



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 09:33 PM EDT

PDB ID : 1GU9
Title : Crystal Structure of Mycobacterium tuberculosis Alkylperoxidase AhpD
Authors : Nunn, C.M.; Djordjevic, S.; Hillas, P.J.; Nishida, C.; Ortiz de Montellano, P.R.
Deposited on : 2002-01-24
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

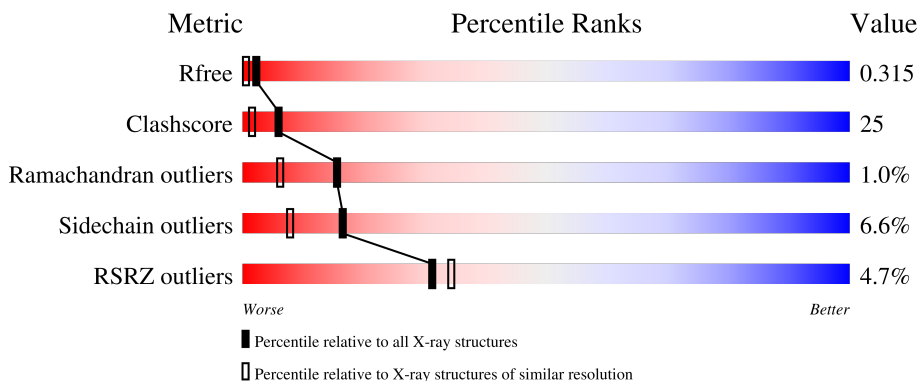
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of 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	177	
1	B	177	
1	C	177	
1	D	177	
1	E	177	

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Mol	Chain	Length	Quality of chain
1	F	177	<p>3% 67% 25% 5%</p>
1	G	177	<p>2% 63% 28% 5%</p>
1	H	177	<p>6% 63% 31% 2%</p>
1	I	177	<p>6% 61% 32% 5%</p>
1	J	177	<p>6% 62% 32% 2%</p>
1	K	177	<p>3% 58% 36% 5%</p>
1	L	177	<p>7% 57% 33% 5% 5%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16174 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 ALKYLHYDROPEROXIDASE D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	172	1284	808	232	239	3	2	0	0	0
1	B	173	1292	814	233	240	3	2	8	0	0
1	C	168	1256	791	228	232	3	2	0	0	0
1	D	172	1284	808	232	239	3	2	0	0	0
1	E	173	1292	814	233	240	3	2	8	0	0
1	F	169	1264	797	229	233	3	2	0	0	0
1	G	168	1256	791	228	232	3	2	11	0	0
1	H	171	1275	803	231	236	3	2	0	0	0
1	I	173	1292	814	233	240	3	2	0	0	0
1	J	172	1284	808	232	239	3	2	0	0	0
1	K	173	1292	814	233	240	3	2	0	0	0
1	L	168	1256	791	228	232	3	2	11	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total 61	O 61	0	0
2	B	78	Total 78	O 78	0	0

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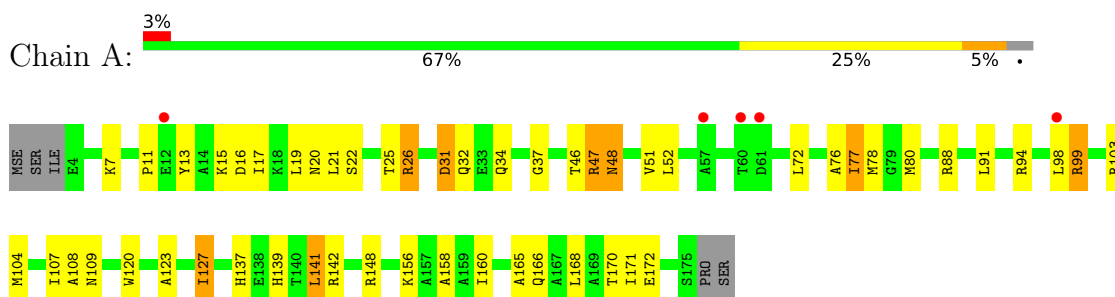
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	88	Total 88	O 88	0	0
2	D	70	Total 70	O 70	0	0
2	E	53	Total 53	O 53	0	0
2	F	108	Total 108	O 108	0	0
2	G	66	Total 66	O 66	0	0
2	H	65	Total 65	O 65	0	0
2	I	57	Total 57	O 57	0	0
2	J	76	Total 76	O 76	0	0
2	K	58	Total 58	O 58	0	0
2	L	67	Total 67	O 67	0	0

