



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:18 am BST

PDB ID : 4M64
Title : 3D crystal structure of Na⁺/melibiose symporter of Salmonella typhimurium
Authors : Ethayathulla, A.S.; Guan, L.
Deposited on : 2013-08-08
Resolution : 3.35 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

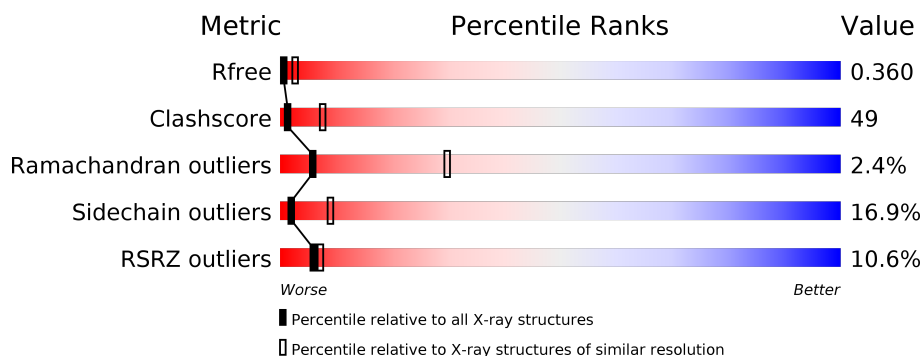
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	A	486	<div> <div>6%</div> <div>32% 51% 9% 8%</div> </div>
1	B	486	<div> <div>16%</div> <div>38% 40% 10% 12%</div> </div>
1	C	486	<div> <div>5%</div> <div>32% 45% 12% 11%</div> </div>
1	D	486	<div> <div>9%</div> <div>34% 37% 7% 21%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12982 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 Melibiose carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3442	2295	540	585	22			
1	B	426	Total	C	N	O	S	0	0	0
			3258	2176	503	558	21			
1	C	431	Total	C	N	O	S	0	0	0
			3352	2242	520	568	22			
1	D	382	Total	C	N	O	S	0	0	0
			2930	1965	449	497	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
A	477	HIS	-	EXPRESSION TAG	UNP P30878
A	478	HIS	-	EXPRESSION TAG	UNP P30878
A	479	HIS	-	EXPRESSION TAG	UNP P30878
A	480	HIS	-	EXPRESSION TAG	UNP P30878
A	481	HIS	-	EXPRESSION TAG	UNP P30878
A	482	HIS	-	EXPRESSION TAG	UNP P30878
A	483	HIS	-	EXPRESSION TAG	UNP P30878
A	484	HIS	-	EXPRESSION TAG	UNP P30878
A	485	HIS	-	EXPRESSION TAG	UNP P30878
A	486	HIS	-	EXPRESSION TAG	UNP P30878
B	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
B	477	HIS	-	EXPRESSION TAG	UNP P30878
B	478	HIS	-	EXPRESSION TAG	UNP P30878
B	479	HIS	-	EXPRESSION TAG	UNP P30878
B	480	HIS	-	EXPRESSION TAG	UNP P30878
B	481	HIS	-	EXPRESSION TAG	UNP P30878
B	482	HIS	-	EXPRESSION TAG	UNP P30878
B	483	HIS	-	EXPRESSION TAG	UNP P30878
B	484	HIS	-	EXPRESSION TAG	UNP P30878
B	485	HIS	-	EXPRESSION TAG	UNP P30878

