Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 05:53 AM EDT

PDB ID	:	3BLC
Title	:	Crystal structure of the periplasmic domain of the Escherichia Coli YIDC
Authors	:	Paetzel, M.; Oliver, D.C.
Deposited on	:	2007-12-10
Resolution	:	2.50 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 (i) symbol.

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

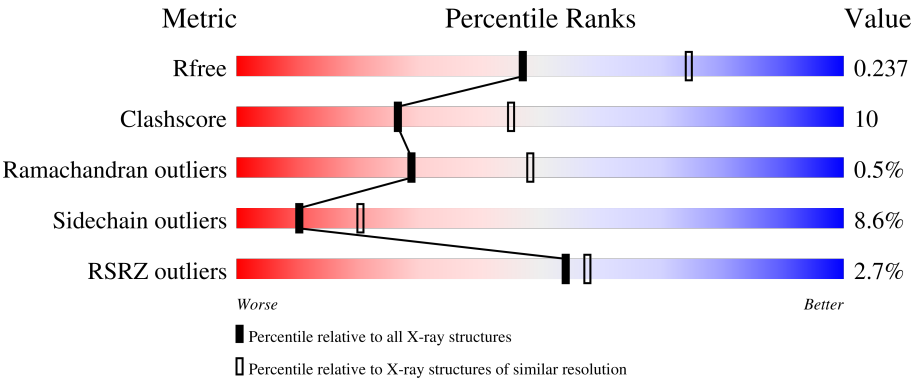
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	330	3% 64% 19% · 15%
1	B	330	2% 66% 15% · 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4371 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 Inner membrane protein oxaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	Se	0	0	0
			2154	1373	359	418	4			
1	B	278	Total	C	N	O	Se	0	0	0
			2137	1364	354	415	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MSE	-	expression tag	UNP P25714
A	228	ALA	GLU	engineered mutation	UNP P25714
A	229	ALA	LYS	engineered mutation	UNP P25714
A	231	ALA	GLU	engineered mutation	UNP P25714
A	232	ALA	LYS	engineered mutation	UNP P25714
A	234	ALA	LYS	engineered mutation	UNP P25714
A	341	LEU	-	expression tag	UNP P25714
A	342	VAL	-	expression tag	UNP P25714
A	343	PRO	-	expression tag	UNP P25714
A	344	ARG	-	expression tag	UNP P25714
A	345	GLY	-	expression tag	UNP P25714
A	346	SER	-	expression tag	UNP P25714
A	347	LEU	-	expression tag	UNP P25714
A	348	GLU	-	expression tag	UNP P25714
A	349	HIS	-	expression tag	UNP P25714
A	350	HIS	-	expression tag	UNP P25714
A	351	HIS	-	expression tag	UNP P25714
A	352	HIS	-	expression tag	UNP P25714
A	353	HIS	-	expression tag	UNP P25714
A	354	HIS	-	expression tag	UNP P25714
B	25	MSE	-	expression tag	UNP P25714
B	228	ALA	GLU	engineered mutation	UNP P25714
B	229	ALA	LYS	engineered mutation	UNP P25714
B	231	ALA	GLU	engineered mutation	UNP P25714
B	232	ALA	LYS	engineered mutation	UNP P25714

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Chain	Residue	Modelled	Actual	Comment	Reference
B	234	ALA	LYS	engineered mutation	UNP P25714
B	341	LEU	-	expression tag	UNP P25714
B	342	VAL	-	expression tag	UNP P25714
B	343	PRO	-	expression tag	UNP P25714
B	344	ARG	-	expression tag	UNP P25714
B	345	GLY	-	expression tag	UNP P25714
B	346	SER	-	expression tag	UNP P25714
B	347	LEU	-	expression tag	UNP P25714
B	348	GLU	-	expression tag	UNP P25714
B	349	HIS	-	expression tag	UNP P25714
B	350	HIS	-	expression tag	UNP P25714
B	351	HIS	-	expression tag	UNP P25714
B	352	HIS	-	expression tag	UNP P25714
B	353	HIS	-	expression tag	UNP P25714
B	354	HIS	-	expression tag	UNP P25714

