



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:19 am BST

PDB ID : 3OPO
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli
Authors : Su, C.-C.
Deposited on : 2010-09-01
Resolution : 3.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

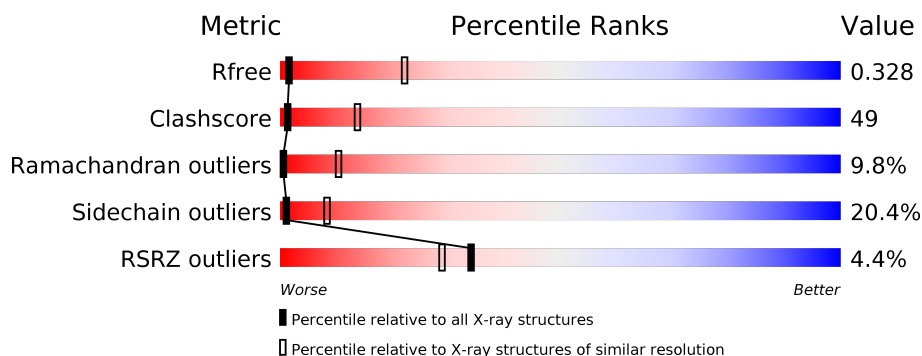
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)

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 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 $\leq 5\%$. 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	413	<div> <div>2%</div> <div> <div></div> <div>22%</div> <div>36%</div> <div>12%</div> <div>•</div> <div>28%</div> </div> </div>
1	B	413	<div> <div>4%</div> <div> <div></div> <div>22%</div> <div>36%</div> <div>12%</div> <div>•</div> <div>28%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AG	A	414	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4543 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 Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2267	1444	391	427	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

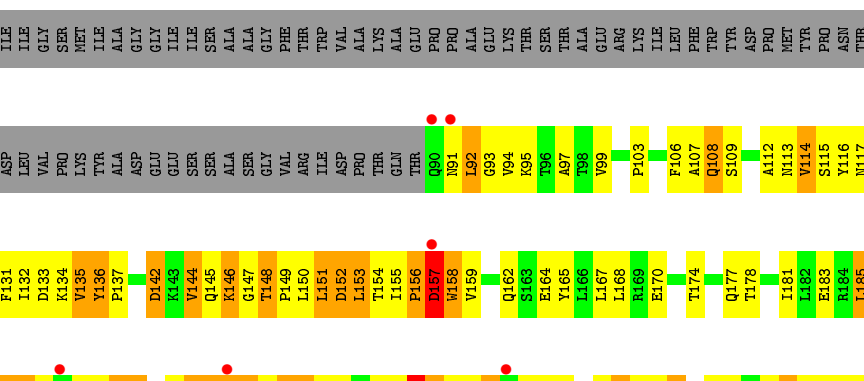
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	EXPRESSION TAG	UNP P77239
A	409	HIS	-	EXPRESSION TAG	UNP P77239
A	410	HIS	-	EXPRESSION TAG	UNP P77239
A	411	HIS	-	EXPRESSION TAG	UNP P77239
A	412	HIS	-	EXPRESSION TAG	UNP P77239
A	413	HIS	-	EXPRESSION TAG	UNP P77239
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ag	0	0
			1	1		
2	A	1	Total	Ag	0	0
			1	1		

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 

- Chain B:

Amino Acid	Count	Percentage
Met	1	4%
Lys	1	
Ile	1	
Leu	1	
Ile	1	
Gly	1	
Met	1	
Ser	1	
Ile	1	
Ala	1	
Gly	1	
Ile	1	
Ser	1	
Ala	1	
Gly	1	
Phe	1	
Thr	1	
Val	1	
Lys	1	
Ala	1	
Leu	1	
Pro	1	
Thr	1	
Ala	1	
Gly	1	
Lys	1	
Thr	1	
Ser	1	
Thr	1	
Ala	1	
Gly	1	
Arg	1	
Lys	1	
Ile	1	
Leu	1	
Phe	1	
Trp	1	
Tyr	1	
Asp	1	
Pro	1	
Met	1	
Tyr	1	
Pro	1	
Asn	1	
Thr	1	
Arg	1	
Phe	1	
Asp	1	
Lys	1	
Pro	1	
Gly	1	
Lys	1	