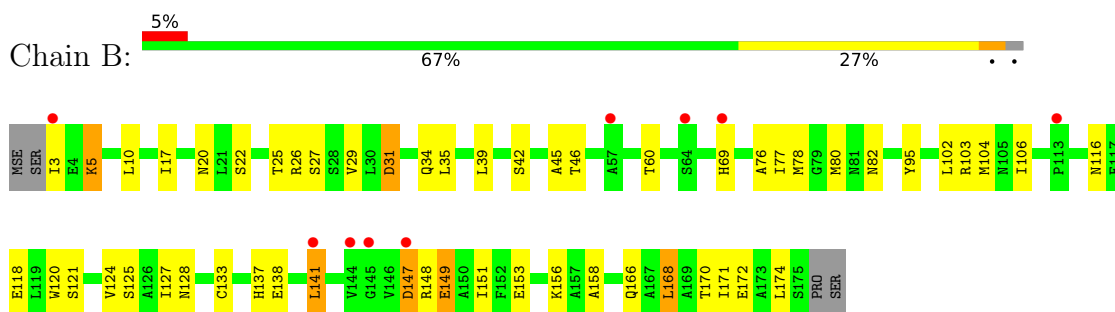
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

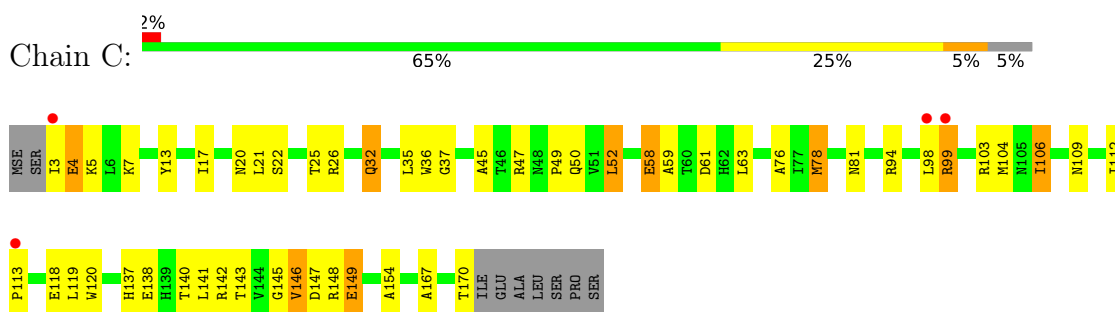
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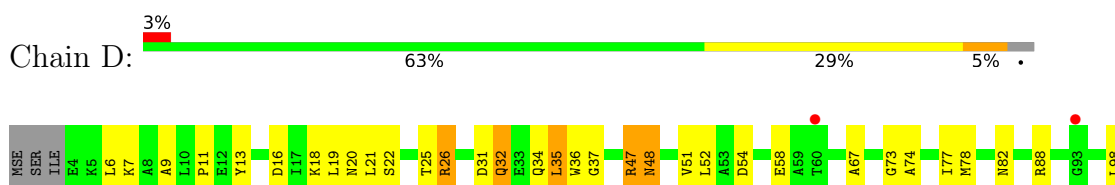
• Molecule 1: ALKYLHYDROPEROXIDASE D

