



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2017 – 08:57 PM EDT

PDB ID : 5KHS  
Title : Crystal structures of the Burkholderia multivorans hopanoid transporter HpnN  
Authors : Su, C.-C.; Yu, E.W.  
Deposited on : 2016-06-15  
Resolution : 3.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029077

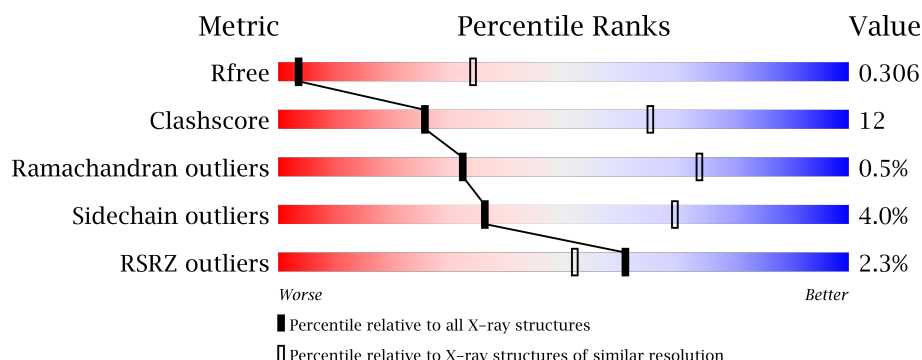
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.76 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))
$R_{free}$	100719	1423 (4.02-3.50)
Clashscore	112137	1087 (4.00-3.52)
Ramachandran outliers	110173	1047 (4.00-3.52)
Sidechain outliers	110143	1041 (4.00-3.52)
RSRZ outliers	101464	1011 (4.00-3.52)

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	883	<div> <div>2%</div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
1	B	883	<div> <div>2%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12679 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 Putative RND superfamily efflux pump membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	853	Total	C	N	O	S	0	0	0
			6342	4094	1087	1143	18			
1	A	852	Total	C	N	O	S	0	0	0
			6337	4091	1086	1142	18			

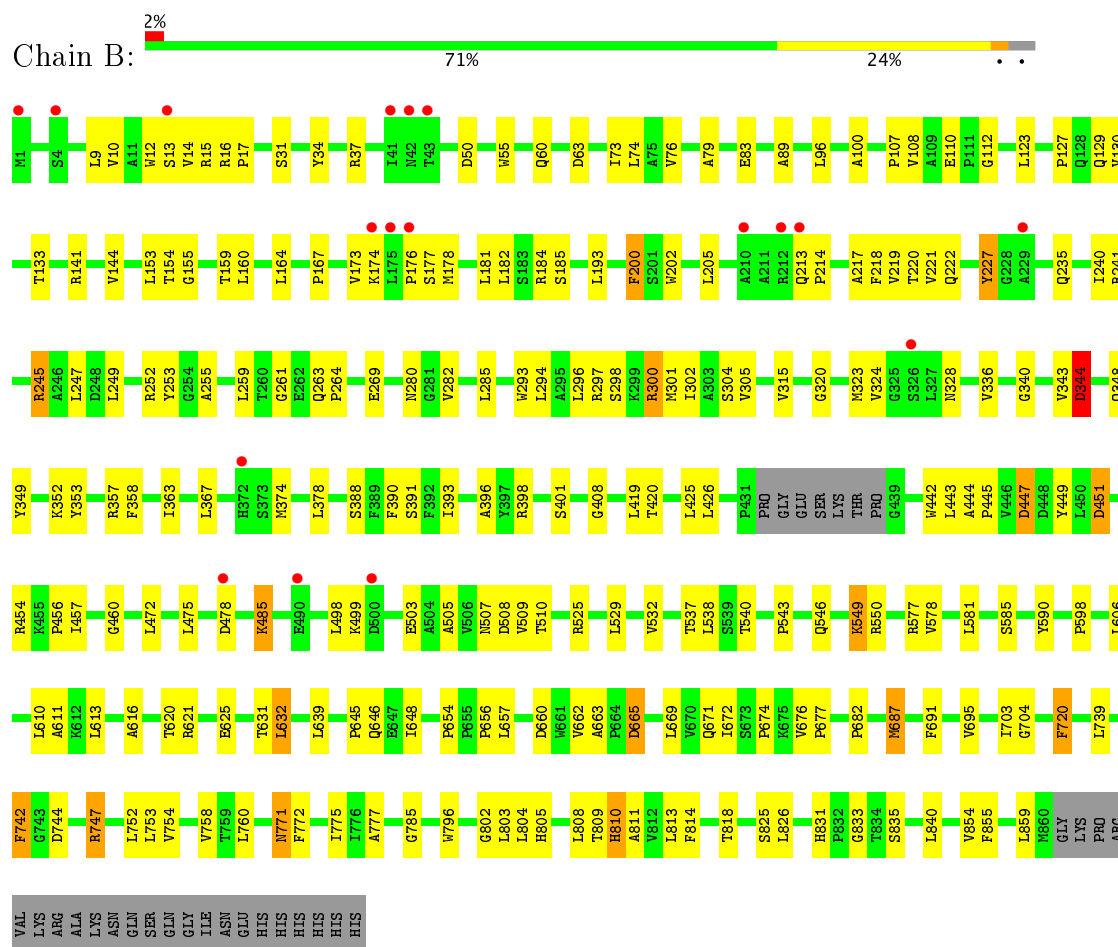
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	360	GLY	ASP	engineered mutation	UNP A0A0H3KP92
B	362	ALA	ARG	engineered mutation	UNP A0A0H3KP92
B	365	ALA	HIS	engineered mutation	UNP A0A0H3KP92
B	878	HIS	-	expression tag	UNP A0A0H3KP92
B	879	HIS	-	expression tag	UNP A0A0H3KP92
B	880	HIS	-	expression tag	UNP A0A0H3KP92
B	881	HIS	-	expression tag	UNP A0A0H3KP92
B	882	HIS	-	expression tag	UNP A0A0H3KP92
B	883	HIS	-	expression tag	UNP A0A0H3KP92
A	360	GLY	ASP	engineered mutation	UNP A0A0H3KP92
A	362	ALA	ARG	engineered mutation	UNP A0A0H3KP92
A	365	ALA	HIS	engineered mutation	UNP A0A0H3KP92
A	878	HIS	-	expression tag	UNP A0A0H3KP92
A	879	HIS	-	expression tag	UNP A0A0H3KP92
A	880	HIS	-	expression tag	UNP A0A0H3KP92
A	881	HIS	-	expression tag	UNP A0A0H3KP92
A	882	HIS	-	expression tag	UNP A0A0H3KP92
A	883	HIS	-	expression tag	UNP A0A0H3KP92

