



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:25 AM UTC

PDB ID : 4AH6 / pdb_00004ah6
Title : Human mitochondrial aspartyl-tRNA synthetase
Authors : Neuenfeldt, A.; Sissler, M.; Lorber, B.; Florentz, C.; Sauter, C.
Deposited on : 2012-02-03
Resolution : 3.70 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

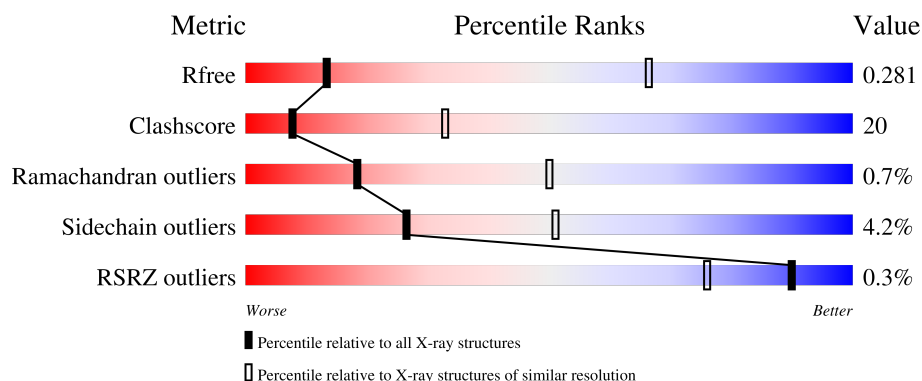
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 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	617	56% 36% • 5%
1	B	617	55% 37% • 5%
1	C	617	55% 37% • 5%
1	D	617	55% 38% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18840 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 ASPARTATE-TRNA LIGASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			
1	B	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			
1	C	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			
1	D	589	Total	C	N	O	S	0	0	0
			4710	3007	813	867	23			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP Q6PI48
A	646	VAL	-	expression tag	UNP Q6PI48
A	647	MET	-	expression tag	UNP Q6PI48
A	648	TYR	-	expression tag	UNP Q6PI48
A	649	LEU	-	expression tag	UNP Q6PI48
A	650	GLU	-	expression tag	UNP Q6PI48
A	651	HIS	-	expression tag	UNP Q6PI48
A	652	HIS	-	expression tag	UNP Q6PI48
A	653	HIS	-	expression tag	UNP Q6PI48
A	654	HIS	-	expression tag	UNP Q6PI48
A	655	HIS	-	expression tag	UNP Q6PI48
A	656	HIS	-	expression tag	UNP Q6PI48
B	40	MET	-	expression tag	UNP Q6PI48
B	646	VAL	-	expression tag	UNP Q6PI48
B	647	MET	-	expression tag	UNP Q6PI48
B	648	TYR	-	expression tag	UNP Q6PI48
B	649	LEU	-	expression tag	UNP Q6PI48
B	650	GLU	-	expression tag	UNP Q6PI48
B	651	HIS	-	expression tag	UNP Q6PI48
B	652	HIS	-	expression tag	UNP Q6PI48
B	653	HIS	-	expression tag	UNP Q6PI48