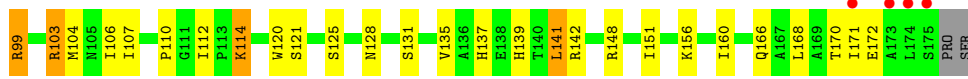


• Molecule 1: ALKYLHYDROPEROXIDASE D



• Molecule 1: ALKYLHYDROPEROXIDASE D

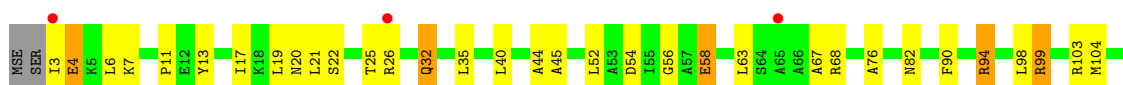




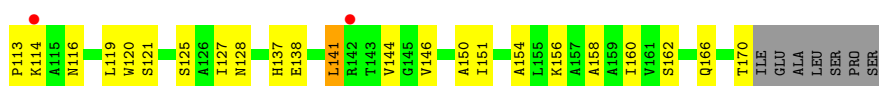
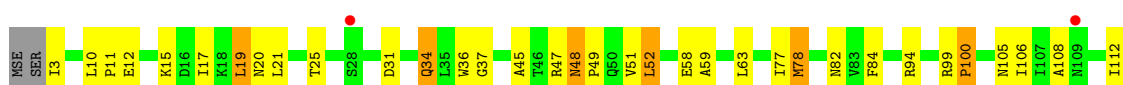
• Molecule 1: ALKYLHYDROPEROXIDASE D



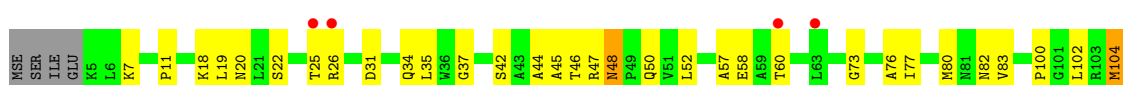
• Molecule 1: ALKYLHYDROPEROXIDASE D



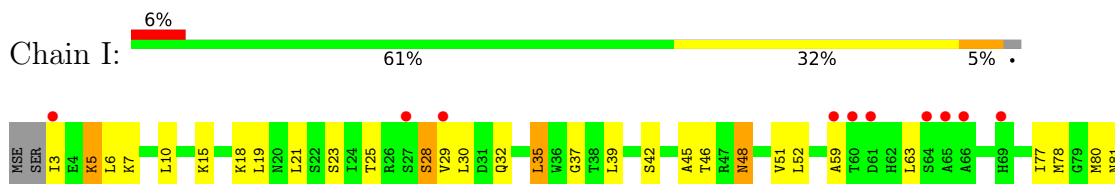
• Molecule 1: ALKYLHYDROPEROXIDASE D



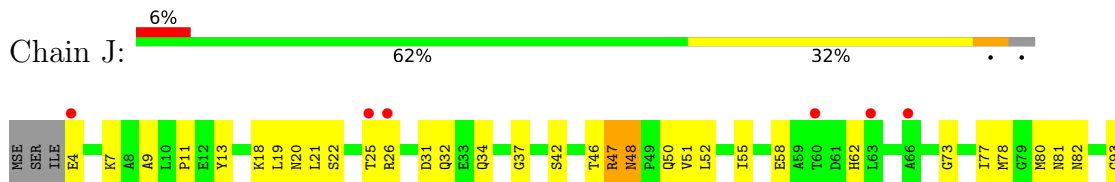
• Molecule 1: ALKYLHYDROPEROXIDASE D



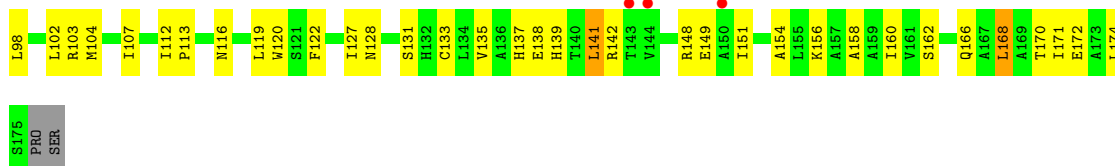
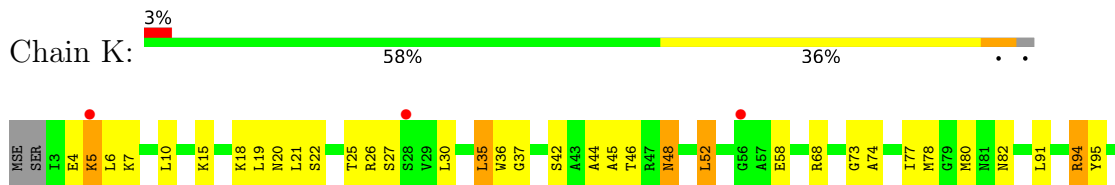
• Molecule 1: ALKYLHYDROPEROXIDASE D



