WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:22 AM GMT

PDB ID	:	3EFC
Title	:	Crystal Structure of YaeT periplasmic domain
Authors	:	Gatzeva-Topalova, P.Z.; Walton, T.A.; Sousa, M.C.
Deposited on	:	2008-09-08
Resolution	:	3.30 Å(reported)

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

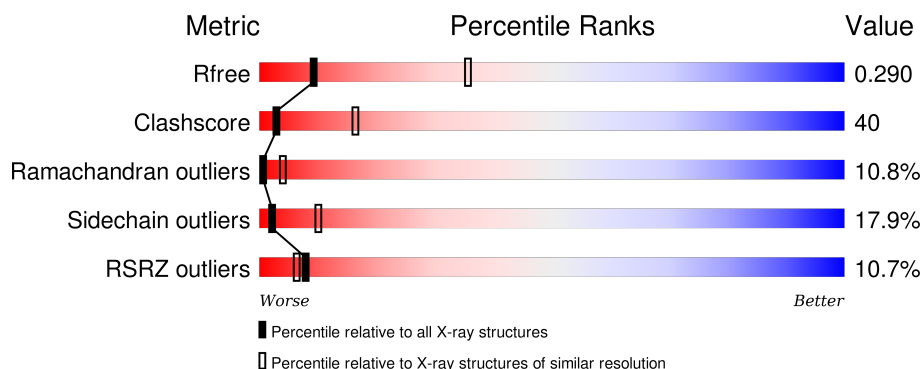|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 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	Percentile Ranks	Value
Rfree		0.290
Clashscore		40
Ramachandran outliers		10.8%
Sidechain outliers		17.9%
RSRZ outliers		10.7%

Worse　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	395	9% / 31% / 39% / 11% / · / 17%

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2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2514 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
			Total	C	N	O	S			
1	A	327	2514	1576	430	504	4	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	EXPRESSION TAG	UNP P0A940
A	19	ALA	-	EXPRESSION TAG	UNP P0A940
A	20	MET	-	EXPRESSION TAG	UNP P0A940
A	411	PRO	-	EXPRESSION TAG	UNP P0A940
A	412	GLY	-	EXPRESSION TAG	UNP P0A940

3 Residue-property plots ⓘ

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
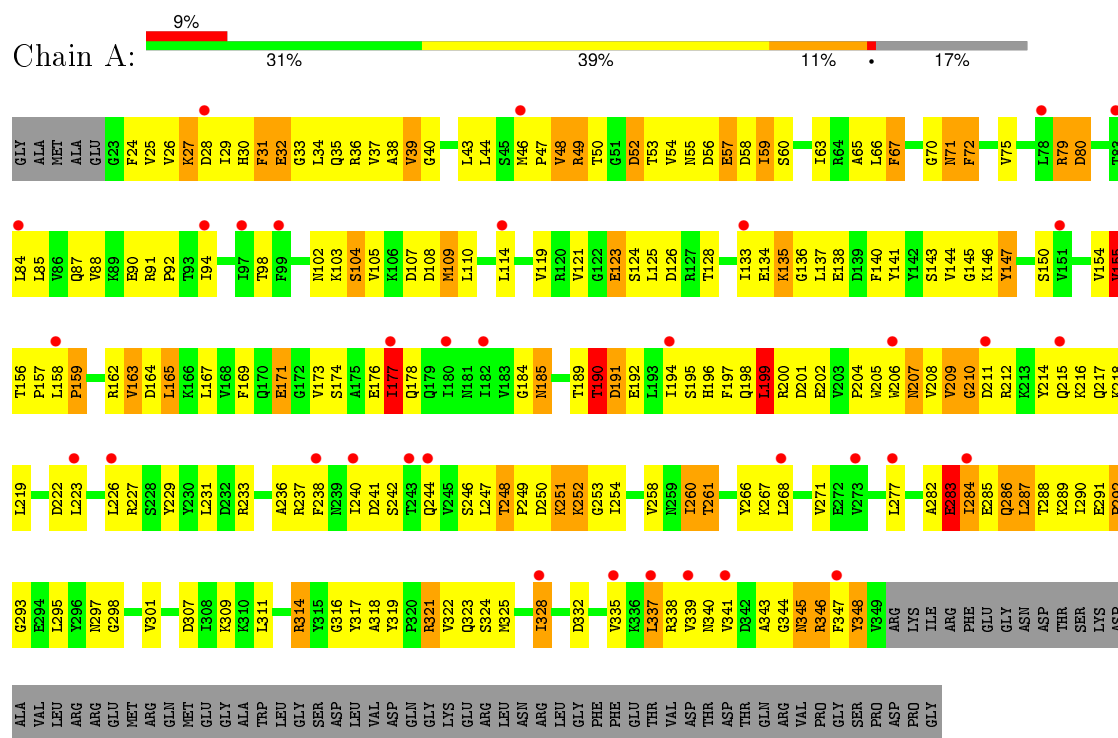
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.51Å 92.51Å 142.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.50 – 3.30 69.83 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.50-3.30) 99.5 (69.83-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.33Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.267 , 0.295 0.256 , 0.290	Depositor DCC
R_{free} test set	1125 reflections (10.20%)	DCC
Wilson B-factor (Å^2)	99.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 77.6	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 11065 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2514	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0/2554	0.67	1/3474 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	LEU	CA-CB-CG	5.44	127.80	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2514	0	2420	195	0
All	All	2514	0	2420	195	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 40.

