



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:33 am BST

PDB ID : 1E2T
Title : Arylamine N-acetyltransferase (NAT) from Salmonella typhimurium
Authors : Sinclair, J.C.; Sandy, J.; Delgoda, R.; Sim, E.; Noble, M.E.M.
Deposited on : 2000-05-24
Resolution : 2.80 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

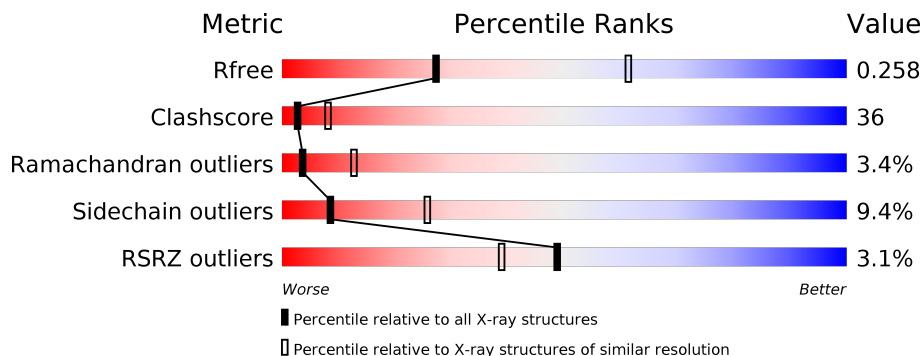
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



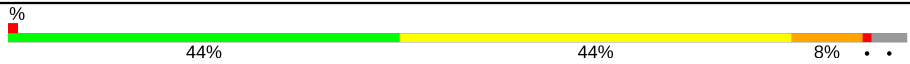

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	284	
1	B	284	
1	C	284	
1	D	284	
1	E	284	
1	F	284	

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Mol	Chain	Length	Quality of chain
1	G	284	 <p>%</p> <p>44% 44% 8% . .</p>
1	H	284	 <p>4%</p> <p>44% 45% 7% . .</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18260 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 N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2224	1421	403	389	11	0	0	0
1	B	274	2224	1421	403	389	11	0	0	0
1	C	274	2224	1421	403	389	11	0	0	0
1	D	274	2224	1421	403	389	11	0	0	0
1	E	274	2224	1421	403	389	11	0	0	0
1	F	274	2224	1421	403	389	11	0	0	0
1	G	274	2224	1421	403	389	11	0	0	0
1	H	274	2224	1421	403	389	11	0	0	0

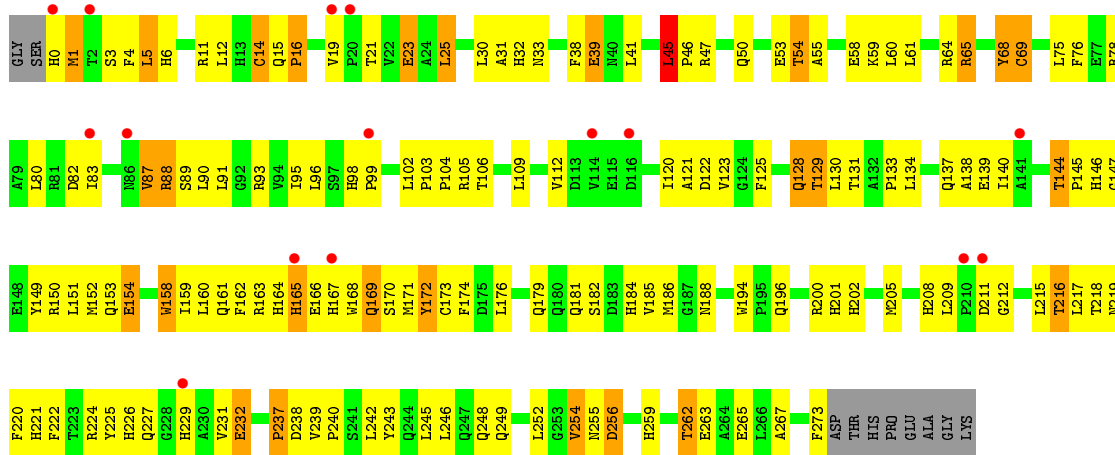
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total 56	O 56	0	0
2	B	51	Total 51	O 51	0	0
2	C	79	Total 79	O 79	0	0
2	D	36	Total 36	O 36	0	0
2	E	92	Total 92	O 92	0	0
2	F	48	Total 48	O 48	0	0

