



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:45 am BST

PDB ID : 3T53
Title : Crystal structures of the extrusion state of the CusBA adaptor-transporter complex
Authors : Su, C.-C.; Long, F.; Yu, E.W.
Deposited on : 2011-07-26
Resolution : 3.37 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

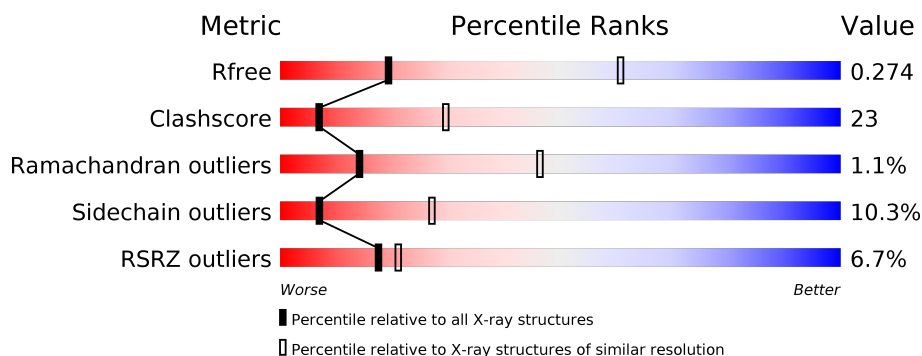
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 ≥ 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	B	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 36%, green 56%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 10% 56% 36% • • </div> </div>
1	C	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 35%, green 57%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 57% 35% • • </div> </div>
2	A	1054	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 41%, green 51%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 10% 51% 41% 5% • </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12876 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	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1028	Total	C	N	O	S	0	0	0
			7923	5124	1330	1433	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	HIS	-	EXPRESSION TAG	UNP P38054

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0

- Molecule 4 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total O 4 4	0	0
4	C	10	Total O 10 10	0	0
4	A	7	Total O 7 7	0	0

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 B:

56% 36%

Chain B: A horizontal bar chart showing a distribution of values. The bar is primarily green, with a small red segment at the far left and a small yellow segment at the far right. The green segment is labeled '56%' and the yellow segment is labeled '36%'. Below the bar, a series of colored squares (red, green, yellow, orange, grey) are arranged in a sequence, each corresponding to a specific value or category.

- Chain C: 

- Chain A: 

L1026	S1027	L1028	F1029	I1030	I1031	P1032	A1033	A1034	Y1035	K1036	L1037	H1038	H1039	H1040	R1041	R1042	H1043	ARG	VAL	ARG	LYS																																			
V955	F956	S957	L958	I959	N960	P961	G962	T963	S964	S965	K966	L969	R969	D970	L973	A977	R980	R982	P983	K984	A985	P986	T987	V988	L989	V989	G990	G991	I992	A993	G994	L995	L996	P997	L998	L999	G1000	G1001	T1002	E1007	R1011	I1012	A1013	A1014	N1015	P1016	I1017	M1020	I1021	T1022	A1023	P1024	L1025			
T979	L980	M981	I982	I983	F984	V985	L986	L987	V988	L989	R990	R991	R992	R993	G995	B996	A997	L998	L999	I990	V904	P905	P906	A907	L908	V909	G910	G911	I912	N913	H921	A925	T926	G927	I931	A937	P940	G941	V942	V943	N944	L945	N946	Y947	L948	R949	R950	A951	B953	A954						
L783	L786	P787	L788	L789	T796	T797	L798	V801	R804	R805	R806	R812	L813	B816	N817	I824	D827	V834	V837	H838	Q841	R842	B846	R847	Q849	L850	R851	G853	T854	Q861	R862	B863	L864	A868	R871	L872	R873	L874	R875	R876	R877	D778	Q781	A782												
M696	T700	E701	F702	V703	A704	R705	T706	V707	P708	S712	A715	L718	R722	T723	N725	N729	K732	Y736	V740	Q744	L745	F746	V747	T748	S749	A750	V756	A764	R765	Y766	P767	M668	R669	I670	L673	S679	V685	G607	K608	K611	T614															
D617	A619	P620	L621	B622	M623	V624	E625	T626	T627	T628	Q629	L630	Q633	E634	Q635	M636	P637	P638	M640	T641	M642	D643	K644	L649	T652	V653	G657	L658	A659	M660	L661	M662	V663	P664	P665	I666	R667	M668	I670	L673	S679	V685	G607	K608	K611	T614										
T539	L540	L541	L545	S546	S547	L548	T549	V550	L551	M552	P553	L554	V557	F561	L562	P563	E567	G568	D569	L570	L571	Y572	M573	P574	S575	I580	A586	S587	M588	L589	Q590	K591	T592	D593	K594	L595	I596	M597	S598	V599	P600	E601	V602	A603	R604	V605	F606	G607	K608	K611	T614					
G476	P477	F480	T481	K482	T483	Y484	A485	M486	A487	G488	L492	A493	I494	V495	V496	I497	P498	I499	M501	G502	V503	H504	I505	ARG	GLY	LYS	V444	F445	V446	G447	P448	A449	L450	F451	L452	S453	L454	L455	L456	I457	T458	L459	S460	F461	L462	P463	L464	F465	T466	L467	Q470	R471	G472	R473	L474	F475
H415	R416	R417	E419	P420	V421	Q422	R423	Q424	R425	P426	A428	T429	L430	D431	N432	K433	T434	R435	W436	Q437	V438	L439	T440	D441	A442	S443	V444	F445	V446	G447	P448	A449	L450	F451	L452	S453	L454	L455	L456	I457	T458	L459	S460	F461	L462	P463	L464	F465	T466	L467	Q470	R471	G472	R473	L474	F475
L343	E344	V349	L355	F356	R359	V360	R361	L364	V365	A366	I367	I368	S369	L370	P371	L374	C375	I376	A377	F378	I379	V380	N381	Q384	G385	L386	N387	A388	N389	I390	M391	S392	G395	I396	A397	I398	A399	V400	G401	A402	M403	V404	D405	A406	A407	I408	V409	M410	I411	E412	M413	V414	A414			
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342								
L337	M338	I339	Y140	E141	Y142	A143	L144	V145	D146	L153	R157	A178	V184	K185	E186	V189	V190	I191	D192	P193	Q194	R195	I201	S202	L203	V206	D211	A212	D102	P103	Y104	W105	A106	L114	I222	E223	L224	Y229	T324	Y325	D326	R327	S328	Q329	L330	I331	L338	S339	G340	K341	V247	L342				
V255	P256	L259	R260	D261	V265	Q266	G268	P269	E270	M271	R272	I275	A276	E277	L278	N279	E283	V284	V288	V289	I290	L291	K295	N296	A297	R298	E299	V300	I301	V304	L315	I321	V322	T323	T324	Y325	D326																			