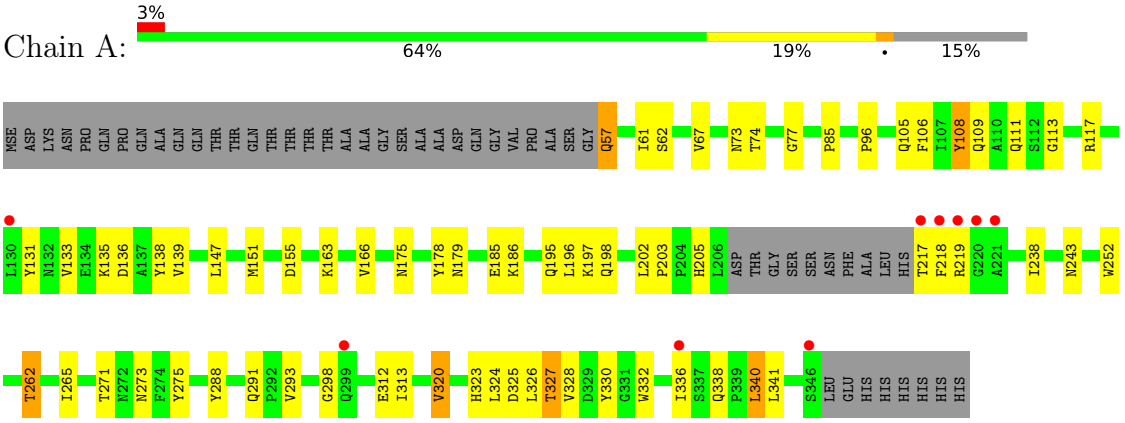
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	43	Total O 43 43	0	0
2	B	37	Total O 37 37	0	0

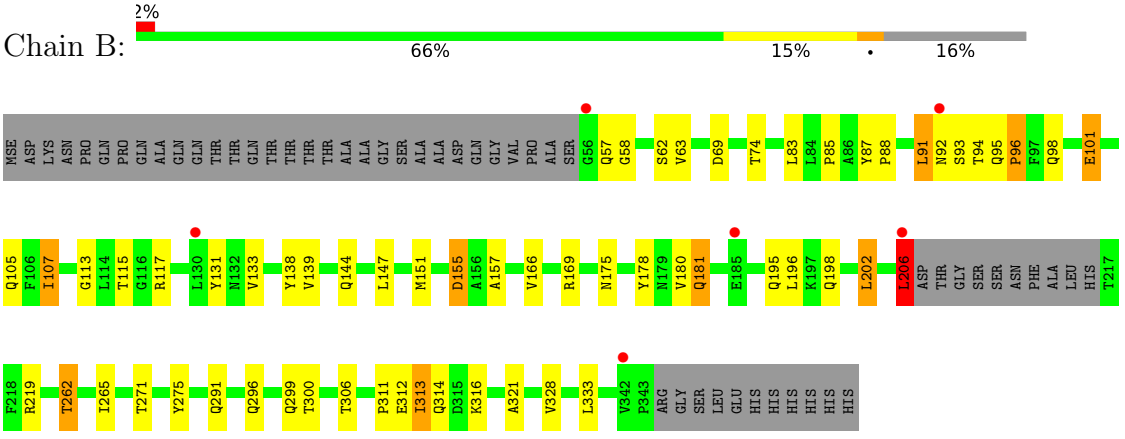
3 Residue-property plots (i)

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: Inner membrane protein oxaA



• Molecule 1: Inner membrane protein oxaA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.13Å 126.13Å 288.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.50) 99.0 (48.65-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.249 0.203 , 0.237	Depositor DCC
R_{free} test set	2021 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4371	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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	0.66	0/2205	0.74	1/3009 (0.0%)
1	B	0.83	2/2188 (0.1%)	0.69	0/2987
All	All	0.75	2/4393 (0.0%)	0.72	1/5996 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	LEU	C-O	23.56	1.68	1.23
1	B	105	GLN	CB-CG	6.31	1.69	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	LEU	CA-CB-CG	5.51	127.97	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	GLY	Peptide

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	2154	0	2085	52	0
1	B	2137	0	2067	37	0
2	A	43	0	0	1	0
2	B	37	0	0	1	0
All	All	4371	0	4152	87	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 10.