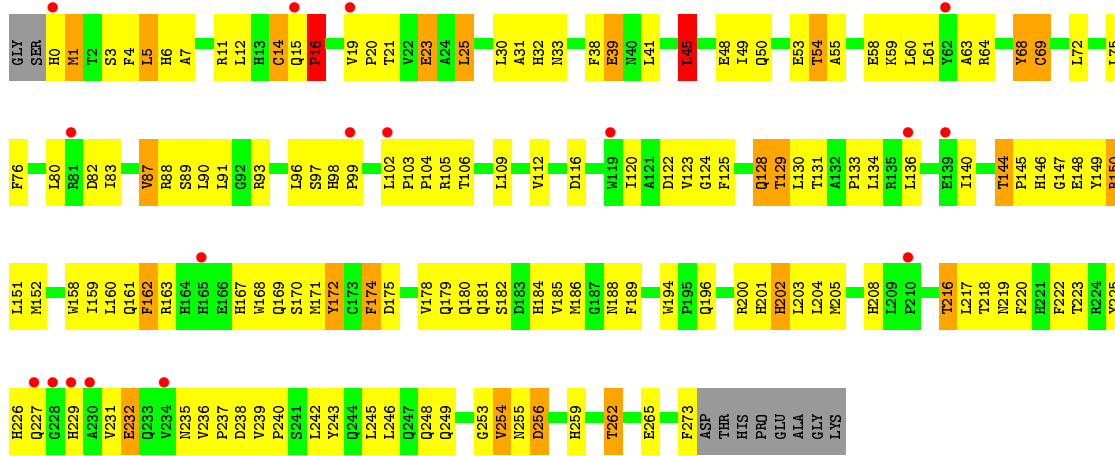
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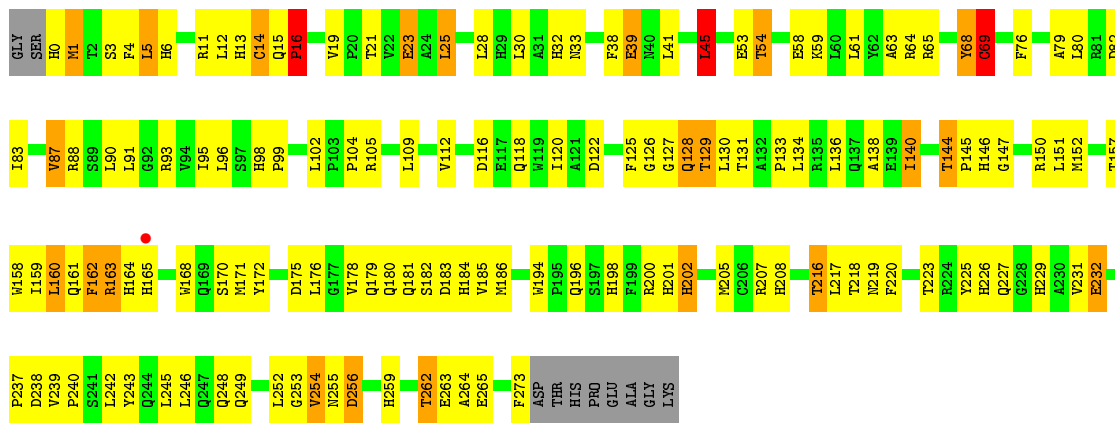
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	56	Total	O	0	0
			56	56		
2	H	50	Total	O	0	0
			50	50		