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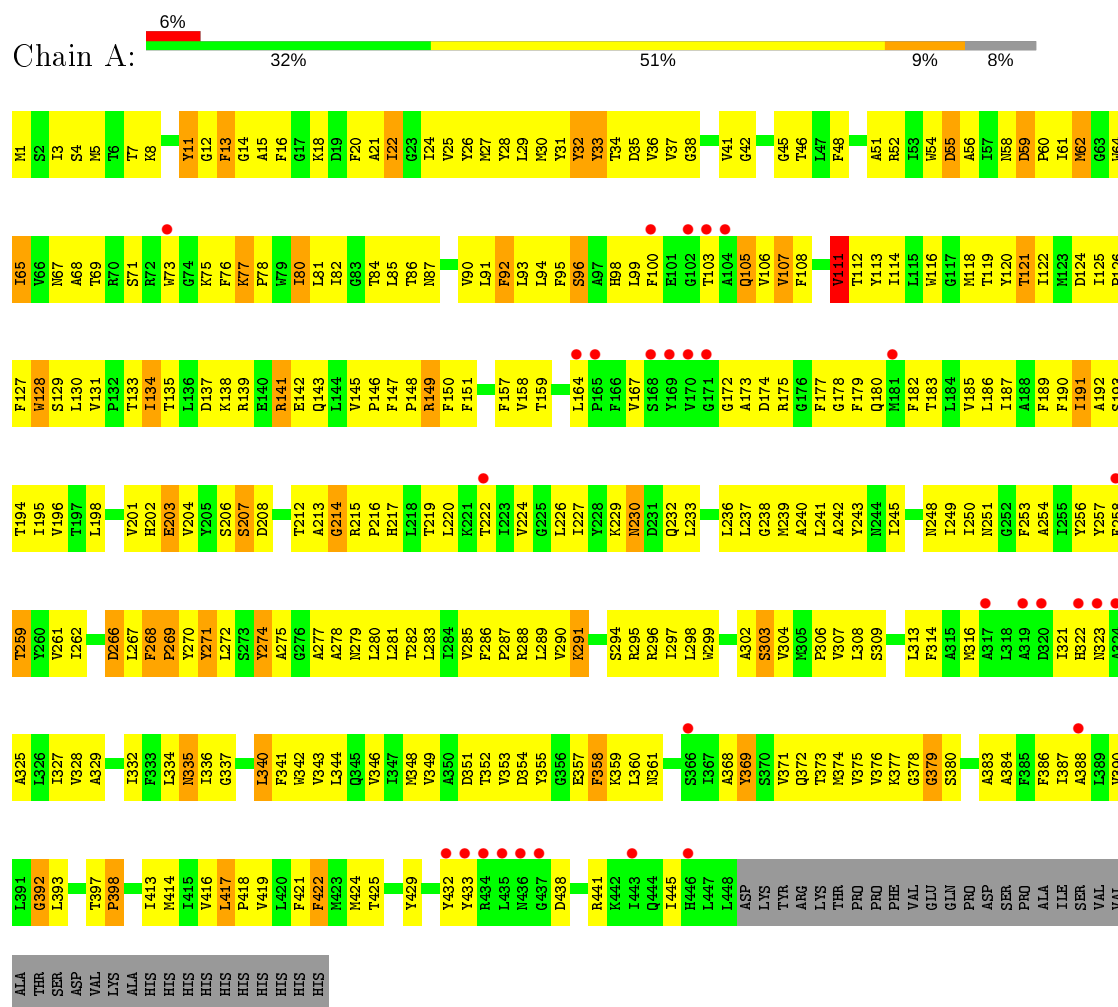
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Chain	Residue	Modelled	Actual	Comment	Reference
B	486	HIS	-	EXPRESSION TAG	UNP P30878
C	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
C	477	HIS	-	EXPRESSION TAG	UNP P30878
C	478	HIS	-	EXPRESSION TAG	UNP P30878
C	479	HIS	-	EXPRESSION TAG	UNP P30878
C	480	HIS	-	EXPRESSION TAG	UNP P30878
C	481	HIS	-	EXPRESSION TAG	UNP P30878
C	482	HIS	-	EXPRESSION TAG	UNP P30878
C	483	HIS	-	EXPRESSION TAG	UNP P30878
C	484	HIS	-	EXPRESSION TAG	UNP P30878
C	485	HIS	-	EXPRESSION TAG	UNP P30878
C	486	HIS	-	EXPRESSION TAG	UNP P30878
D	5	MET	LEU	ENGINEERED MUTATION	UNP P30878
D	477	HIS	-	EXPRESSION TAG	UNP P30878
D	478	HIS	-	EXPRESSION TAG	UNP P30878
D	479	HIS	-	EXPRESSION TAG	UNP P30878
D	480	HIS	-	EXPRESSION TAG	UNP P30878
D	481	HIS	-	EXPRESSION TAG	UNP P30878
D	482	HIS	-	EXPRESSION TAG	UNP P30878
D	483	HIS	-	EXPRESSION TAG	UNP P30878
D	484	HIS	-	EXPRESSION TAG	UNP P30878
D	485	HIS	-	EXPRESSION TAG	UNP P30878
D	486	HIS	-	EXPRESSION TAG	UNP P30878