All (195) 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:79:ARG:HG3	1:A:80:ASP:N	1.83	0.92
1:A:72:PHE:HB3	1:A:90:GLU:HA	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:SER:HB3	1:A:339:VAL:HG22	1.54	0.88
1:A:135:LYS:HA	1:A:138:GLU:HB2	1.55	0.88
1:A:141:TYR:HE2	1:A:171:GLU:HG3	1.40	0.86
1:A:79:ARG:HG3	1:A:80:ASP:H	1.37	0.86
1:A:209:VAL:HG22	1:A:212:ARG:HA	1.58	0.86
1:A:248:THR:HG22	1:A:249:PRO:HD2	1.59	0.85
1:A:286:GLN:HG3	1:A:286:GLN:O	1.74	0.85
1:A:32:GLU:OE2	1:A:32:GLU:HA	1.81	0.79
1:A:158:LEU:HB3	1:A:159:PRO:HD2	1.63	0.78
1:A:126:ASP:OD1	1:A:128:THR:HB	1.84	0.77
1:A:209:VAL:HG13	1:A:212:ARG:H	1.49	0.77
1:A:322:VAL:HG22	1:A:341:VAL:HG22	1.68	0.76
1:A:176:GLU:O	1:A:178:GLN:HG3	1.87	0.75
1:A:189:THR:C	1:A:191:ASP:H	1.90	0.74
1:A:184:GLY:HA3	1:A:260:ILE:HG22	1.69	0.74
1:A:345:ASN:N	1:A:345:ASN:HD22	1.85	0.73
1:A:189:THR:O	1:A:191:ASP:N	2.21	0.73
1:A:238:PHE:HE1	1:A:260:ILE:HG12	1.53	0.73
1:A:238:PHE:CE1	1:A:260:ILE:HG12	2.25	0.71
1:A:32:GLU:O	1:A:33:GLY:C	2.29	0.70
1:A:72:PHE:HA	1:A:91:ARG:H	1.56	0.69
1:A:26:VAL:HG12	1:A:27:LYS:H	1.56	0.69
1:A:79:ARG:CG	1:A:80:ASP:N	2.57	0.68
1:A:60:SER:HA	1:A:63:ILE:HD12	1.75	0.67
1:A:345:ASN:O	1:A:346:ARG:C	2.33	0.66
1:A:238:PHE:HE1	1:A:260:ILE:CG1	2.09	0.66
1:A:209:VAL:HG22	1:A:212:ARG:CA	2.25	0.66
1:A:72:PHE:CD2	1:A:88:VAL:HG11	2.31	0.65
1:A:347:PHE:O	1:A:348:TYR:HB2	1.96	0.64
1:A:54:VAL:HG21	1:A:84:LEU:HD11	1.79	0.64
1:A:46:MET:HG2	1:A:66:LEU:HD21	1.79	0.64
1:A:328:ILE:HG23	1:A:335:VAL:HG22	1.79	0.64
1:A:27:LYS:NZ	1:A:29:ILE:HG12	2.12	0.63
1:A:92:PRO:HB2	1:A:163:VAL:CG2	2.28	0.63
1:A:48:VAL:HG11	1:A:54:VAL:HG22	1.81	0.63
1:A:209:VAL:CG2	1:A:212:ARG:HA	2.29	0.62
1:A:205:TRP:O	1:A:205:TRP:CD1	2.53	0.62
1:A:346:ARG:HB3	1:A:348:TYR:HE2	1.63	0.62
1:A:248:THR:HG22	1:A:249:PRO:CD	2.29	0.61
1:A:317:TYR:CD2	1:A:343:ALA:HB1	2.35	0.61
1:A:140:PHE:O	1:A:143:SER:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD23	1:A:287:LEU:O	1.99	0.61
1:A:261:THR:HG22	1:A:261:THR:O	2.01	0.59
1:A:199:LEU:HD23	1:A:199:LEU:O	2.04	0.58
1:A:317:TYR:HD2	1:A:344:GLY:H	1.49	0.58
1:A:250:ASP:O	1:A:252:LYS:N	2.36	0.58
1:A:137:LEU:HD11	1:A:167:LEU:HD13	1.86	0.57
1:A:159:PRO:HD2	1:A:162:ARG:HH21	1.66	0.57
1:A:317:TYR:HD2	1:A:344:GLY:N	2.03	0.56
1:A:185:ASN:ND2	1:A:185:ASN:O	2.35	0.56
1:A:155:VAL:HG23	1:A:156:THR:N	2.20	0.56
1:A:297:ASN:O	1:A:301:VAL:HG23	2.05	0.56
1:A:158:LEU:HB3	1:A:159:PRO:CD	2.34	0.56
1:A:26:VAL:O	1:A:27:LYS:C	2.43	0.55
1:A:301:VAL:HG13	1:A:337:LEU:HD11	1.89	0.55
1:A:137:LEU:CD1	1:A:167:LEU:HD13	2.37	0.55
1:A:271:VAL:HB	1:A:288:THR:HG22	1.90	0.54
1:A:40:GLY:O	1:A:44:LEU:HD12	2.07	0.54
1:A:197:PHE:HB3	1:A:222:ASP:OD2	2.07	0.54
1:A:283:GLU:O	1:A:285:GLU:N	2.41	0.54
1:A:155:VAL:O	1:A:156:THR:OG1	2.25	0.54
1:A:145:GLY:C	1:A:147:TYR:H	2.10	0.54