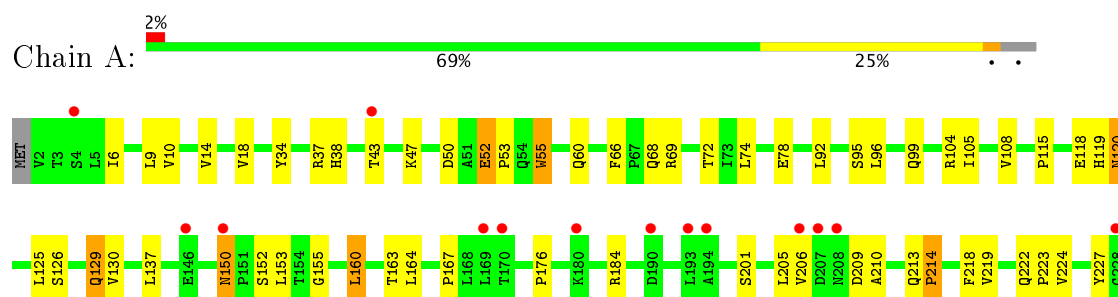
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Putative RND superfamily efflux pump membrane protein



- Molecule 1: Putative RND superfamily efflux pump membrane protein



T821	A692	F541	F440	L229	L230	K231	A232	G233	R241	R245	A246	L247	D248	L249	R252	Y253	G254	A255	R258	Q263	P264	L265	A266	D267	D268	E269	G276	N280	T284	V288	L292	W293	L294	R300	N301	I302	T308	G312	N328	S331	V336
A622	V695	P542	P441	L231	L232	A233	G234	R242	R246	A247	L248	D249	L250	R251	Y254	G255	A256	R259	Q264	P265	L266	A267	D268	E269	G277	N281	T285	V289	L293	W294	L295	R301	N302	I303	T309	G313	N329	S332	V337		
S825	E689	P543	R442	L233	L234	A234	G235	R243	R247	A248	L249	D250	L251	R252	Y255	G256	A257	R260	Q265	P266	L267	A268	D269	E270	G278	N282	T286	V290	L294	W295	L296	R302	N303	I304	T310	G314	N330	S333	V338		
S829	I703	L560	D447	L235	L236	A235	G236	R244	D448	A249	L250	D251	L252	R253	Y256	G257	A258	R261	Q266	P267	L268	A269	D270	E271	G279	N283	T287	V291	L295	W296	L297	R303	N304	I305	T311	G315	N331	S334	V339		
H830	G704	T565	Y449	L237	L238	A236	G237	R245	Y449	A250	L251	D252	L253	R254	Y257	G258	A259	R262	Q267	P268	L269	A270	D271	E272	G280	N284	T288	V292	L296	W297	L298	R304	N305	I306	T312	G316	N332	S335	V340		
H831	P706	L581	D451	L239	L240	A237	G238	R246	D451	A251	L252	D253	L254	R255	Y258	G259	A260	R263	Q268	P269	L270	A271	D272	E273	G281	N285	T289	V293	L297	W298	L299	R305	N306	I307	T313	G317	N333	S336	V341		
L840	I707	L582	R454	L241	L242	A238	G239	R247	R454	A252	L253	D254	L255	R256	Y259	G260	A261	R264	Q269	P270	L271	A272	D273	E274	G282	N286	T290	V294	L298	W299	L300	R306	N307	I308	T314	G318	N334	S337	V342		
Q856	S712	L583	K455	L243	L244	A239	G240	R248	K455	A253	L254	D255	L256	R257	Y260	G261	A262	R265	Q270	P271	L272	A273	D274	E275	G283	N287	T291	V295	L299	W300	L301	R307	N308	I309	T315	G319	N335	S338	V343		
P857	L716	L584	P456	L245	L246	A240	G241	R249	P456	A254	L255	D256	L257	R258	Y261	G262	A263	R266	Q271	P272	L273	A274	D275	E276	G284	N288	T292	V296	L300	W301	L302	R308	N309	I310	T316	G320	N336	S339	V344		
V858	I717	L585	I457	L247	L248	A241	G242	R250	I457	A255	L256	D257	L258	R259	Y262	G263	A264	R267	Q272	P273	L274	A275	D276	E277	G285	N289	T293	V297	L301	W302	L303	R309	N310	I311	T317	G321	N337	S340	V345		
L859	S718	L586	L458	L249	L250	A242	G243	R251	L458	A256	L257	D258	L259	R260	Y263	G264	A265	R268	Q273	P274	L275	A276	D277	E278	G286	N290	T294	V298	L302	W303	L304	R310	N311	I312	T318	G322	N338	S341	V346		
GLY	I719	L587	L460	L251	L252	A243	G244	R252	L460	A257	L258	D259	L260	R261	Y264	G265	A266	R269	Q274	P275	L276	A277	D278	E279	G287	N291	T295	V299	L303	W304	L305	R311	N312	I313	T319	G323	N339	S342	V347		