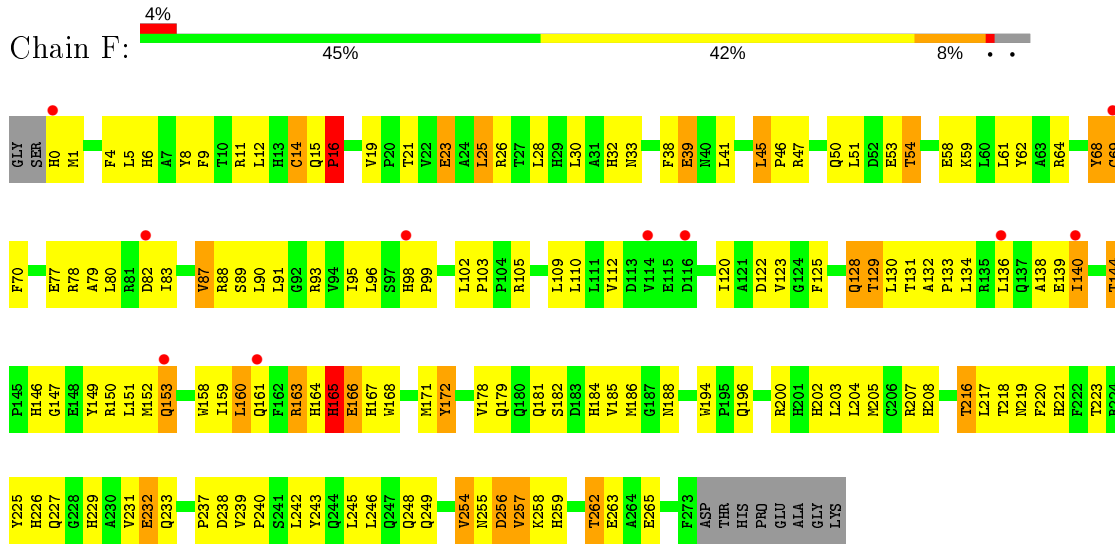
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



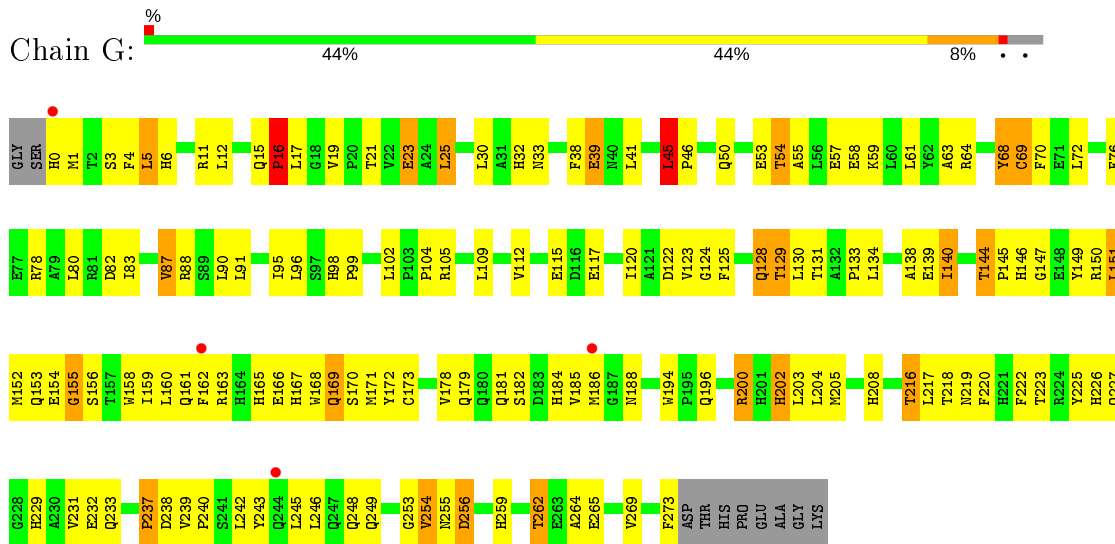
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



