Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:10 PM GMT

PDB ID	:	3WDO
Title	:	Structure of E. coli YajR transporter
Authors	:	Jiang, D.
Deposited on	:	2013-06-19
Resolution	:	3.15 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:

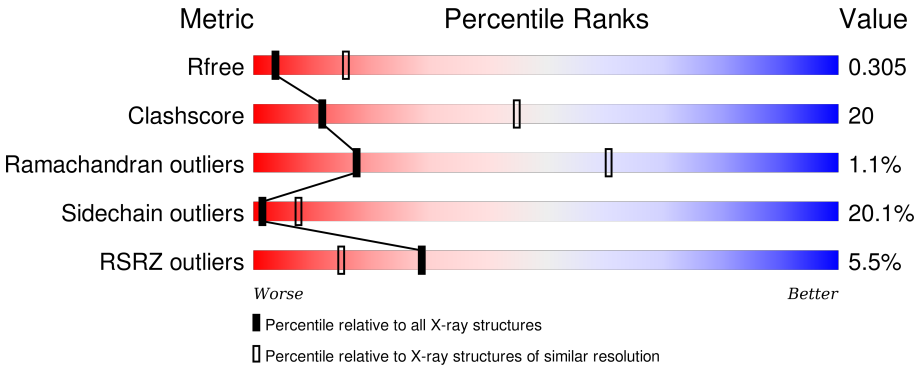
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	453	6% 53% 37% 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3419 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 MFS Transporter.

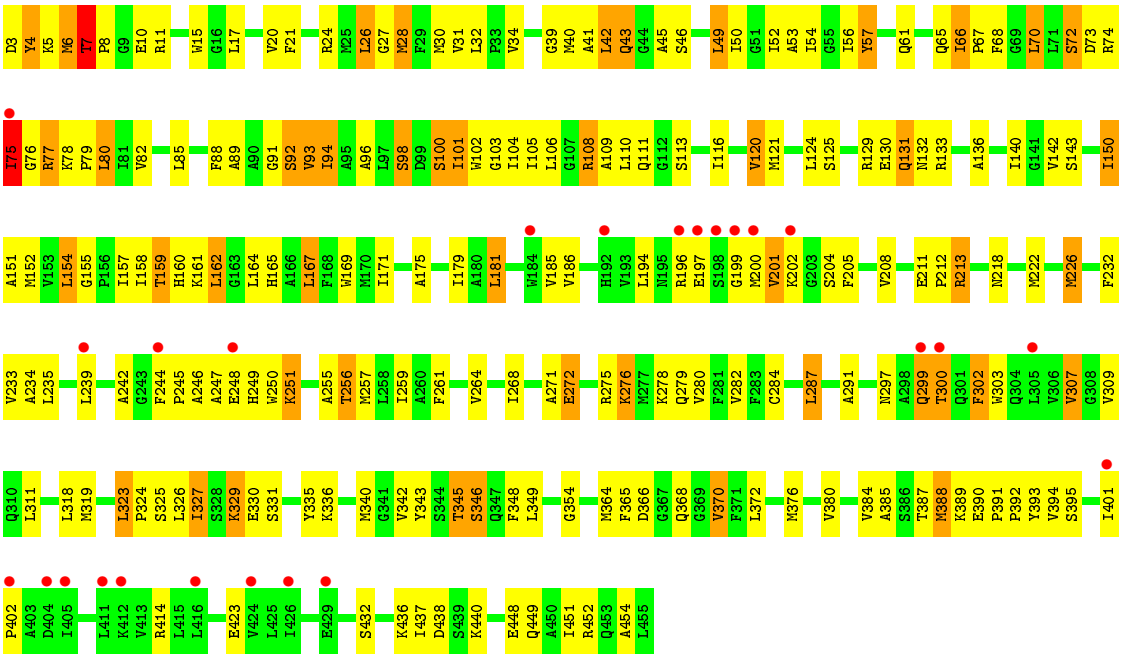
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	453	3419	2243	560	594	22	0	0	0