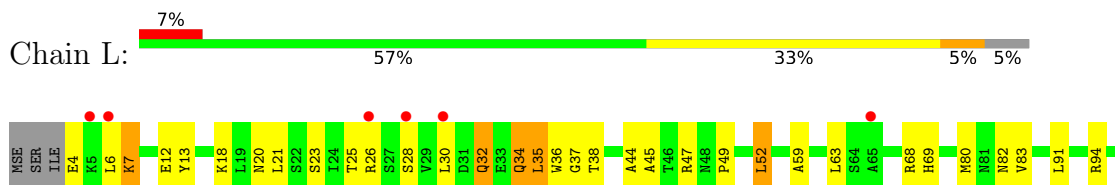
- Molecule 1: ALKYLHYDROPEROXIDASE D



- Molecule 1: ALKYLHYDROPEROXIDASE D



- Molecule 1: ALKYLHYDROPEROXIDASE D



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.38Å 117.28Å 88.99Å 90.00° 113.97° 90.00°	Depositor
Resolution (Å)	29.60 – 1.90 29.59 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.60-1.90) 99.4 (29.59-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.91Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.243 , 0.313 0.245 , 0.315	Depositor DCC
R_{free} test set	13616 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtrriage
Anisotropy	0.227	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.9	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	0.95	EDS
Total number of atoms	16174	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.34 % 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 5.0701e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.45	0/1303	0.65	0/1764
1	B	0.44	0/1311	0.64	0/1775
1	C	0.46	0/1275	0.66	0/1726
1	D	0.47	0/1303	0.64	0/1764
1	E	0.44	0/1311	0.64	0/1775
1	F	0.45	0/1283	0.65	0/1737
1	G	0.47	0/1275	0.66	1/1726 (0.1%)
1	H	0.45	0/1294	0.65	1/1752 (0.1%)
1	I	0.41	0/1311	0.66	0/1775
1	J	0.44	0/1303	0.63	0/1764
1	K	0.43	0/1311	0.64	0/1775
1	L	0.43	0/1275	0.64	0/1726
All	All	0.45	0/15555	0.65	2/21059 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	104	MET	CG-SD-CE	-5.99	90.62	100.20
1	G	78	MSE	CG-SE-CE	-5.94	85.84	98.90

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	1284	0	1296	75	0
1	B	1292	0	1307	59	0
1	C	1256	0	1269	66	0
1	D	1284	0	1296	75	0
1	E	1292	0	1307	81	0
1	F	1264	0	1280	56	0
1	G	1256	0	1269	59	0
1	H	1275	0	1290	74	0
1	I	1292	0	1307	79	0
1	J	1284	0	1296	84	0
1	K	1292	0	1307	72	0
1	L	1256	0	1269	79	0
2	A	61	0	0	4	0
2	B	78	0	0	6	0
2	C	88	0	0	6	0
2	D	70	0	0	3	0
2	E	53	0	0	4	0
2	F	108	0	0	2	0
2	G	66	0	0	2	0
2	H	65	0	0	6	0
2	I	57	0	0	7	0
2	J	76	0	0	3	0
2	K	58	0	0	5	0
2	L	67	0	0	5	0
All	All	16174	0	15493	769	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 25.