LYS	A719	L588	L461	L253	L254	A244	G245	R253	L461	A258	L259	D260	L261	R262	Y265	G266	A267	R270	Q275	P276	L277	A278	D279	E280	G288	N292	T296	V300	L304	W305	L306	R312	N313	I314	T320	G324	N340	S343	V348		
PRO	F720	L589	L462	L255	L256	A245	G246	R254	L462	A259	L260	D261	L262	R263	Y266	G267	A268	R271	Q276	P277	L278	A279	D280	E281	G289	N293	T297	V301	L305	W306	L307	R313	N314	I315	T321	G325	N341	S344	V349		
ARG	L721	L590	L463	L257	L258	A246	G247	R255	L463	A260	L261	D262	L263	R264	Y267	G268	A269	R272	Q277	P278	L279	A280	D281	E282	G290	N294	T298	V302	L306	W307	L308	R314	N315	I316	T322	G326	N342	S345	V350		
VAL	H722	L591	L464	L259	L260	A247	G248	R256	L464	A261	L262	D263	L264	R265	Y268	G269	A270	R273	Q278	P279	L280	A281	D282	E283	G291	N295	T299	V303	L307	W308	L309	R315	N316	I317	T323	G327	N343	S346	V351		
LYS	I728	L592	L465	L261	L262	A248	G249	R257	L465	A262	L263	D264	L265	R266	Y269	G270	A271	R274	Q279	P280	L281	A282	D283	E284	G292	N296	T300	V304	L308	W309	L310	R316	N317	I318	T324	G328	N344	S347	V352		
ASN	L734	L593	L466	L263	L264	A249	G250	R258	L466	A263	L264	D265	L266	R267	Y270	G271	A272	R275	Q280	P281	L282	A283	D284	E285	G293	N297	T301	V305	L309	W310	L311	R317	N318	I319	T325	G329	N345	S348	V353		
GLN	T738	L594	L467	L265	L266	A250	G251	R259	L467	A264	L265	D266	L267	R268	Y271	G272	A273	R276	Q281	P282	L283	A284	D285	E286	G294	N298	T302	V306	L310	W311	L312	R318	N319	I320	T326	G330	N346	S349	V354		
GLY	L739	L595	L468	L267	L268	A251	G252	R260	L468	A265	L266	D267	L268	R269	Y272	G273	A274	R277	Q282	P283	L284	A285	D286	E287	G295	N299	T303	V307	L311	W312	L313	R319	N320	I321	T327	G331	N347	S350	V355		
ILE	F742	L596	L469	L269	L270	A252	G253	R261	L469	A266	L267	D268	L269	R270	Y273	G274	A275	R278	Q283	P284	L285	A286	D287	E288	G296	N300	T304	V308	L312	W313	L314	R320	N321	I322	T328	G332	N348	S351	V356		
ASN	R747	L597	L470	L271	L272	A253	G254	R262	L470	A267	L268	D269	L270	R271	Y274	G275	A276	R279	Q284	P285	L286	A287	D288	E289	G297	N301	T305	V309	L313	W314	L315	R321	N322	I323	T329	G333	N349	S352	V357		
GLU	T738	L598	L471	L273	L274	A254	G255	R263	L471	A268	L269	D270	L271	R272	Y275	G276	A277	R280	Q285	P286	L287	A288	D289	E290	G298	N302	T306	V310	L314	W315	L316	R322	N323	I324	T330	G334	N350	S353	V358		
HIS	L734	L599	L472	L275	L276	A255	G256	R264	L472	A269	L270	D271	L272	R273	Y276	G277	A278	R281	Q286	P287	L288	A289	D290	E291	G299	N303	T307	V311	L315	W316	L317	R323	N324	I325	T331	G335	N351	S354	V359		
HIS	T738	L600	L473	L277	L278	A256	G257	R265	L473	A270	L271	D272	L273	R274	Y277	G278	A279	R282	Q287	P288	L289	A290	D291	E292	G300	N304	T308	V312	L316	W317	L318	R324	N325	I326	T332	G336	N352	S355	V360		