1:A:318:ALA:HB3	1:A:319:TYR:CD1	2.43	0.54
1:A:287:LEU:HD21	1:A:307:ASP:HB3	1.89	0.53
1:A:317:TYR:CE2	1:A:343:ALA:HB1	2.44	0.53
1:A:328:ILE:HG23	1:A:335:VAL:CG2	2.37	0.53
1:A:345:ASN:ND2	1:A:345:ASN:N	2.49	0.53
1:A:164:ASP:OD1	1:A:165:LEU:N	2.42	0.53
1:A:283:GLU:O	1:A:284:ILE:C	2.46	0.52
1:A:55:ASN:O	1:A:57:GLU:N	2.43	0.52
1:A:198:GLN:O	1:A:199:LEU:CB	2.57	0.52
1:A:316:GLY:O	1:A:346:ARG:HG3	2.10	0.52
1:A:33:GLY:HA2	1:A:88:VAL:O	2.09	0.52
1:A:189:THR:C	1:A:191:ASP:N	2.56	0.52
1:A:271:VAL:HG13	1:A:337:LEU:HB3	1.91	0.52
1:A:236:ALA:O	1:A:237:ARG:HB2	2.10	0.52
1:A:246:SER:OG	1:A:247:LEU:N	2.43	0.51
1:A:159:PRO:HD2	1:A:162:ARG:NH2	2.25	0.51
1:A:146:LYS:O	1:A:147:TYR:C	2.49	0.51
1:A:72:PHE:HA	1:A:91:ARG:N	2.25	0.51
1:A:227:ARG:HA	1:A:238:PHE:CE2	2.46	0.51
1:A:219:LEU:HD13	1:A:219:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLY:CA	1:A:88:VAL:O	2.59	0.50
1:A:209:VAL:HG23	1:A:214:TYR:HB3	1.93	0.50
1:A:184:GLY:CA	1:A:260:ILE:HG22	2.39	0.50
1:A:67:PHE:CE1	1:A:75:VAL:HB	2.47	0.50
1:A:34:LEU:HD13	1:A:39:VAL:HA	1.94	0.49
1:A:223:LEU:HD21	1:A:258:VAL:CG2	2.42	0.49
1:A:125:LEU:HD13	1:A:125:LEU:C	2.32	0.49
1:A:260:ILE:HG23	1:A:261:THR:N	2.27	0.49
1:A:200:ARG:C	1:A:202:GLU:H	2.15	0.49
1:A:27:LYS:CE	1:A:29:ILE:HG12	2.42	0.49
1:A:340:ASN:OD1	1:A:340:ASN:C	2.51	0.49
1:A:209:VAL:CG1	1:A:210:GLY:N	2.75	0.48
1:A:287:LEU:HD21	1:A:307:ASP:CB	2.42	0.48
1:A:49:ARG:HG2	1:A:52:ASP:OD1	2.13	0.48
1:A:55:ASN:O	1:A:58:ASP:N	2.32	0.48
1:A:25:VAL:HG21	1:A:54:VAL:HG23	1.95	0.48
1:A:328:ILE:HA	1:A:335:VAL:HG22	1.95	0.48
1:A:209:VAL:HG12	1:A:210:GLY:N	2.28	0.48
1:A:283:GLU:O	1:A:286:GLN:N	2.47	0.48
1:A:185:ASN:OD1	1:A:190:THR:HA	2.13	0.48
1:A:126:ASP:C	1:A:126:ASP:OD1	2.53	0.47
1:A:271:VAL:HB	1:A:288:THR:CG2	2.44	0.47
1:A:37:VAL:HG23	1:A:90:GLU:OE2	2.15	0.47
1:A:238:PHE:CE1	1:A:260:ILE:CG1	2.91	0.47
1:A:49:ARG:CG	1:A:52:ASP:OD1	2.63	0.47
1:A:27:LYS:HZ2	1:A:29:ILE:HG12	1.77	0.47
1:A:38:ALA:C	1:A:40:GLY:N	2.63	0.47
1:A:110:LEU:HD13	1:A:169:PHE:CZ	2.50	0.47
1:A:27:LYS:HZ1	1:A:29:ILE:HG23	1.78	0.47
1:A:134:GLU:C	1:A:136:GLY:H	2.18	0.47
1:A:240:ILE:O	1:A:242:SER:N	2.48	0.47
1:A:290:ILE:O	1:A:291:GLU:HB3	2.15	0.46
1:A:119:VAL:HG21	1:A:133:ILE:HD13	1.97	0.46
1:A:134:GLU:O	1:A:136:GLY:N	2.49	0.46
1:A:277:LEU:CD2	1:A:341:VAL:HB	2.46	0.46
1:A:177:ILE:HA	1:A:254:ILE:HB	1.96	0.45
1:A:94:ILE:O	1:A:121:VAL:O	2.34	0.45
1:A:346:ARG:HB3	1:A:348:TYR:CE2	2.46	0.45
1:A:156:THR:HB	1:A:164:ASP:HB3	1.97	0.45
1:A:248:THR:OG1	1:A:253:GLY:O	2.35	0.45
1:A:92:PRO:HD2	1:A:125:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PRO:HB2	1:A:163:VAL:HG21	1.98	0.45
1:A:218:LYS:HA	1:A:218:LYS:HD3	1.80	0.45
1:A:63:ILE:HG23	1:A:75:VAL:HG12	1.99	0.45
1:A:25:VAL:HG11	1:A:84:LEU:HG	1.99	0.45
1:A:268:LEU:HD13	1:A:290:ILE:HD13	1.98	0.45