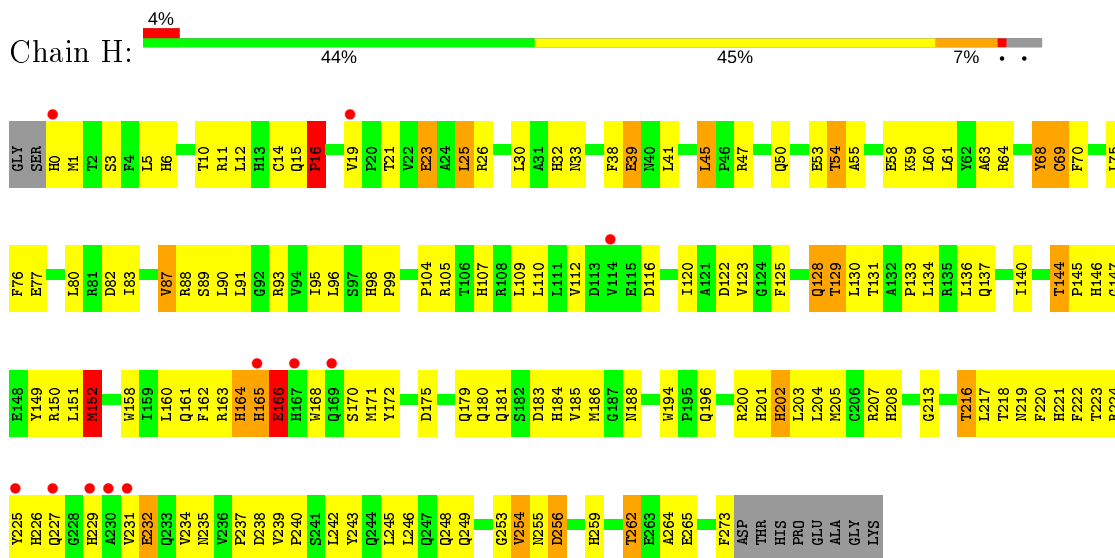
• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



• Molecule 1: N-HYDROXYARYLAMINE O-ACETYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.53Å 222.42Å 104.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 40.75 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.80) 78.7 (40.75-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.65Å)	Xtrriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.264 , 0.302 0.267 , 0.258	Depositor DCC
R_{free} test set	6188 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtrriage
Anisotropy	0.642	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18260	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% 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](#)

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	0.78	0/2290	0.87	2/3113 (0.1%)
1	B	0.82	1/2290 (0.0%)	0.91	2/3113 (0.1%)
1	C	0.79	2/2290 (0.1%)	0.90	2/3113 (0.1%)
1	D	0.70	1/2290 (0.0%)	0.85	1/3113 (0.0%)
1	E	0.92	2/2290 (0.1%)	0.94	2/3113 (0.1%)
1	F	0.84	1/2290 (0.0%)	0.88	2/3113 (0.1%)
1	G	0.78	1/2290 (0.0%)	0.88	2/3113 (0.1%)
1	H	0.78	0/2290	0.89	2/3113 (0.1%)
All	All	0.80	8/18320 (0.0%)	0.89	15/24904 (0.1%)

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	B	0	1
1	F	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	CYS	CB-SG	-8.15	1.68	1.82
1	F	14	CYS	CB-SG	-7.24	1.70	1.82
1	E	14	CYS	CB-SG	-6.82	1.70	1.82
1	G	173	CYS	CB-SG	-6.71	1.70	1.82
1	E	69	CYS	CB-SG	-5.71	1.72	1.81

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	45	LEU	N-CA-C	-8.12	89.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	LEU	N-CA-C	-8.07	89.22	111.00
1	B	45	LEU	N-CA-C	-7.72	90.14	111.00
1	C	45	LEU	N-CA-C	-7.62	90.42	111.00
1	B	150	ARG	NE-CZ-NH1	7.62	124.11	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	TYR	Sidechain
1	F	172	TYR	Sidechain

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	2224	0	2149	156	0
1	B	2224	0	2149	179	1
1	C	2224	0	2149	177	2
1	D	2224	0	2149	157	0
1	E	2224	0	2149	145	0
1	F	2224	0	2149	151	1
1	G	2224	0	2149	167	0
1	H	2224	0	2149	161	2
2	A	56	0	0	13	0
2	B	51	0	0	26	0
2	C	79	0	0	29	0
2	D	36	0	0	18	0
2	E	92	0	0	19	0
2	F	48	0	0	13	0
2	G	56	0	0	19	0
2	H	50	0	0	13	0
All	All	18260	0	17192	1252	4

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 36.

