



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DKL  
Title : CRYSTAL STRUCTURE OF ESCHERICHIA COLI PHYTASE AT PH 4.5  
(NO LIGAND BOUND)  
Authors : Lim, D.; Golovan, S.; Forsberg, C.W.; Jia, Z.  
Deposited on : 1999-12-08  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

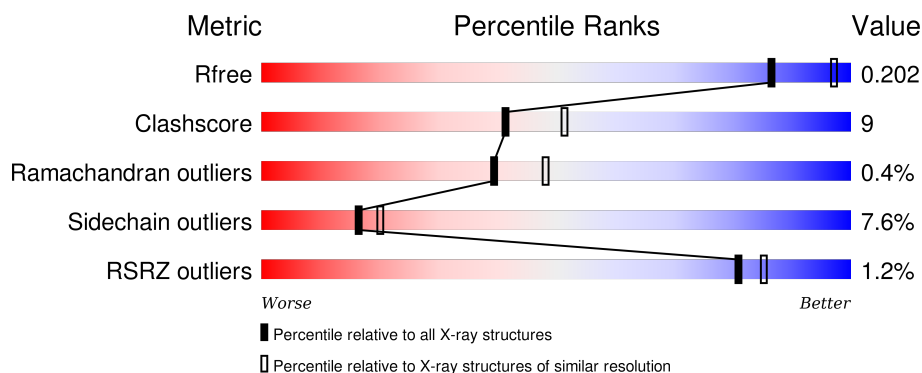
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	410	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>77%</span> <span>18%</span> <span>..</span> </div> </div>
1	B	410	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>80%</span> <span>15%</span> <span>..</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6508 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 PHYTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3090	1942	550	585	13			
1	B	402	Total	C	N	O	S	0	0	0
			3075	1934	548	580	13			

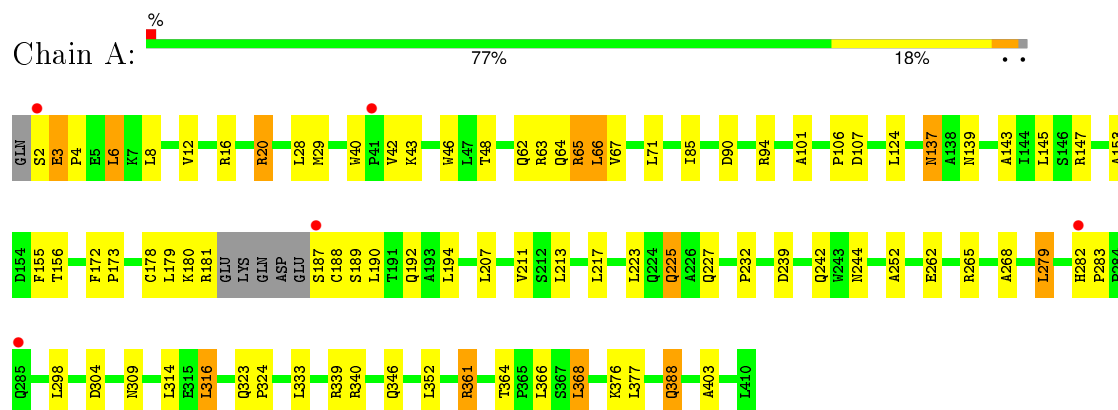
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	181	Total	O	0	0
			181	181		
2	B	162	Total	O	0	0
			162	162		