All (87) 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:206:LEU:O	1:B:206:LEU:C	1.68	1.30
1:A:196:LEU:HD13	1:A:262:THR:CG2	2.05	0.86
1:A:323:HIS:O	1:A:323:HIS:CG	2.32	0.82
1:A:218:PHE:CZ	1:A:330:TYR:HD2	2.03	0.76
1:B:144:GLN:O	1:B:169:ARG:NH1	2.18	0.76
1:A:133:VAL:HG23	1:A:138:TYR:OH	1.87	0.74
1:B:202:LEU:H	1:B:202:LEU:HD23	1.53	0.73
1:B:312:GLU:HG3	1:B:328:VAL:HG22	1.71	0.73
1:A:218:PHE:HZ	1:A:330:TYR:HD2	1.35	0.71
1:A:325:ASP:OD1	1:A:327:THR:HB	1.91	0.70
1:B:271:THR:H	1:B:291:GLN:NE2	1.89	0.69
1:B:196:LEU:HD22	1:B:262:THR:HG23	1.74	0.68
1:A:131:TYR:HB3	1:A:151:MSE:HB2	1.76	0.67
1:A:196:LEU:HD13	1:A:262:THR:HG23	1.75	0.67
1:A:196:LEU:HD13	1:A:262:THR:HG22	1.80	0.64
1:A:238:ILE:HG23	1:A:243:ASN:HD21	1.63	0.64
1:B:180:VAL:O	1:B:300:THR:HA	1.97	0.63
1:B:131:TYR:HB3	1:B:151:MSE:HB2	1.82	0.61
1:A:312:GLU:OE2	1:A:330:TYR:CE1	2.55	0.59
1:B:196:LEU:HD22	1:B:262:THR:CG2	2.33	0.59
1:B:93:SER:HB3	1:B:95:GLN:H	1.68	0.58
1:A:198:GLN:NE2	1:A:219:ARG:HH11	2.01	0.58
1:A:113:GLY:HA2	1:A:178:TYR:OH	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:CG2	1:A:138:TYR:OH	2.53	0.57
1:B:113:GLY:HA2	1:B:178:TYR:OH	2.04	0.56
1:A:332:TRP:CH2	1:A:336:ILE:HD11	2.41	0.56
1:A:218:PHE:CZ	1:A:330:TYR:CD2	2.90	0.55
1:A:312:GLU:OE2	1:A:330:TYR:HE1	1.88	0.55
1:A:218:PHE:HZ	1:A:330:TYR:CD2	2.20	0.54
1:A:163:LYS:HD3	1:A:178:TYR:CZ	2.43	0.54
1:B:300:THR:HG23	2:B:365:HOH:O	2.08	0.53
1:B:196:LEU:CD2	1:B:262:THR:HG23	2.39	0.52
1:A:196:LEU:HD22	1:A:262:THR:HG23	1.90	0.52
1:B:311:PRO:HG2	1:B:313:ILE:HD13	1.92	0.52
1:A:265:ILE:HD13	1:A:320:VAL:HG12	1.92	0.51
1:B:133:VAL:HG22	1:B:138:TYR:OH	2.10	0.51
1:A:73:ASN:O	1:A:77:GLY:HA2	2.11	0.51
1:B:196:LEU:HD13	1:B:262:THR:HG22	1.91	0.51
1:B:181:GLN:HG3	1:B:300:THR:HG22	1.92	0.51
1:A:271:THR:H	1:A:291:GLN:NE2	2.09	0.51
2:A:363:HOH:O	1:B:314:GLN:HG2	2.10	0.50
1:A:61:ILE:HG22	1:A:136:ASP:HA	1.93	0.50
1:B:196:LEU:HD13	1:B:262:THR:CG2	2.42	0.50
1:A:163:LYS:HD3	1:A:178:TYR:CE1	2.47	0.50
1:A:327:THR:HG22	1:A:328:VAL:HG23	1.95	0.49
1:A:196:LEU:CD1	1:A:262:THR:HG23	2.40	0.48
1:B:69:ASP:HB2	1:B:83:LEU:HB2	1.95	0.48
1:A:332:TRP:O	1:A:336:ILE:HB	2.13	0.48
1:B:271:THR:H	1:B:291:GLN:HE21	1.61	0.48
1:A:85:PRO:HA	1:A:96:PRO:HB3	1.94	0.47
1:B:85:PRO:HA	1:B:96:PRO:HB3	1.97	0.47
1:A:57:GLN:HE21	1:A:57:GLN:N	2.11	0.47
1:B:202:LEU:HD22	1:B:219:ARG:CZ	2.46	0.46
1:B:195:GLN:NE2	1:B:275:TYR:OH	2.46	0.45
1:B:155:ASP:HB3	1:B:157:ALA:H	1.81	0.45
1:B:98:GLN:NE2	1:B:101:GLU:HB2	2.32	0.45
1:A:265:ILE:HD13	1:A:320:VAL:CG1	2.47	0.44
1:A:271:THR:H	1:A:291:GLN:HE21	1.63	0.44
1:B:57:GLN:NE2	1:B:58:GLY:H	2.15	0.44
1:A:57:GLN:HG2	1:A:57:GLN:O	2.18	0.44
1:A:133:VAL:HG23	1:A:138:TYR:HH	1.81	0.44
1:A:195:GLN:NE2	1:A:275:TYR:OH	2.47	0.44
1:A:273:ASN:O	1:A:288:TYR:HA	2.17	0.44
1:A:313:ILE:HD12	1:B:91:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD22	1:A:262:THR:CG2	2.48	0.43
1:B:202:LEU:H	1:B:202:LEU:CD2	2.27	0.43
1:B:166:VAL:HB	1:B:175:ASN:HB2	2.00	0.43
1:B:87:TYR:HA	1:B:88:PRO:HD3	1.89	0.43
1:A:108:TYR:HA	1:A:197:LYS:O	2.19	0.43
1:A:108:TYR:OH	1:A:262:THR:HB	2.19	0.42
1:B:175:ASN:ND2	1:B:306:THR:OG1	2.53	0.42
1:B:107:ILE:O	1:B:198:GLN:HA	2.19	0.42
1:A:327:THR:HG22	1:A:328:VAL:N	2.34	0.42
1:A:323:HIS:O	1:A:323:HIS:CD2	2.71	0.41
1:A:338:GLN:OE1	1:B:314:GLN:HB2	2.20	0.41
1:A:106:PHE:HZ	1:A:198:GLN:HE21	1.69	0.41
1:A:109:GLN:NE2	1:A:197:LYS:HE3	2.36	0.41
1:A:252:TRP:CZ2	1:A:324:LEU:HD22	2.55	0.41
1:A:202:LEU:HB3	1:A:203:PRO:HD2	2.02	0.41
1:B:265:ILE:HG21	1:B:321:ALA:HB2	2.03	0.41
1:A:133:VAL:HG22	1:A:135:LYS:O	2.21	0.41
1:A:111:GLN:NE2	1:A:197:LYS:HE2	2.35	0.41
1:B:115:THR:O	1:B:115:THR:OG1	2.28	0.41
1:B:316:LYS:HA	1:B:316:LYS:HD3	1.81	0.41
1:A:166:VAL:HB	1:A:175:ASN:HB2	2.03	0.41
1:A:67:VAL:O	1:A:85:PRO:HD2	2.21	0.40
1:A:196:LEU:CD2	1:A:262:THR:HG23	2.51	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	276/330 (84%)	262 (95%)	13 (5%)	1 (0%)	34	54
1	B	274/330 (83%)	262 (96%)	10 (4%)	2 (1%)	22	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	550/660 (83%)	524 (95%)	23 (4%)	3 (0%)	29 48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	91	LEU
1	B	92	ASN
1	A	155	ASP