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: MFS Transporter

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	128.72Å 128.72Å 165.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.17 – 3.15 39.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.17-3.15) 99.4 (39.17-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.271 , 0.290 0.280 , 0.305	Depositor DCC
R_{free} test set	708 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	109.4	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 14475 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3419	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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, 0.375 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	0.54	0/3491	0.84	3/4737 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	LEU	CA-CB-CG	-6.31	100.78	115.30
1	A	213	ARG	CB-CG-CD	-5.17	98.15	111.60
1	A	194	LEU	CA-CB-CG	5.12	127.08	115.30

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	3419	0	3557	141	0
All	All	3419	0	3557	141	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 20.

All (141) 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:276:LYS:HB3	1:A:279:GLN:HG3	1.58	0.84
1:A:46:SER:HB3	1:A:49:LEU:HB2	1.60	0.81
1:A:66:ILE:HD13	1:A:66:ILE:H	1.46	0.79
1:A:7:THR:HG22	1:A:8:PRO:HD2	1.68	0.73
1:A:331:SER:HB2	1:A:336:LYS:HE2	1.70	0.71
1:A:52:ILE:HG22	1:A:105:ILE:HD11	1.74	0.70
1:A:245:PRO:HD2	1:A:248:GLU:HB2	1.76	0.68
1:A:102:TRP:HA	1:A:105:ILE:HG22	1.76	0.68
1:A:20:VAL:HG12	1:A:181:LEU:HD23	1.77	0.67
1:A:26:LEU:O	1:A:30:MET:HG3	1.95	0.67
1:A:98:SER:OG	1:A:103:GLY:HA3	1.94	0.67
1:A:56:ILE:HD13	1:A:109:ALA:HB2	1.77	0.67
1:A:302:PHE:HE1	1:A:303:TRP:CE2	2.15	0.65
1:A:394:VAL:HA	1:A:437:ILE:O	1.97	0.64
1:A:10:GLU:OE1	1:A:132:ASN:ND2	2.31	0.63
1:A:30:MET:HE3	1:A:154:LEU:HG	1.79	0.63
1:A:66:ILE:HG12	1:A:67:PRO:HD3	1.80	0.62
1:A:27:GLY:O	1:A:31:VAL:HG23	2.00	0.61
1:A:275:ARG:NH1	1:A:440:LYS:HA	2.15	0.60
1:A:155:GLY:O	1:A:159:THR:HG22	2.01	0.59
1:A:234:ALA:HB2	1:A:370:VAL:CG2	2.33	0.59
1:A:255:ALA:O	1:A:259:ILE:HG12	2.02	0.58
1:A:54:ILE:HA	1:A:108:ARG:HE	1.68	0.58
1:A:34:VAL:HG22	1:A:159:THR:HG21	1.85	0.58
1:A:205:PHE:O	1:A:208:VAL:HG12	2.04	0.57
1:A:30:MET:CE	1:A:154:LEU:HG	2.34	0.56
1:A:53:ALA:O	1:A:56:ILE:HG22	2.05	0.56
1:A:234:ALA:HB2	1:A:370:VAL:HG21	1.86	0.56
1:A:91:GLY:HA3	1:A:110:LEU:HB2	1.88	0.56
1:A:423:GLU:HB3	1:A:436:LYS:HB2	1.88	0.56
1:A:10:GLU:OE2	1:A:129:ARG:N	2.33	0.55