1:A:309:LYS:HE3	1:A:322:VAL:HB	1.98	0.44
1:A:227:ARG:HG2	1:A:231:LEU:HD11	1.99	0.44
1:A:156:THR:O	1:A:157:PRO:C	2.56	0.44
1:A:134:GLU:O	1:A:137:LEU:N	2.50	0.44
1:A:38:ALA:O	1:A:39:VAL:C	2.54	0.44
1:A:266:TYR:O	1:A:295:LEU:HD23	2.17	0.44
1:A:28:ASP:HB2	1:A:84:LEU:HB2	1.99	0.44
1:A:43:LEU:C	1:A:43:LEU:HD13	2.37	0.44
1:A:114:LEU:HD11	1:A:167:LEU:HD12	1.98	0.44
1:A:46:MET:HA	1:A:47:PRO:HD2	1.61	0.44
1:A:59:ILE:HG22	1:A:63:ILE:HD11	2.00	0.44
1:A:291:GLU:N	1:A:292:PRO:HD3	2.33	0.44
1:A:337:LEU:HD13	1:A:339:VAL:HG23	2.00	0.44
1:A:344:GLY:C	1:A:345:ASN:HD22	2.21	0.43
1:A:289:LYS:O	1:A:290:ILE:HG12	2.18	0.43
1:A:154:VAL:O	1:A:154:VAL:HG13	2.18	0.43
1:A:288:THR:O	1:A:288:THR:HG22	2.18	0.43
1:A:214:TYR:CE1	1:A:218:LYS:HE3	2.54	0.43
1:A:189:THR:HG23	1:A:192:GLU:H	1.83	0.43
1:A:125:LEU:HD22	1:A:125:LEU:HA	1.72	0.43
1:A:30:HIS:O	1:A:31:PHE:O	2.37	0.43
1:A:291:GLU:O	1:A:293:GLY:N	2.51	0.43
1:A:104:SER:OG	1:A:171:GLU:OE2	2.35	0.43
1:A:209:VAL:HG23	1:A:214:TYR:CB	2.49	0.43
1:A:219:LEU:CD1	1:A:223:LEU:HD12	2.49	0.43
1:A:205:TRP:O	1:A:207:ASN:N	2.52	0.42
1:A:231:LEU:C	1:A:233:ARG:H	2.23	0.42
1:A:268:LEU:HB3	1:A:290:ILE:HD13	2.02	0.42
1:A:72:PHE:HA	1:A:91:ARG:HB2	2.00	0.42
1:A:298:GLY:O	1:A:301:VAL:HB	2.19	0.42
1:A:141:TYR:CE2	1:A:171:GLU:HG3	2.33	0.42
1:A:250:ASP:C	1:A:252:LYS:N	2.72	0.42
1:A:289:LYS:HD3	1:A:289:LYS:HA	1.62	0.42
1:A:37:VAL:CG2	1:A:71:ASN:HD22	2.32	0.42
1:A:214:TYR:CZ	1:A:218:LYS:HE3	2.54	0.42
1:A:318:ALA:CB	1:A:319:TYR:CD1	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:MET:HA	1:A:109:MET:CE	2.50	0.42
1:A:70:GLY:O	1:A:91:ARG:NH2	2.53	0.42
1:A:248:THR:HB	1:A:252:LYS:H	1.84	0.42
1:A:346:ARG:CB	1:A:348:TYR:HE2	2.29	0.42
1:A:185:ASN:ND2	1:A:185:ASN:C	2.73	0.42
1:A:321:ARG:HD2	1:A:323:GLN:OE1	2.20	0.42
1:A:114:LEU:HD11	1:A:167:LEU:CD1	2.50	0.42
1:A:36:ARG:H	1:A:90:GLU:CD	2.22	0.41
1:A:211:ASP:O	1:A:212:ARG:CB	2.68	0.41
1:A:223:LEU:HD21	1:A:258:VAL:HG22	2.02	0.41
1:A:102:ASN:N	1:A:102:ASN:OD1	2.53	0.41
1:A:198:GLN:O	1:A:199:LEU:HB2	2.20	0.41
1:A:35:GLN:HB3	1:A:90:GLU:OE1	2.19	0.41
1:A:250:ASP:O	1:A:251:LYS:C	2.59	0.41
1:A:317:TYR:CD2	1:A:344:GLY:N	2.87	0.41
1:A:65:ALA:O	1:A:66:LEU:C	2.55	0.41
1:A:105:VAL:HG12	1:A:109:MET:HB2	2.01	0.41
1:A:216:LYS:O	1:A:217:GLN:C	2.59	0.41
1:A:226:LEU:HD22	1:A:238:PHE:CZ	2.56	0.41
1:A:167:LEU:HA	1:A:167:LEU:HD23	1.84	0.41
1:A:58:ASP:O	1:A:59:ILE:C	2.59	0.41
1:A:223:LEU:HD21	1:A:258:VAL:HG21	2.02	0.41
1:A:267:LYS:HA	1:A:295:LEU:HA	2.02	0.41
1:A:43:LEU:O	1:A:43:LEU:HD13	2.21	0.41
1:A:194:ILE:O	1:A:196:HIS:N	2.53	0.41
1:A:314:ARG:C	1:A:316:GLY:H	2.24	0.41
1:A:92:PRO:CB	1:A:163:VAL:CG2	2.99	0.41
1:A:205:TRP:CG	1:A:205:TRP:O	2.75	0.40
1:A:134:GLU:C	1:A:136:GLY:N	2.74	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	325/395 (82%)	223 (69%)	67 (21%)	35 (11%)	0	4