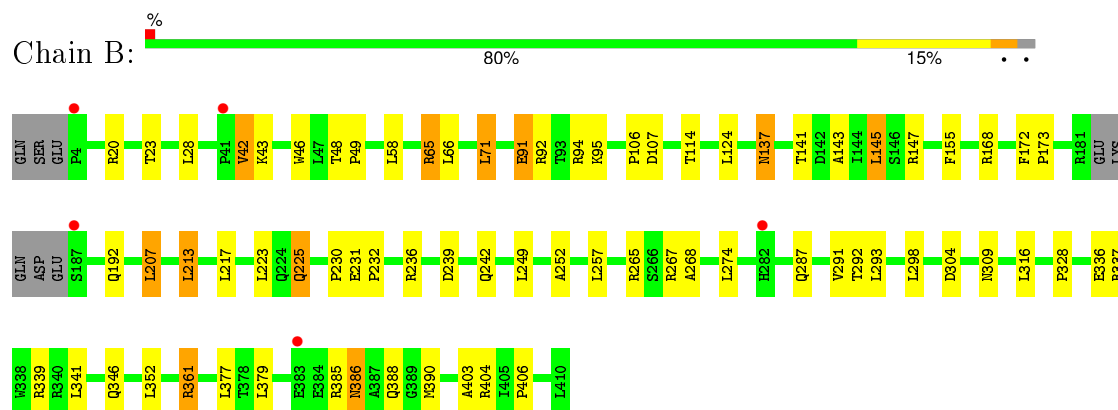
### 3 Residue-property plots

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: PHYTASE



#### • Molecule 1: PHYTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.80Å 72.13Å 82.43Å 90.00° 92.04° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 19.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (25.00-2.30) 94.7 (19.91-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 2.30Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.157 , 0.202 0.156 , 0.202	Depositor DCC
$R_{free}$ test set	3710 reflections (10.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.4	EDS
Estimated twinning fraction	0.017 for k,h,-l 0.015 for -k,-h,-l 0.074 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 37040 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.38	0/3156	0.65	0/4304
1	B	0.38	0/3141	0.64	0/4283
All	All	0.38	0/6297	0.64	0/8587

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 [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	3090	0	3088	62	0
1	B	3075	0	3078	47	0
2	A	181	0	0	8	0
2	B	162	0	0	3	0
All	All	6508	0	6166	105	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 9.