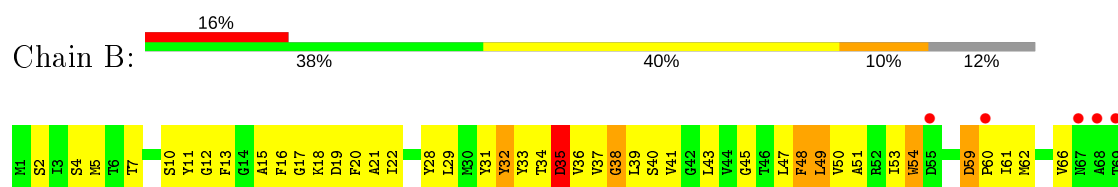
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Melibiose carrier protein



• Molecule 1: Melibiose carrier protein

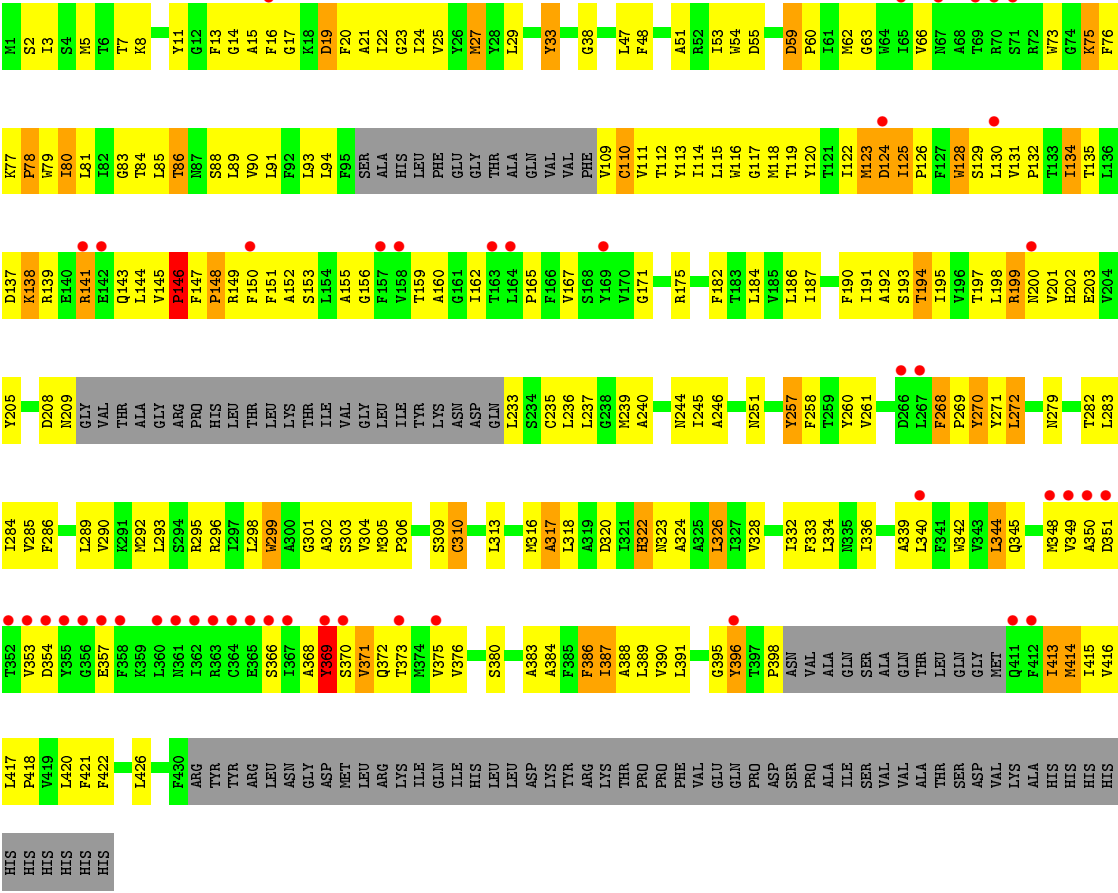




V416	Q345	T282	V201	I134	R70	M1
L417	V346	L283	H202	T135	S71	I3
P418	I347	L283	E203	R136	R72	S2
V419	V348		V204	D137	W73	S4
L420	V349	F286	Y205	K138	G74	S5
F421	A350	F287		R139	K75	T6
F422	D351	R288	M209	E140	F76	T7
M423	T352		G210	R141	K77	
M424	V353	L293	V211	E142	F78	S10
T425	D354	S294	T212	Q143	W79	Y11
L426	V355	R295	A213	L144	I80	
V427	G356	R296	G214	V145	L81	G14
L428	E357	I297	R215	P146	I82	A15
F429	F358	L298	P216	G83	F147	A16
F430	R359	N299	H217	P148	G17	G17
R431	L360	A300	L218		L85	K18
TTR	N361	G301	T219	F151	T86	D19
TTR	L362	A302			N87	F20
ARG	R363	S303	I227	A155	S88	A21
LEU		V304	Y228	G156	L89	I22
ASN	I367	R305	K229	F157	V90	G23
GLY	A368	P306	N230	V158	L91	G23
ASP	Y369	V307	D231	T159	F92	I24
MET	S370	L308	Q232	A160	L93	M27
LEU	V371	S309	L233	G161	L94	Y28
ARG	Q372	C310	S234	I162	F95	L29