The worst 5 of 1252 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:F:46:PRO:HD2	2:F:2011:HOH:O	1.24	1.34
1:F:186:MET:CE	1:H:186:MET:HE3	1.63	1.27
1:F:186:MET:HE2	1:H:186:MET:CE	1.70	1.20
1:B:186:MET:HE3	1:C:186:MET:CE	1.79	1.11
1:B:186:MET:CE	1:C:186:MET:HE3	1.80	1.10

All (4) 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:F:6:HIS:ND1	1:F:62:TYR:OH[2_665]	1.90	0.30
1:C:211:ASP:OD2	1:H:10:THR:O[4_556]	1.92	0.28
1:B:6:HIS:ND1	1:B:62:TYR:OH[2_665]	1.98	0.22
1:C:209:LEU:CD1	1:H:6:HIS:NE2[4_556]	2.19	0.01

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	272/284 (96%)	225 (83%)	38 (14%)	9 (3%)	4	13
1	B	272/284 (96%)	216 (79%)	44 (16%)	12 (4%)	2	8
1	C	272/284 (96%)	223 (82%)	41 (15%)	8 (3%)	4	15
1	D	272/284 (96%)	217 (80%)	46 (17%)	9 (3%)	4	13
1	E	272/284 (96%)	229 (84%)	35 (13%)	8 (3%)	4	15
1	F	272/284 (96%)	223 (82%)	40 (15%)	9 (3%)	4	13
1	G	272/284 (96%)	221 (81%)	44 (16%)	7 (3%)	5	18
1	H	272/284 (96%)	226 (83%)	35 (13%)	11 (4%)	3	9
All	All	2176/2272 (96%)	1780 (82%)	323 (15%)	73 (3%)	3	13

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
1	A	256	ASP
1	B	69	CYS
1	B	140	ILE
1	B	165	HIS

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	236/243 (97%)	213 (90%)	23 (10%)	8 24
1	B	236/243 (97%)	215 (91%)	21 (9%)	9 28
1	C	236/243 (97%)	214 (91%)	22 (9%)	9 26
1	D	236/243 (97%)	211 (89%)	25 (11%)	6 20
1	E	236/243 (97%)	211 (89%)	25 (11%)	6 20
1	F	236/243 (97%)	216 (92%)	20 (8%)	10 31
1	G	236/243 (97%)	215 (91%)	21 (9%)	9 28
1	H	236/243 (97%)	216 (92%)	20 (8%)	10 31
All	All	1888/1944 (97%)	1711 (91%)	177 (9%)	8 26

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	150	ARG
1	E	76	PHE
1	H	68	TYR
1	D	162	PHE
1	D	254	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	161	GLN
1	E	184	HIS
1	H	165	HIS
1	D	188	ASN
1	D	226	HIS

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	274/284 (96%)	0.22	4 (1%) 73 68	47, 79, 110, 122	0
1	B	274/284 (96%)	0.23	6 (2%) 62 52	54, 77, 106, 119	0
1	C	274/284 (96%)	0.30	15 (5%) 25 16	54, 79, 113, 121	0
1	D	274/284 (96%)	0.45	17 (6%) 20 13	49, 93, 116, 121	0
1	E	274/284 (96%)	-0.09	1 (0%) 92 91	37, 59, 87, 119	0
1	F	274/284 (96%)	0.23	10 (3%) 42 32	45, 70, 104, 119	0
1	G	274/284 (96%)	0.13	4 (1%) 73 68	39, 77, 106, 120	0
1	H	274/284 (96%)	0.16	11 (4%) 38 28	47, 78, 109, 120	0
All	All	2192/2272 (96%)	0.20	68 (3%) 49 39	37, 76, 110, 122	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.5
1	A	0	HIS	6.5
1	H	0	HIS	5.7
1	F	0	HIS	5.3
1	G	0	HIS	5.2

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.