All (105) 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:316:LEU:HD11	1:B:379:LEU:HD23	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:CZ3	1:A:227:GLN:HG3	2.08	0.87
1:A:388:GLN:HE21	1:A:388:GLN:HA	1.53	0.73
1:A:225:GLN:HE21	1:A:232:PRO:HG2	1.54	0.72
1:A:239:ASP:OD2	1:A:242:GLN:HG3	1.91	0.71
1:A:3:GLU:HB3	1:A:4:PRO:HD3	1.72	0.71
1:B:265:ARG:HD2	1:B:403:ALA:O	1.90	0.70
1:A:189:SER:HB3	1:A:192:GLN:HB2	1.74	0.69
1:A:244:ASN:HD22	1:A:324:PRO:HB3	1.57	0.68
1:B:339:ARG:HG3	1:B:346:GLN:NE2	2.08	0.68
1:B:46:TRP:CD1	1:B:91:GLU:HG2	2.31	0.66
1:A:2:SER:CB	1:B:361:ARG:HE	2.10	0.64
1:A:265:ARG:HD2	1:A:403:ALA:O	1.96	0.64
1:A:156:THR:HG23	2:A:685:HOH:O	1.97	0.63
1:A:172:PHE:N	1:A:173:PRO:HD2	2.13	0.62
1:B:20:ARG:HD3	1:B:92:ARG:HD3	1.81	0.62
1:A:388:GLN:HE22	1:B:168:ARG:NH1	1.97	0.61
1:B:386:ASN:HD22	1:B:386:ASN:C	2.03	0.61
1:A:20:ARG:HD2	2:A:720:HOH:O	2.00	0.61
1:A:155:PHE:HZ	1:A:252:ALA:HB1	1.66	0.61
1:B:225:GLN:HE21	1:B:232:PRO:HG2	1.64	0.61
1:B:137:ASN:N	1:B:137:ASN:HD22	2.00	0.60
1:A:16:ARG:HD2	1:A:304:ASP:HB3	1.85	0.58
1:A:181:ARG:HH12	1:A:187:SER:HB3	1.67	0.58
1:A:225:GLN:NE2	1:A:232:PRO:HG2	2.19	0.57
1:A:244:ASN:ND2	1:A:324:PRO:HB3	2.19	0.57
1:A:339:ARG:HG3	1:A:346:GLN:NE2	2.20	0.57
1:A:213:LEU:HD13	1:A:217:LEU:HD22	1.85	0.57
1:A:178:CYS:O	1:A:181:ARG:HB2	2.06	0.56
1:B:172:PHE:N	1:B:173:PRO:HD2	2.21	0.55
1:B:65:ARG:HD2	1:B:65:ARG:C	2.26	0.55
1:A:106:PRO:O	1:A:107:ASP:HB2	2.06	0.55
1:A:314:LEU:HB2	1:A:316:LEU:HD22	1.89	0.54
1:A:65:ARG:HD2	1:A:65:ARG:C	2.27	0.54
1:A:153:ALA:O	1:A:156:THR:HG22	2.07	0.54
1:A:48:THR:OG1	1:A:227:GLN:NE2	2.40	0.54
1:B:42:VAL:HG11	1:B:48:THR:HG22	1.90	0.54
1:A:137:ASN:HD22	1:A:137:ASN:N	2.06	0.54
1:A:6:LEU:HD12	1:A:340:ARG:HA	1.90	0.54
1:B:106:PRO:O	1:B:107:ASP:HB2	2.08	0.53
1:B:143:ALA:O	1:B:147:ARG:HG3	2.08	0.53
1:A:339:ARG:HG3	1:A:346:GLN:HE22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASN:HD21	1:B:390:MET:H	1.57	0.53
1:A:388:GLN:HE22	1:B:168:ARG:HH12	1.57	0.52
1:A:225:GLN:HE21	1:A:225:GLN:HA	1.75	0.51
1:A:156:THR:HG21	2:A:663:HOH:O	2.10	0.51
1:B:386:ASN:ND2	1:B:390:MET:H	2.07	0.51
1:B:213:LEU:HD22	1:B:217:LEU:HD22	1.93	0.51
1:A:90:ASP:O	1:A:94:ARG:HG3	2.10	0.51
1:B:94:ARG:HD3	1:B:114:THR:HG21	1.93	0.50
1:B:239:ASP:OD2	1:B:242:GLN:HG3	2.11	0.50
1:A:282:HIS:HB3	2:A:819:HOH:O	2.12	0.50
1:B:388:GLN:OE1	1:B:388:GLN:N	2.41	0.50
1:B:207:LEU:HD22	1:B:257:LEU:HD21	1.93	0.50
1:B:291:VAL:HG12	1:B:293:LEU:CD1	2.43	0.49
1:A:181:ARG:NH2	1:A:188:CYS:HB2	2.28	0.49
1:B:385:ARG:HA	1:B:390:MET:O	2.13	0.49
1:B:141:THR:O	1:B:145:LEU:HD22	2.13	0.49
1:A:155:PHE:CZ	1:A:252:ALA:HB1	2.45	0.48
1:B:316:LEU:CD1	1:B:379:LEU:HD23	2.34	0.48
1:B:337:ARG:HD2	1:B:346:GLN:OE1	2.13	0.47
1:A:63:ARG:O	1:A:67:VAL:HG23	2.15	0.47
1:B:267:ARG:HG2	1:B:267:ARG:HH11	1.78	0.47
2:A:840:HOH:O	1:B:230:PRO:HA	2.14	0.47
1:B:192:GLN:HG3	2:B:754:HOH:O	2.14	0.47
1:A:282:HIS:CE1	1:A:283:PRO:HG2	2.50	0.46
1:B:137:ASN:H	1:B:137:ASN:HD22	1.63	0.46
1:A:207:LEU:HD13	1:A:211:VAL:HG11	1.96	0.46
1:B:225:GLN:HA	1:B:225:GLN:HE21	1.81	0.46
1:A:40:TRP:CZ3	1:A:227:GLN:CG	2.93	0.46
1:A:190:LEU:HD12	1:A:194:LEU:HD23	1.97	0.46
1:A:213:LEU:CD1	1:A:217:LEU:HD22	2.46	0.46
1:A:225:GLN:NE2	1:A:361:ARG:NH1	2.65	0.45
1:B:42:VAL:O	1:B:43:LYS:C	2.56	0.44
1:B:49:PRO:HG2	2:B:579:HOH:O	2.18	0.44
1:A:42:VAL:O	1:A:43:LYS:C	2.56	0.44
1:A:85:ILE:CD1	1:A:101:ALA:HB2	2.48	0.44
1:A:2:SER:OG	1:A:3:GLU:N	2.51	0.43
1:B:339:ARG:NH1	1:B:341:LEU:HD23	2.33	0.43
1:B:268:ALA:HB2	1:B:309:ASN:HB3	2.00	0.43
1:A:239:ASP:HB3	2:A:610:HOH:O	2.18	0.43
1:B:386:ASN:C	1:B:386:ASN:ND2	2.68	0.43
1:A:340:ARG:NH1	2:A:832:HOH:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:HA	1:B:95:LYS:HD3	1.84	0.43
1:A:64:GLN:NE2	1:A:368:LEU:H	2.17	0.43
1:B:292:THR:O	1:B:293:LEU:HD12	2.18	0.43
1:B:339:ARG:HG3	1:B:346:GLN:HE22	1.83	0.43
1:B:406:PRO:HG2	2:B:721:HOH:O	2.18	0.43
1:A:29:MET:HE1	2:A:773:HOH:O	2.18	0.42
1:B:231:GLU:HG3	1:B:231:GLU:O	2.19	0.42
1:A:143:ALA:O	1:A:147:ARG:HG3	2.19	0.42
1:B:155:PHE:CZ	1:B:252:ALA:HB1	2.53	0.42
1:A:62:GLN:O	1:A:66:LEU:HB2	2.18	0.42
1:A:2:SER:CB	1:B:361:ARG:NE	2.81	0.41
1:A:323:GLN:HA	1:A:324:PRO:HD2	1.94	0.41
1:A:282:HIS:ND1	1:A:283:PRO:O	2.51	0.41
1:A:268:ALA:HB2	1:A:309:ASN:HB3	2.02	0.41
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.88	0.41
1:A:376:LYS:HA	1:A:376:LYS:HD3	1.86	0.41
1:A:12:VAL:CG2	1:A:279:LEU:HD13	2.50	0.41
1:A:64:GLN:HE22	1:A:368:LEU:H	1.69	0.41
1:A:43:LYS:HD2	1:A:46:TRP:CH2	2.56	0.41
1:B:65:ARG:NH1	1:B:336:GLU:OE2	2.48	0.40
1:A:368:LEU:HD12	1:A:368:LEU:HA	1.91	0.40
1:A:179:LEU:C	1:A:181:ARG:H	2.24	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	400/410 (98%)	393 (98%)	5 (1%)	2 (0%)	34	41
1	B	398/410 (97%)	387 (97%)	10 (2%)	1 (0%)	46	57
All	All	798/820 (97%)	780 (98%)	15 (2%)	3 (0%)	39	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	B	42	VAL
1	A	180	LYS