LYS	T373	A311	G235	T163	S96	M30
ILE	M374	G312	L236	L164	A97	V31
GLN	V375	L313	L237	P165	H98	X32
ILE	V376	F314	G238	F166	L99	Y33
HIS		A315	M239	V167	T34	T34
LEU	G379	N316	A240	S168	D35	D35
LEU	S380	A317	L241	V169	V36	V36
ASP		L318	A242	G171	V106	V37
LYS	A383	A319		G171		
TTR	A384	B320	I245	G172		V41
ARG	F385	I321			V109	G42
LYS	F386	H322	M248	R175	C110	
TTR	I387	N323	I249	G176	V111	L43
PRO		A324	I250	F177	T112	V44
PRO	L391	A325		G178	Y113	
PHE	G392	L326	F253	F179	I114	F48
VAL	L393	I327	A254	Q180	L115	L49
GLU		V328	T255	M181	W116	V50
GLN	Y396	A329			G117	A51
PRO	T397	A330	F258	L184	M118	R52
ASP	P398	G331	T259	V185	T119	I53
SER	N399	L332	Y260	L186	C120	N54
PRO	V400	F333		I187	T121	D55
ALA	A401	L334	F268		I122	A96
ILE	Q402	N335	P269	I191	M123	I57
SER	S403	G337	Y270	A192	D124	N58
VAL		T338	L272	S193	I125	D59
VAL	Q408	T339		T194	P126	P60
ALA	G409	A339	A275	I195	F127	I61
THR	M410	L340	T276	S129	W128	M62
SER	Q411	F341	G276	V196	L130	V66
ASP	F412	N342	A277	L198	L131	N67
VAL	I413	V343	A278	F199	V130	A68
VAL		T344	N270	R200	F432	M60