The worst 5 of 769 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:J:78:MSE:HE2	1:J:82:ASN:ND2	1.58	1.19
1:G:78:MSE:HE2	1:G:121:SER:HB3	1.15	1.14
1:K:5:LYS:HA	1:K:5:LYS:HE3	1.32	1.10
1:C:3:ILE:HG22	1:C:4:GLU:H	1.16	1.10
1:F:99:ARG:H	1:F:99:ARG:HD2	1.07	1.10

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	170/177 (96%)	162 (95%)	6 (4%)	2 (1%)	13	4
1	B	171/177 (97%)	165 (96%)	6 (4%)	0	100	100
1	C	166/177 (94%)	157 (95%)	7 (4%)	2 (1%)	13	4
1	D	170/177 (96%)	164 (96%)	5 (3%)	1 (1%)	25	15
1	E	171/177 (97%)	157 (92%)	10 (6%)	4 (2%)	6	1
1	F	167/177 (94%)	165 (99%)	1 (1%)	1 (1%)	25	15
1	G	166/177 (94%)	155 (93%)	9 (5%)	2 (1%)	13	4
1	H	169/177 (96%)	161 (95%)	7 (4%)	1 (1%)	25	15
1	I	171/177 (97%)	160 (94%)	10 (6%)	1 (1%)	25	15
1	J	170/177 (96%)	158 (93%)	9 (5%)	3 (2%)	8	2
1	K	171/177 (97%)	163 (95%)	7 (4%)	1 (1%)	25	15
1	L	166/177 (94%)	155 (93%)	8 (5%)	3 (2%)	8	2
All	All	2028/2124 (96%)	1922 (95%)	85 (4%)	21 (1%)	15	6

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	E	64	SER
1	E	115	ALA
1	G	100	PRO
1	J	109	ASN

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	128/130 (98%)	119 (93%)	9 (7%)	15	7
1	B	129/130 (99%)	123 (95%)	6 (5%)	26	16
1	C	125/130 (96%)	115 (92%)	10 (8%)	12	5
1	D	128/130 (98%)	118 (92%)	10 (8%)	12	5
1	E	129/130 (99%)	121 (94%)	8 (6%)	18	9
1	F	126/130 (97%)	116 (92%)	10 (8%)	12	5
1	G	125/130 (96%)	117 (94%)	8 (6%)	17	8
1	H	127/130 (98%)	119 (94%)	8 (6%)	18	8
1	I	129/130 (99%)	118 (92%)	11 (8%)	10	4
1	J	128/130 (98%)	123 (96%)	5 (4%)	32	23
1	K	129/130 (99%)	121 (94%)	8 (6%)	18	9
1	L	125/130 (96%)	117 (94%)	8 (6%)	17	8
All	All	1528/1560 (98%)	1427 (93%)	101 (7%)	16	8

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	47	ARG
1	I	35	LEU
1	L	98	LEU
1	G	52	LEU
1	H	114	LYS

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

Mol	Chain	Res	Type
1	I	81	ASN
1	K	32	GLN
1	I	105	ASN
1	J	48	ASN
1	K	105	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 monosaccharides 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	170/177 (96%)	0.23	5 (2%) 51 54	9, 26, 59, 73	0
1	B	170/177 (96%)	0.38	9 (5%) 26 29	10, 30, 56, 71	0
1	C	166/177 (93%)	0.21	4 (2%) 59 62	9, 25, 50, 69	0
1	D	170/177 (96%)	0.16	6 (3%) 44 47	7, 24, 54, 67	0
1	E	170/177 (96%)	0.57	12 (7%) 16 17	10, 35, 63, 73	0
1	F	167/177 (94%)	0.11	5 (2%) 50 53	7, 24, 53, 69	0
1	G	165/177 (93%)	0.23	4 (2%) 59 62	11, 29, 55, 72	0
1	H	169/177 (95%)	0.27	11 (6%) 18 21	9, 27, 56, 75	0
1	I	171/177 (96%)	0.51	11 (6%) 19 22	11, 34, 59, 74	0
1	J	170/177 (96%)	0.34	11 (6%) 18 21	10, 31, 61, 73	0
1	K	171/177 (96%)	0.32	6 (3%) 44 47	11, 33, 59, 76	0
1	L	165/177 (93%)	0.58	12 (7%) 15 16	14, 33, 59, 77	0
All	All	2024/2124 (95%)	0.33	96 (4%) 31 34	7, 30, 59, 77	0

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	109	ASN	5.7
1	F	3	ILE	4.9
1	K	28	SER	4.7
1	J	108	ALA	4.7
1	B	3	ILE	4.6

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 monosaccharides 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.