HIS	L734	L601	L474	L279	L280	A257	G258	R266	L474	A271	L272	D273	L274	R275	Y278	G279	A280	R283	Q288	P289	L290	A291	D292	E293	G301	N305	T309	V313	L317	W318	L319	R325	N326	I327	T333	G337	N353	S356	V361		
HIS	T738	L602	L475	L281	L282	A258	G259	R267	L475	A272	L273	D274	L275	R276	Y279	G280	A281	R284	Q289	P290	L291	A292	D293	E294	G302	N306	T310	V314	L318	W319	L320	R326	N327	I328	T334	G338	N354	S357	V362		
HIS	L734	L603	L476	L283	L284	A259	G260	R268	L476	A273	L274	D275	L276	R277	Y280	G281	A282	R285	Q290	P291	L292	A293	D294	E295	G303	N307	T311	V315	L319	W320	L321	R327	N328	I329	T335	G339	N355	S358	V363		
HIS	T738	L604	L477	L285	L286	A260	G261	R269	L477	A274	L275	D276	L277	R278	Y281	G282	A283	R286	Q291	P292	L293	A294	D295	E296	G304	N308	T312	V316	L320	W321	L322	R328	N329	I330	T336	G340	N356	S359	V364		
HIS	L734	L605	L478	L287	L288	A261	G262	R270	L478	A275	L276	D277	L278	R279	Y282	G283	A284	R287	Q292	P293	L294	A295	D296	E297	G305	N309	T313	V317	L321	W322	L323	R329	N330	I331	T337	G341	N357	S360	V365		
HIS	T738	L606	L479	L289	L290	A262	G263	R271	L479	A276	L277	D278	L279	R280	Y283	G284	A285	R288	Q293	P294	L295	A296	D297	E298	G306	N310	T314	V318	L322	W323	L324	R330	N331	I332	T338	G342	N358	S361	V366		
HIS	L734	L607	L480	L291	L292	A263	G264	R272	L480	A277	L278	D279	L280	R281	Y284	G285	A286	R289	Q294	P295	L296	A297	D298	E299	G307	N311	T315	V319	L323	W324	L325	R331	N332	I333	T339	G343	N359	S362	V367		
HIS	T738	L608	L481	L293	L294	A264	G265	R273	L481	A278	L279	D280	L281	R282	Y285	G286	A287	R290	Q295	P296	L297	A298	D299	E300	G308	N312	T316	V320	L324	W325	L326	R332	N333	I334	T340	G344	N360	S363	V368		
HIS	L734	L609	L482	L295	L296	A265	G266	R274	L482	A279	L280	D281	L282	R283	Y286	G287	A288	R291	Q296	P297	L298	A299	D300	E301	G309	N313	T317	V321	L325	W326	L327	R333	N334	I335	T341	G345	N361	S364	V369		
HIS	T738	L610	L483	L297	L298	A266	G267	R275	L483	A280	L281	D282	L283	R284	Y287	G288	A289	R292	Q297	P298	L299	A300	D301	E302	G310	N314	T318	V322	L326	W327	L328	R334	N335	I336	T342	G346	N362	S365	V370		
HIS	L734	L611	L484	L299	L300	A267	G268	R276	L484	A281	L282	D283	L284	R285	Y288	G289	A290	R293	Q298	P299	L300	A301	D302	E303	G311	N315	T319	V323	L327	W328	L329	R335	N336	I337	T343	G347	N363	S366	V371		
HIS	T738	L612	L485	L301	L302	A268	G269	R277	L485	A282	L283	D284	L285	R286	Y289	G290	A291	R294	Q299	P300	L301	A302	D303	E304	G312	N316	T320	V324	L328	W329	L330	R336	N337	I338	T344	G348	N364	S367	V372		
HIS	L734	L613	L486	L303	L304	A269	G270	R278	L486	A283	L284	D285	L286	R287	Y290	G291	A292	R295	Q300	P301	L302	A303	D304	E305	G313	N317	T321	V3													