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	228/262 (87%)	208 (91%)	20 (9%)	10 19
1	B	226/262 (86%)	207 (92%)	19 (8%)	11 21
All	All	454/524 (87%)	415 (91%)	39 (9%)	10 20

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	62	SER
1	A	74	THR
1	A	105	GLN
1	A	108	TYR
1	A	117	ARG
1	A	139	VAL
1	A	147	LEU
1	A	179	ASN
1	A	185	GLU
1	A	186	LYS
1	A	205	HIS
1	A	217	THR
1	A	262	THR
1	A	293	VAL

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Mol	Chain	Res	Type
1	A	320	VAL
1	A	326	LEU
1	A	327	THR
1	A	340	LEU
1	A	341	LEU
1	B	62	SER
1	B	63	VAL
1	B	74	THR
1	B	94	THR
1	B	96	PRO
1	B	101	GLU
1	B	107	ILE
1	B	117	ARG
1	B	139	VAL
1	B	147	LEU
1	B	155	ASP
1	B	181	GLN
1	B	202	LEU
1	B	206	LEU
1	B	262	THR
1	B	296	GLN
1	B	299	GLN
1	B	313	ILE
1	B	333	LEU

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

Mol	Chain	Res	Type
1	A	109	GLN
1	A	111	GLN
1	A	145	ASN
1	A	175	ASN
1	A	179	ASN
1	A	195	GLN
1	A	198	GLN
1	A	243	ASN
1	A	273	ASN
1	A	291	GLN
1	A	296	GLN
1	A	304	ASN
1	B	57	GLN
1	B	109	GLN

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Mol	Chain	Res	Type
1	B	111	GLN
1	B	125	ASN
1	B	175	ASN
1	B	181	GLN
1	B	195	GLN
1	B	258	GLN
1	B	273	ASN
1	B	291	GLN
1	B	296	GLN
1	B	323	HIS
1	B	338	GLN

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 monosaccharides 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, 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	276/330 (83%)	0.36	9 (3%) 46 50	26, 34, 39, 46	0
1	B	274/330 (83%)	0.22	6 (2%) 62 65	28, 34, 40, 43	0
All	All	550/660 (83%)	0.29	15 (2%) 54 58	26, 34, 39, 46	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	5.2
1	B	206	LEU	4.1
1	A	218	PHE	3.7
1	A	346	SER	3.2
1	B	56	GLY	2.7
1	A	130	LEU	2.6
1	A	336	ILE	2.6
1	A	299	GLN	2.6
1	B	130	LEU	2.4
1	A	220	GLY	2.4
1	B	185	GLU	2.4
1	A	219	ARG	2.3
1	B	342	VAL	2.1
1	A	221	ALA	2.1
1	B	92	ASN	2.1

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 monosaccharides 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.