### 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	338/344 (98%)	313 (93%)	25 (7%)	17	21
1	B	336/344 (98%)	310 (92%)	26 (8%)	16	20
All	All	674/688 (98%)	623 (92%)	51 (8%)	16	20

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	8	LEU
1	A	20	ARG
1	A	28	LEU
1	A	65	ARG
1	A	66	LEU
1	A	71	LEU
1	A	124	LEU
1	A	137	ASN
1	A	139	ASN
1	A	145	LEU
1	A	223	LEU
1	A	225	GLN
1	A	262	GLU
1	A	279	LEU
1	A	298	LEU
1	A	316	LEU
1	A	333	LEU
1	A	352	LEU
1	A	361	ARG

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Mol	Chain	Res	Type
1	A	364	THR
1	A	366	LEU
1	A	368	LEU
1	A	377	LEU
1	A	388	GLN
1	B	23	THR
1	B	28	LEU
1	B	58	LEU
1	B	65	ARG
1	B	66	LEU
1	B	71	LEU
1	B	91	GLU
1	B	124	LEU
1	B	137	ASN
1	B	145	LEU
1	B	207	LEU
1	B	213	LEU
1	B	223	LEU
1	B	225	GLN
1	B	236	ARG
1	B	249	LEU
1	B	274	LEU
1	B	287	GLN
1	B	298	LEU
1	B	304	ASP
1	B	328	PRO
1	B	352	LEU
1	B	361	ARG
1	B	377	LEU
1	B	386	ASN
1	B	404	ARG

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	27	GLN
1	A	30	GLN
1	A	64	GLN
1	A	134	GLN
1	A	137	ASN
1	A	139	ASN
1	A	158	HIS

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	225	GLN
1	A	227	GLN
1	A	244	ASN
1	A	287	GLN
1	A	358	GLN
1	A	369	ASN
1	A	388	GLN
1	B	64	GLN
1	B	134	GLN
1	B	137	ASN
1	B	139	ASN
1	B	158	HIS
1	B	225	GLN
1	B	244	ASN
1	B	285	GLN
1	B	287	GLN
1	B	386	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/410 (98%)	-0.52	5 (1%) 81 85	12, 26, 53, 70	0
1	B	402/410 (98%)	-0.53	5 (1%) 81 85	12, 28, 55, 73	0
All	All	806/820 (98%)	-0.52	10 (1%) 81 85	12, 27, 55, 73	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	5.4
1	A	41	PRO	3.1
1	B	4	PRO	3.0
1	B	41	PRO	2.9
1	A	187	SER	2.8
1	B	187	SER	2.5
1	B	282	HIS	2.5
1	B	383	GLU	2.3
1	A	285	GLN	2.2
1	A	282	HIS	2.1

### 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.