46
1:A:237:ARG:NH1	1:A:330:ASP:OD1	2.47	0.46
1:B:331:ALA:O	1:B:334:THR:HG23	2.15	0.46
1:B:219:LEU:HD22	1:B:223:LEU:HD22	1.97	0.46
1:A:226:LEU:CD1	1:A:238:PHE:HZ	2.28	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:CG	1:B:162:ARG:HH11	2.29	0.46
1:B:323:GLN:HE21	1:B:340:ASN:HD22	1.64	0.46
1:B:103:LYS:H	1:B:171:GLU:CD	2.17	0.46
1:A:189:THR:O	1:A:192:GLU:N	2.47	0.46
1:B:330:ASP:N	1:B:330:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:120:ARG:O	1:B:123:GLU:HB2	2.16	0.45
1:A:157:PRO:HA	1:A:163:VAL:HG23	1.97	0.45
1:A:291:GLU:CD	1:A:292:PRO:HD2	2.37	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
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:244:GLN:H	1:A:244:GLN:HG2	1.56	0.44
1:A:160:ARG:HB3	1:A:161:ASN:H	1.53	0.44
1:A:79:ARG:HG3	1:A:80:ASP:N	2.33	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:A:37:VAL:HG23	1:A:90:GLU:CD	2.39	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: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:A:305:GLU:HG2	1:A:322:VAL:HG12	2.00	0.43
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:B:247:LEU:HA	1:B:254:ILE:HG22	2.01	0.42
1:B:93:THR:O	1:B:163:VAL:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:HA	1:A:288:THR:HG23	2.01	0.42
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.93	0.42
1:A:273:VAL:HG21	1:A:284:ILE:HD12	2.00	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:B:280:HIS:O	1:B:284:ILE:HG23	2.21	0.41
1:B:237:ARG:CZ	1:B:328:ILE:CG2	2.99	0.41
1:B:113:ASN:ND2	1:B:140:PHE:CD2	2.89	0.41
1:B:84:LEU:HA	1:B:84:LEU:HD12	1.90	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: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
1:B:106:LYS:HB3	1:B:106:LYS:HZ2	1.84	0.40
1:A:24:PHE:HE2	1:A:82:ASP:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	8 20
1	B	302/335 (90%)	270 (89%)	25 (8%)	7 (2%)	8 20
All	All	604/670 (90%)	548 (91%)	42 (7%)	14 (2%)	8 20

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
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 (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	264/288 (92%)	232 (88%)	32 (12%)	6 14
1	B	264/288 (92%)	240 (91%)	24 (9%)	12 26
All	All	528/576 (92%)	472 (89%)	56 (11%)	8 19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	PHE
1	A	27	LYS
1	A	44	LEU
1	A	56	ASP
1	A	67	PHE
1	A	72	PHE
1	A	79	ARG
1	A	85	LEU
1	A	88	VAL
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	119	VAL
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
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	330	ASP
1	A	351	LYS
1	B	29	ILE
1	B	30	HIS
1	B	53	THR
1	B	60	SER
1	B	62	THR
1	B	67	PHE
1	B	78	LEU
1	B	79	ARG
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	237	ARG
1	B	248	THR
1	B	272	GLU

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Mol	Chain	Res	Type
1	B	286	GLN
1	B	289	LYS
1	B	330	ASP
1	B	338	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	71	ASN
1	A	102	ASN
1	A	112	GLN
1	A	113	ASN
1	A	170	GLN
1	A	179	GLN
1	A	217	GLN
1	A	276	ASN
1	A	323	GLN
1	A	345	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	276	ASN
1	B	286	GLN
1	B	340	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	310/335 (92%)	0.12	2 (0%)	90	91	33, 53, 79, 100	0
1	B	310/335 (92%)	0.29	6 (1%)	70	70	41, 70, 95, 108	0
All	All	620/670 (92%)	0.20	8 (1%)	79	79	33, 62, 89, 108	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	LEU	4.7
1	B	26	VAL	3.0
1	A	349	VAL	2.5
1	B	190	THR	2.4
1	B	155	VAL	2.2
1	B	291	GLU	2.2
1	A	346	ARG	2.0
1	B	99	PHE	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.