1:A:7:THR:CB	1:A:10:GLU:HG3	2.37	0.55
1:A:438:ASP:OD1	1:A:440:LYS:HB2	2.07	0.54
1:A:40:MET:HG2	1:A:45:ALA:HB1	1.90	0.54
1:A:7:THR:HB	1:A:10:GLU:HG3	1.89	0.54
1:A:40:MET:HA	1:A:45:ALA:HB1	1.91	0.53
1:A:82:VAL:HG13	1:A:179:ILE:HG23	1.90	0.53
1:A:326:LEU:HD22	1:A:391:PRO:HG3	1.91	0.53
1:A:303:TRP:O	1:A:307:VAL:HG12	2.07	0.53
1:A:242:ALA:HB2	1:A:300:THR:HA	1.90	0.53
1:A:226:MET:HA	1:A:354:GLY:HA3	1.89	0.53
1:A:40:MET:HG2	1:A:45:ALA:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HD3	1:A:330:GLU:OE1	2.09	0.53
1:A:387:THR:O	1:A:387:THR:OG1	2.27	0.52
1:A:154:LEU:O	1:A:158:ILE:HG22	2.10	0.52
1:A:197:GLU:OE1	1:A:201:VAL:HA	2.09	0.52
1:A:271:ALA:HB2	1:A:280:VAL:HG21	1.91	0.52
1:A:150:ILE:HG22	1:A:154:LEU:HD23	1.91	0.51
1:A:121:MET:HE3	1:A:140:ILE:HD12	1.92	0.51
1:A:390:GLU:HG3	1:A:391:PRO:HD2	1.91	0.51
1:A:124:LEU:HD11	1:A:136:ALA:HB1	1.92	0.51
1:A:247:ALA:O	1:A:250:TRP:CD1	2.64	0.51
1:A:385:ALA:O	1:A:388:MET:HG3	2.11	0.51
1:A:380:VAL:O	1:A:384:VAL:HG23	2.10	0.51
1:A:96:ALA:O	1:A:165:HIS:HB3	2.11	0.51
1:A:390:GLU:CG	1:A:391:PRO:HD2	2.41	0.50
1:A:272:GLU:OE2	1:A:329:LYS:NZ	2.39	0.50
1:A:7:THR:HG22	1:A:8:PRO:CD	2.38	0.50
1:A:213:ARG:HB3	1:A:330:GLU:OE1	2.12	0.50
1:A:53:ALA:HA	1:A:105:ILE:HG13	1.93	0.49
1:A:324:PRO:HG3	1:A:343:TYR:OH	2.12	0.49
1:A:372:LEU:O	1:A:376:MET:HG3	2.11	0.49
1:A:261:PHE:HA	1:A:264:VAL:HG12	1.94	0.49
1:A:92:SER:HB2	1:A:111:GLN:OE1	2.12	0.49
1:A:66:ILE:CD1	1:A:66:ILE:H	2.21	0.49
1:A:68:PHE:O	1:A:80:LEU:HD23	2.13	0.49
1:A:395:SER:O	1:A:436:LYS:HA	2.14	0.48
1:A:364:MET:HG3	1:A:365:PHE:CE2	2.48	0.48
1:A:88:PHE:HD2	1:A:175:ALA:HB2	1.78	0.48
1:A:291:ALA:HB2	1:A:311:LEU:HB3	1.95	0.48
1:A:130:GLU:HA	1:A:133:ARG:HG3	1.96	0.48
1:A:211:GLU:OE1	1:A:212:PRO:HD2	2.14	0.47
1:A:204:SER:HB3	1:A:335:TYR:CE2	2.49	0.47
1:A:96:ALA:HB1	1:A:169:TRP:CD1	2.50	0.47
1:A:319:MET:HG3	1:A:323:LEU:HD12	1.96	0.47
1:A:72:SER:HA	1:A:76:GLY:O	2.14	0.47
1:A:52:ILE:HG22	1:A:105:ILE:CD1	2.43	0.47
1:A:142:VAL:HG22	1:A:261:PHE:CD1	2.50	0.47
1:A:94:ILE:HG21	1:A:106:LEU:HD22	1.96	0.47
1:A:158:ILE:HG23	1:A:167:LEU:HD12	1.97	0.46
1:A:7:THR:OG1	1:A:10:GLU:HG3	2.14	0.46
1:A:26:LEU:HD23	1:A:151:ALA:HB2	1.97	0.46
1:A:239:LEU:HB3	1:A:249:HIS:NE2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HA	1:A:157:ILE:HB	1.97	0.46
1:A:57:TYR:CD1	1:A:57:TYR:C	2.88	0.46
1:A:246:ALA:O	1:A:249:HIS:HB2	2.16	0.46
1:A:6:MET:O	1:A:10:GLU:HB2	2.16	0.46
1:A:17:LEU:HD13	1:A:124:LEU:HB2	1.98	0.45
1:A:89:ALA:HB2	1:A:175:ALA:HB3	1.98	0.45