GLU	I195	L257	I327	ARG	R196	V258	A331	ARG	R197	V259	L260	I332	GLU	D334	F264	T267	V268	P269	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	A290	T291	R292	T293	L294	R297	L298	M302	E305	A306	L307	K308	P309	M312	A313	W314	L317	M318	T319	A320	S321	E322	P323	M324	I325	L326
ARG	I196	K259	A332	ARG	R198	A261	I333	SER	L198	D260	A261	I333	GLU	D334	F264	T267	V268	P269	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	A290	T291	R292	T293	L294	R297	L298	M302	E305	A306	L307	K308	P309	M312	A313	W314	L317	M318	T319	A320	S321	E322	P323	M324	I325	L326
THR	Q202	A261	T335	SER	T201	F264	D334	GLU	A200	T201	F264	D334	GLU	D334	F264	T267	V268	P269	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	A290	T291	R292	T293	L294	R297	L298	M302	E305	A306	L307	K308	P309	M312	A313	W314	L317	M318	T319	A320	S321	E322	P323	M324	I325	L326
ALA	R203	T267	G336	ALA	Q202	F264	D334	ALA	R203	T267	V268	P269	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	A290	T291	R292	T293	L294	R297	L298	M302	E305	A306	L307	K308	P309	M312	A313	W314	L317	M318	T319	A320	S321	E322	P323	M324	I325	L326						
HIS	R205	T269	E338	HIS	Q203	T267	E338	ALA	R206	T269	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	A290	T291	R292	T293	L294	R297	L298	M302	E305	A306	L307	K308	P309	M312	A313	W314	L317	M318	T319	A320	S321	E322	P323	M324	I325	L326								
HIS	T206	R270	Q339	HIS	Q206	A270	Q339	HIS	T206	R270	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	A290	T291	R292	T293	L294	R297	L298	M302	E305	A306	L307	K308	P309	M312	A313	W314	L317	M318	T319	A320	S321	E322	P323	M324	I325	L326								
HIS	R207	T271	V341	HIS	F208	R271	V341	HIS	R207	T271	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	A290	T291	R292	T293	L294	R297	L298	M302	E305	A306	L307	K308	P309	M312	A313	W314	L317	M318	T319	A320	S321	E322	P323	M324	I325	L326								
HIS	T209	L210	T342	HIS	F208	T272	T342	HIS	T209	L210	T342	T343	V344	D345	A346	D347	G348	R349	F350	V351	P352	K353	R354	V355	A356	V357	F358	Q362	T365	A366	L367	R368	L371	A372	V377	V378	S379	S380	G381	L382	F383	L384	I385	ASP	SER	GLU	ALA	ASN	ILE	SER	GLY	ALA	LEU								
HIS	T211	R212	T343	HIS	T209	L210	T343	HIS	T211	R212	T343	T343	V344	D345	A346	D347	G348	R349	F350	V351	P352	K353	R354	V355	A356	V357	F358	Q362	T365	A366	L367	R368	L371	A372	V377	V378	S379	S380	G381	L382	F383	L384	I385	ASP	SER	GLU	ALA	ASN	ILE	SER	GLY	ALA	LEU								
HIS	P213	I214	D215	HIS	T211	R212	T343	HIS	P213	I214	D215	T343	V344	D345	A346	D347	G348	R349	F350	V351	P352	K353	R354	V355	A356	V357	F358	Q362	T365	A366	L367	R368	L371	A372	V377	V378	S379	S380	G381	L382	F383	L384	I385	ASP	SER	GLU	ALA	ASN	ILE	SER	GLY	ALA	LEU								
HIS	I218	T219	A220	HIS	T218	T219	A220	HIS	I218	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256															
HIS	T219	A220	F221	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	A220	F221	D222	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T220	R221	L223	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T221	D222	L223	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T222	L223	R224	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T223	R224	A225	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T224	A225	G226	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T225	G226	M227	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T226	M227	R228	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T227	R228	I229	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T228	I229	A230	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T229	A230	R231	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T230	R231	D232	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T231	D232	L223	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T232	L223	R224	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T233	R224	A225	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T234	A225	G226	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T235	G226	M227	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T236	M227	R228	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T237	R228	I229	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227	R228	I229	A230	R231	D232	R233	V234	V235	A236	K237	I238	Q239	G240	M241	D242	P243	V244	W245	V246	A249	I250	P251	E252	S253	I254	A255	W256																
HIS	T238	I229	A230	HIS	T218	T219	A220	HIS	T219	A220	T220	R221	D222	L223	R224	A225	G226	M227</																																											

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.80Å 114.68Å 259.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.31 – 3.85 39.31 – 3.85	Depositor EDS
% Data completeness (in resolution range)	90.9 (39.31-3.85) 98.8 (39.31-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.87Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.295 , 0.340 0.282 , 0.328	Depositor DCC
R_{free} test set	586 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	159.3	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 239.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å ²)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AG

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	0.32	1/2306 (0.0%)	0.53	0/3142
1	B	0.27	0/2313	0.54	0/3152
All	All	0.30	1/4619 (0.0%)	0.53	0/6294

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	GLU	CB-CG	5.26	1.62	1.52

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	2267	0	2336	233	0
1	B	2274	0	2343	227	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4543	0	4679	449	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 49.

The worst 5 of 449 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:332:LEU:HA	1:A:341:VAL:HG11	1.32	1.08
1:A:117:ASN:HD21	1:A:243:PRO:HG2	1.21	1.01
1:A:122:ALA:HB3	1:A:214:ILE:HD12	1.49	0.94
1:A:106:PHE:CD2	1:B:253:SER:HA	2.06	0.89
1:A:249:ALA:HB1	1:A:293:THR:HG21	1.52	0.89

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	294/413 (71%)	220 (75%)	45 (15%)	29 (10%)	0	10
1	B	295/413 (71%)	218 (74%)	48 (16%)	29 (10%)	0	10
All	All	589/826 (71%)	438 (74%)	93 (16%)	58 (10%)	0	10

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	146	LYS
1	A	156	PRO
1	A	157	ASP
1	A	206	THR

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	242/338 (72%)	192 (79%)	50 (21%)	1	8
1	B	243/338 (72%)	194 (80%)	49 (20%)	1	9
All	All	485/676 (72%)	386 (80%)	99 (20%)	1	8

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	LEU
1	B	142	ASP
1	B	345	ASP
1	A	375	GLU
1	B	92	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN
1	A	339	GLN
1	B	162	GLN
1	A	318	ASN
1	B	91	ASN

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	296/413 (71%)	0.11	10 (3%) 45 37	112, 202, 318, 446	0
1	B	297/413 (71%)	0.28	16 (5%) 25 21	120, 214, 362, 581	0
All	All	593/826 (71%)	0.19	26 (4%) 34 29	112, 209, 343, 581	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	THR	7.5
1	A	90	GLN	3.4
1	B	200	ALA	3.3
1	B	158	TRP	3.1
1	B	223	LEU	2.8

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AG	A	414	1/1	0.77	1.35	400,400,400,400	0
2	AG	B	414	1/1	0.80	1.07	268,268,268,268	0

6.5 Other polymers [i](#)

There are no such residues in this entry.