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	52	ASP
1	A	56	ASP
1	A	147	TYR
1	A	171	GLU
1	A	177	ILE
1	A	190	THR
1	A	199	LEU
1	A	206	TRP
1	A	251	LYS
1	A	284	ILE
1	A	292	PRO
1	A	24	PHE
1	A	124	SER
1	A	204	PRO
1	A	241	ASP
1	A	244	GLN
1	A	103	LYS
1	A	135	LYS
1	A	159	PRO
1	A	195	SER
1	A	201	ASP
1	A	207	ASN
1	A	282	ALA
1	A	283	GLU
1	A	27	LYS
1	A	104	SER
1	A	208	VAL
1	A	229	TYR
1	A	346	ARG
1	A	123	GLU
1	A	252	LYS
1	A	348	TYR
1	A	210	GLY
1	A	155	VAL

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	268/338 (79%)	220 (82%)	48 (18%)	2 10

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	39	VAL
1	A	48	VAL
1	A	49	ARG
1	A	50	THR
1	A	53	THR
1	A	57	GLU
1	A	59	ILE
1	A	67	PHE
1	A	71	ASN
1	A	72	PHE
1	A	79	ARG
1	A	80	ASP
1	A	85	LEU
1	A	87	GLN
1	A	98	THR
1	A	107	ASP
1	A	108	ASP
1	A	109	MET
1	A	123	GLU
1	A	144	VAL
1	A	150	SER
1	A	155	VAL
1	A	163	VAL
1	A	165	LEU
1	A	173	VAL
1	A	174	SER
1	A	177	ILE
1	A	185	ASN
1	A	190	THR