1:A:161:LYS:C	1:A:162:LEU:HD12	2.36	0.45
1:A:158:ILE:CG2	1:A:167:LEU:HD12	2.47	0.45
1:A:342:VAL:O	1:A:346:SER:HB3	2.16	0.45
1:A:414:ARG:HH22	1:A:454:ALA:HB3	1.82	0.45
1:A:131:GLN:HG3	1:A:131:GLN:H	1.45	0.45
1:A:42:LEU:HD23	1:A:101:ILE:HA	1.98	0.45
1:A:278:LYS:O	1:A:282:VAL:HG23	2.17	0.44
1:A:74:ARG:HD3	1:A:75:ILE:HG12	2.00	0.44
1:A:116:ILE:O	1:A:120:VAL:HG12	2.17	0.44
1:A:299:GLN:NE2	1:A:368:GLN:HB2	2.33	0.44
1:A:448:GLU:O	1:A:451:ILE:HB	2.17	0.44
1:A:401:ILE:HG13	1:A:432:SER:HA	2.00	0.44
1:A:102:TRP:O	1:A:105:ILE:HG22	2.18	0.44
1:A:11:ARG:O	1:A:15:TRP:HD1	2.01	0.43
1:A:372:LEU:HA	1:A:372:LEU:HD12	1.80	0.43
1:A:116:ILE:HG13	1:A:120:VAL:CG1	2.48	0.43
1:A:287:LEU:HA	1:A:287:LEU:HD23	1.84	0.43
1:A:66:ILE:HG23	1:A:345:THR:HG21	2.01	0.43
1:A:93:VAL:HG22	1:A:169:TRP:CZ3	2.53	0.43
1:A:392:PRO:O	1:A:393:TYR:HB2	2.19	0.43
1:A:185:VAL:HG12	1:A:186:VAL:H	1.84	0.43
1:A:66:ILE:CG1	1:A:67:PRO:HD3	2.45	0.42
1:A:393:TYR:O	1:A:394:VAL:HG13	2.20	0.42
1:A:167:LEU:O	1:A:171:ILE:HG13	2.20	0.42
1:A:185:VAL:HG12	1:A:186:VAL:N	2.35	0.42
1:A:72:SER:O	1:A:77:ARG:NH1	2.53	0.42
1:A:77:ARG:N	1:A:79:PRO:HD2	2.34	0.42
1:A:70:LEU:O	1:A:73:ASP:HB2	2.19	0.42
1:A:250:TRP:CE3	1:A:251:LYS:HA	2.54	0.42
1:A:340:MET:O	1:A:343:TYR:HB3	2.19	0.42
1:A:401:ILE:HG22	1:A:402:PRO:O	2.20	0.42
1:A:239:LEU:HA	1:A:239:LEU:HD23	1.92	0.41
1:A:323:LEU:O	1:A:327:ILE:HD12	2.21	0.41
1:A:28:MET:O	1:A:32:LEU:HG	2.20	0.41
1:A:218:ASN:OD1	1:A:343:TYR:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:CYS:SG	1:A:318:LEU:HD23	2.61	0.41
1:A:43:GLN:HB2	1:A:100:SER:HB2	2.03	0.41
1:A:40:MET:HA	1:A:45:ALA:CB	2.50	0.41
1:A:41:ALA:O	1:A:42:LEU:HB2	2.19	0.41
1:A:200:MET:C	1:A:202:LYS:H	2.23	0.41
1:A:66:ILE:HD12	1:A:345:THR:HG21	2.02	0.41
1:A:284:CYS:HB2	1:A:319:MET:HE1	2.02	0.41
1:A:74:ARG:HD3	1:A:75:ILE:CG1	2.50	0.41
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.88	0.41
1:A:366:ASP:OD1	1:A:366:ASP:N	2.40	0.41
1:A:4:TYR:CD1	1:A:4:TYR:N	2.88	0.40
1:A:256:THR:HG21	1:A:309:VAL:HG13	2.03	0.40
1:A:449:GLN:HA	1:A:452:ARG:CZ	2.52	0.40
1:A:46:SER:O	1:A:50:ILE:HG12	2.21	0.40
1:A:39:GLY:O	1:A:40:MET:HB2	2.22	0.40
1:A:213:ARG:NH1	1:A:330:GLU:HB3	2.35	0.40
1:A:196:ARG:HB3	1:A:196:ARG:HE	1.39	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	451/453 (100%)	415 (92%)	31 (7%)	5 (1%)	17 61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	199	GLY
1	A	42	LEU
1	A	75	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	VAL