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	159.79Å 159.79Å 683.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 3.37 49.12 – 3.37	Depositor EDS
% Data completeness (in resolution range)	87.7 (49.12-3.37) 99.4 (49.12-3.37)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.248 , 0.286 0.241 , 0.274	Depositor DCC
R_{free} test set	2415 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12876	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

5.1 Standard geometry

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

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	B	0.22	0/2498	0.42	0/3401
1	C	0.22	0/2513	0.42	0/3421
2	A	0.21	0/8089	0.40	0/11015
All	All	0.21	0/13100	0.41	0/17837

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

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	B	2458	0	2522	118	0
1	C	2473	0	2533	103	0
2	A	7923	0	8166	408	0
3	A	1	0	0	0	0
4	A	7	0	0	0	0
4	B	4	0	0	0	0
4	C	10	0	0	0	0
All	All	12876	0	13221	600	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 23.

The worst 5 of 600 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:C:256:TRP:CZ3	1:C:257:LEU:HD12	1.45	1.48
2:A:661:LEU:HD23	2:A:662:TRP:N	1.45	1.29
1:C:256:TRP:CZ3	1:C:257:LEU:CD1	2.34	1.11
1:B:120:GLN:HE22	1:B:243:PRO:HD2	1.17	1.05
1:C:256:TRP:CH2	1:C:257:LEU:CD1	2.44	1.01

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	B	320/336 (95%)	284 (89%)	31 (10%)	5 (2%)	9	37
1	C	322/336 (96%)	300 (93%)	19 (6%)	3 (1%)	17	51
2	A	1024/1054 (97%)	923 (90%)	91 (9%)	10 (1%)	15	48
All	All	1666/1726 (96%)	1507 (90%)	141 (8%)	18 (1%)	14	46

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	255	ALA
2	A	638	PRO
2	A	852	PRO
1	B	292	ARG
1	C	172	GLY

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	B	263/275 (96%)	235 (89%)	28 (11%)	6	25
1	C	265/275 (96%)	236 (89%)	29 (11%)	6	24
2	A	847/871 (97%)	762 (90%)	85 (10%)	7	28
All	All	1375/1421 (97%)	1233 (90%)	142 (10%)	7	27

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	65	VAL
2	A	338	LEU
2	A	945	LEU
2	A	105	TRP
2	A	203	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	238	GLN
2	A	413	ASN
2	A	838	HIS
2	A	279	ASN
2	A	329	GLN

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 1 ligands modelled in this entry, 1 is 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	B	322/336 (95%)	-0.06	3 (0%) 84 88	24, 58, 112, 176	0
1	C	324/336 (96%)	-0.01	2 (0%) 89 92	25, 58, 110, 174	0
2	A	1028/1054 (97%)	0.40	107 (10%) 6 8	28, 106, 212, 312	0
All	All	1674/1726 (96%)	0.23	112 (6%) 17 21	24, 79, 194, 312	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	15	LEU	10.7
2	A	890	ALA	8.4
2	A	365	VAL	7.7
2	A	887	LEU	7.7
2	A	495	VAL	5.8

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
3	CU	A	1048	1/1	0.92	0.19	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.