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Mol	Chain	Res	Type
1	A	191	ASP
1	A	199	LEU
1	A	209	VAL
1	A	215	GLN
1	A	248	THR
1	A	260	ILE
1	A	261	THR
1	A	283	GLU
1	A	286	GLN
1	A	311	LEU
1	A	314	ARG
1	A	321	ARG
1	A	325	MET
1	A	328	ILE
1	A	332	ASP
1	A	337	LEU
1	A	338	ARG
1	A	345	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	345	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 carbohydrates 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	327/395 (82%)	0.77	35 (10%)	8	6	70, 92, 118, 163	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	PHE	3.9
1	A	273	VAL	3.6
1	A	206	TRP	3.3
1	A	268	LEU	3.3
1	A	284	ILE	3.2
1	A	347	PHE	2.9
1	A	339	VAL	2.9
1	A	337	LEU	2.9
1	A	226	LEU	2.8
1	A	84	LEU	2.8
1	A	177	ILE	2.7
1	A	97	ILE	2.7
1	A	194	ILE	2.6
1	A	215	GLN	2.6
1	A	158	LEU	2.6
1	A	211	ASP	2.5
1	A	238	PHE	2.5
1	A	180	ILE	2.5
1	A	243	THR	2.4
1	A	83	THR	2.4
1	A	335	VAL	2.3
1	A	46	MET	2.3
1	A	240	ILE	2.3
1	A	114	LEU	2.2
1	A	341	VAL	2.2
1	A	151	VAL	2.2
1	A	277	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	133	ILE	2.1
1	A	28	ASP	2.1
1	A	328	ILE	2.1
1	A	244	GLN	2.0
1	A	94	ILE	2.0
1	A	182	ILE	2.0
1	A	78	LEU	2.0
1	A	223	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.