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.16Å 143.37Å 112.66Å 90.00° 114.10° 90.00°	Depositor
Resolution (Å)	83.57 – 3.76 83.57 – 3.76	Depositor EDS
% Data completeness (in resolution range)	83.0 (83.57-3.76) 82.8 (83.57-3.76)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 3.78Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.263 , 0.307 0.260 , 0.306	Depositor DCC
$R_{free}$ test set	1391 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.9	Xtriage
Anisotropy	1.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , -7.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.387 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	12679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.25	0/6472	0.45	0/8852
1	B	0.26	1/6477 (0.0%)	0.44	1/8859 (0.0%)
All	All	0.25	1/12949 (0.0%)	0.45	1/17711 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	LYS	CE-NZ	-5.12	1.36	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ASP	CB-CG-OD2	6.05	123.75	118.30

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	6337	0	6566	164	1
1	B	6342	0	6571	151	1
All	All	12679	0	13137	308	1

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 12.

The worst 5 of 308 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:269:GLU:HG2	1:A:485:LYS:HE3	1.48	0.95
1:B:127:PRO:HA	1:B:549:LYS:HE2	1.60	0.82
1:A:751:PRO:HG3	1:A:859:LEU:HD13	1.65	0.78
1:A:395:THR:HG21	1:A:719:ALA:HA	1.65	0.76
1:A:751:PRO:HB2	1:A:789:LYS:HE3	1.67	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:TYR:OH	1:A:451:ASP:OD2[1_554]	2.16	0.04

## 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	848/883 (96%)	787 (93%)	58 (7%)	3 (0%)	38	77
1	B	849/883 (96%)	791 (93%)	52 (6%)	6 (1%)	25	68
All	All	1697/1766 (96%)	1578 (93%)	110 (6%)	9 (0%)	32	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	ARG
1	B	811	ALA
1	B	859	LEU
1	B	771	ASN
1	A	214	PRO



### 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	662/690 (96%)	635 (96%)	27 (4%)	35	69
1	B	662/690 (96%)	636 (96%)	26 (4%)	37	70
All	All	1324/1380 (96%)	1271 (96%)	53 (4%)	36	69

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	742	PHE
1	A	120	ASN
1	A	657	LEU
1	B	747	ARG
1	A	52	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	GLN
1	A	150	ASN
1	A	480	ASN
1	A	683	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, 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	852/883 (96%)	-0.04	21 (2%) 58 47	6, 46, 81, 112	0
1	B	853/883 (96%)	-0.01	18 (2%) 64 55	6, 44, 82, 112	0
All	All	1705/1766 (96%)	-0.02	39 (2%) 61 52	6, 45, 82, 112	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ASP	5.8
1	A	170	THR	4.8
1	A	190	ASP	4.4
1	B	174	LYS	3.6
1	A	229	ALA	3.5

### 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.