ALA
HIS
HIS
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● Molecule 1: Melibiose carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	127.21Å 127.21Å 206.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.64 – 3.35 38.64 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.64-3.35) 99.5 (38.64-3.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	47.41 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.312 , 0.359 0.311 , 0.360	Depositor DCC
R_{free} test set	2712 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	94.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.039 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12982	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3433e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

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	0.63	0/3530	0.87	2/4813 (0.0%)
1	B	0.60	0/3342	0.82	3/4561 (0.1%)
1	C	0.66	0/3440	0.91	1/4689 (0.0%)
1	D	0.59	0/3004	0.81	1/4097 (0.0%)
All	All	0.62	0/13316	0.86	7/18160 (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
1	B	0	4
1	C	0	4
1	D	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	55	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	55	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	308	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	340	LEU	CB-CG-CD2	-5.21	102.14	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ILE	Peptide
1	B	254	ALA	Peptide
1	B	38	GLY	Peptide
1	B	429	TYR	Peptide
1	B	74	GLY	Peptide

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	A	3442	0	3479	346	0
1	B	3258	0	3249	299	0
1	C	3352	0	3433	352	0
1	D	2930	0	2965	285	0
All	All	12982	0	13126	1273	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 1273 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:D:299:TRP:CB	1:D:344:LEU:HD13	1.63	1.26
1:D:86:THR:CG2	1:D:115:LEU:HG	1.65	1.26
1:C:75:LYS:HG3	1:C:205:TYR:CB	1.77	1.15
1:D:299:TRP:HB2	1:D:344:LEU:CD1	1.77	1.15
1:C:128:TRP:CH2	1:C:373:THR:HG21	1.83	1.13

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	446/486 (92%)	365 (82%)	65 (15%)	16 (4%)	3	22
1	B	422/486 (87%)	360 (85%)	54 (13%)	8 (2%)	8	34
1	C	429/486 (88%)	358 (83%)	63 (15%)	8 (2%)	8	34
1	D	374/486 (77%)	314 (84%)	52 (14%)	8 (2%)	7	32
All	All	1671/1944 (86%)	1397 (84%)	234 (14%)	40 (2%)	6	30

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ILE
1	A	269	PRO
1	A	271	TYR
1	B	430	PHE
1	C	134	ILE

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	354/406 (87%)	303 (86%)	51 (14%)	3	14
1	B	331/406 (82%)	272 (82%)	59 (18%)	2	7
1	C	353/406 (87%)	281 (80%)	72 (20%)	1	4
1	D	302/406 (74%)	258 (85%)	44 (15%)	3	13
All	All	1340/1624 (82%)	1114 (83%)	226 (17%)	2	9

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	389	LEU
1	C	92	PHE
1	D	208	ASP

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Mol	Chain	Res	Type
1	B	413	ILE
1	C	30	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	B	279	ASN
1	C	230	ASN
1	A	361	ASN
1	C	402	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 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, 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	448/486 (92%)	0.03	30 (6%) 17 20	27, 80, 183, 265	25 (5%)
1	B	426/486 (87%)	0.76	78 (18%) 1 1	28, 89, 247, 360	9 (2%)
1	C	431/486 (88%)	0.03	24 (5%) 24 26	24, 76, 168, 340	0
1	D	382/486 (78%)	0.51	46 (12%) 4 5	31, 85, 220, 331	1 (0%)
All	All	1687/1944 (86%)	0.32	178 (10%) 6 7	24, 82, 213, 360	35 (2%)

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	362	ILE	21.4
1	B	350	ALA	19.3
1	C	321	ILE	16.4
1	B	351	ASP	15.7
1	D	412	PHE	15.5

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.