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	353/354 (100%)	282 (80%)	71 (20%)	1 8

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	4	TYR
1	A	5	LYS
1	A	6	MET
1	A	7	THR
1	A	21	PHE
1	A	24	ARG
1	A	26	LEU
1	A	28	MET
1	A	43	GLN
1	A	49	LEU
1	A	57	TYR
1	A	61	GLN
1	A	65	GLN
1	A	66	ILE
1	A	70	LEU
1	A	72	SER
1	A	75	ILE
1	A	77	ARG
1	A	78	LYS
1	A	85	LEU
1	A	92	SER
1	A	93	VAL
1	A	94	ILE
1	A	98	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	100	SER
1	A	101	ILE
1	A	104	ILE
1	A	108	ARG
1	A	113	SER
1	A	120	VAL
1	A	125	SER
1	A	131	GLN
1	A	143	SER
1	A	150	ILE
1	A	152	MET
1	A	154	LEU
1	A	159	THR
1	A	160	HIS
1	A	162	LEU
1	A	167	LEU
1	A	181	LEU
1	A	222	MET
1	A	226	MET
1	A	232	PHE
1	A	233	VAL
1	A	235	LEU
1	A	244	PHE
1	A	251	LYS
1	A	256	THR
1	A	257	MET
1	A	268	ILE
1	A	272	GLU
1	A	276	LYS
1	A	287	LEU
1	A	297	ASN
1	A	299	GLN
1	A	300	THR
1	A	302	PHE
1	A	307	VAL
1	A	323	LEU
1	A	325	SER
1	A	327	ILE
1	A	329	LYS
1	A	345	THR
1	A	346	SER
1	A	348	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	349	LEU
1	A	370	VAL
1	A	388	MET
1	A	389	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	453/453 (100%)	0.08	25 (5%) 29 15	33, 54, 138, 222	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	ILE	6.3
1	A	202	LYS	5.0
1	A	404	ASP	4.7
1	A	192	HIS	4.4
1	A	248	GLU	4.3
1	A	402	PRO	4.1
1	A	199	GLY	4.0
1	A	198	SER	4.0
1	A	299	GLN	3.5
1	A	200	MET	3.5
1	A	300	THR	3.5
1	A	244	PHE	3.5
1	A	197	GLU	2.8
1	A	426	ILE	2.7
1	A	401	ILE	2.6
1	A	305	LEU	2.5
1	A	412	LYS	2.5
1	A	429	GLU	2.4
1	A	424	VAL	2.3
1	A	75	ILE	2.2
1	A	184	TRP	2.2
1	A	416	LEU	2.1
1	A	196	ARG	2.0
1	A	411	LEU	2.0
1	A	239	LEU	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

There are no such residues in this entry.