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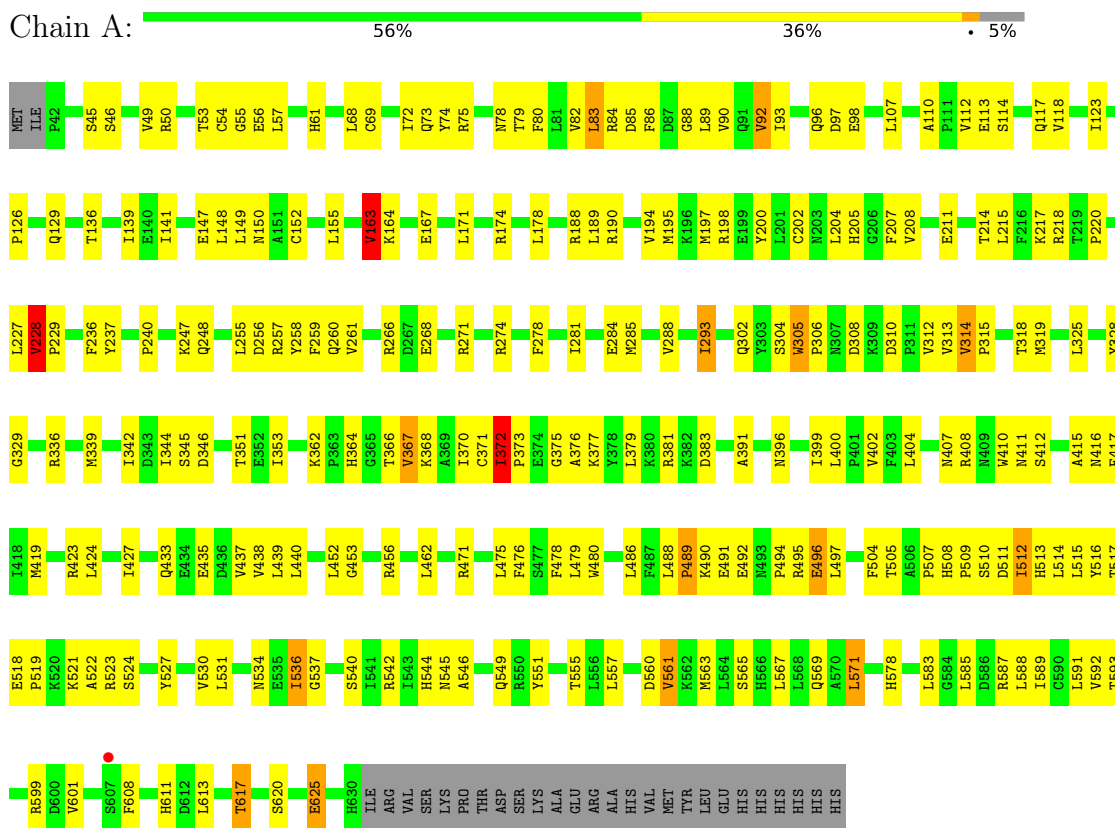
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Chain	Residue	Modelled	Actual	Comment	Reference
B	654	HIS	-	expression tag	UNP Q6PI48
B	655	HIS	-	expression tag	UNP Q6PI48
B	656	HIS	-	expression tag	UNP Q6PI48
C	40	MET	-	expression tag	UNP Q6PI48
C	646	VAL	-	expression tag	UNP Q6PI48
C	647	MET	-	expression tag	UNP Q6PI48
C	648	TYR	-	expression tag	UNP Q6PI48
C	649	LEU	-	expression tag	UNP Q6PI48
C	650	GLU	-	expression tag	UNP Q6PI48
C	651	HIS	-	expression tag	UNP Q6PI48
C	652	HIS	-	expression tag	UNP Q6PI48
C	653	HIS	-	expression tag	UNP Q6PI48
C	654	HIS	-	expression tag	UNP Q6PI48
C	655	HIS	-	expression tag	UNP Q6PI48
C	656	HIS	-	expression tag	UNP Q6PI48
D	40	MET	-	expression tag	UNP Q6PI48
D	646	VAL	-	expression tag	UNP Q6PI48
D	647	MET	-	expression tag	UNP Q6PI48
D	648	TYR	-	expression tag	UNP Q6PI48
D	649	LEU	-	expression tag	UNP Q6PI48
D	650	GLU	-	expression tag	UNP Q6PI48
D	651	HIS	-	expression tag	UNP Q6PI48
D	652	HIS	-	expression tag	UNP Q6PI48
D	653	HIS	-	expression tag	UNP Q6PI48
D	654	HIS	-	expression tag	UNP Q6PI48
D	655	HIS	-	expression tag	UNP Q6PI48
D	656	HIS	-	expression tag	UNP Q6PI48

3 Residue-property plots [i](#)

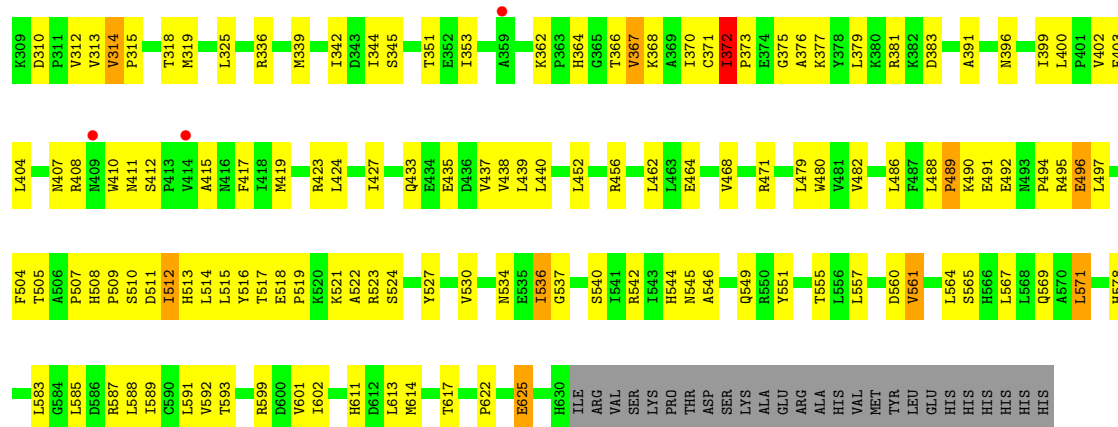
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

• Molecule 1: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL



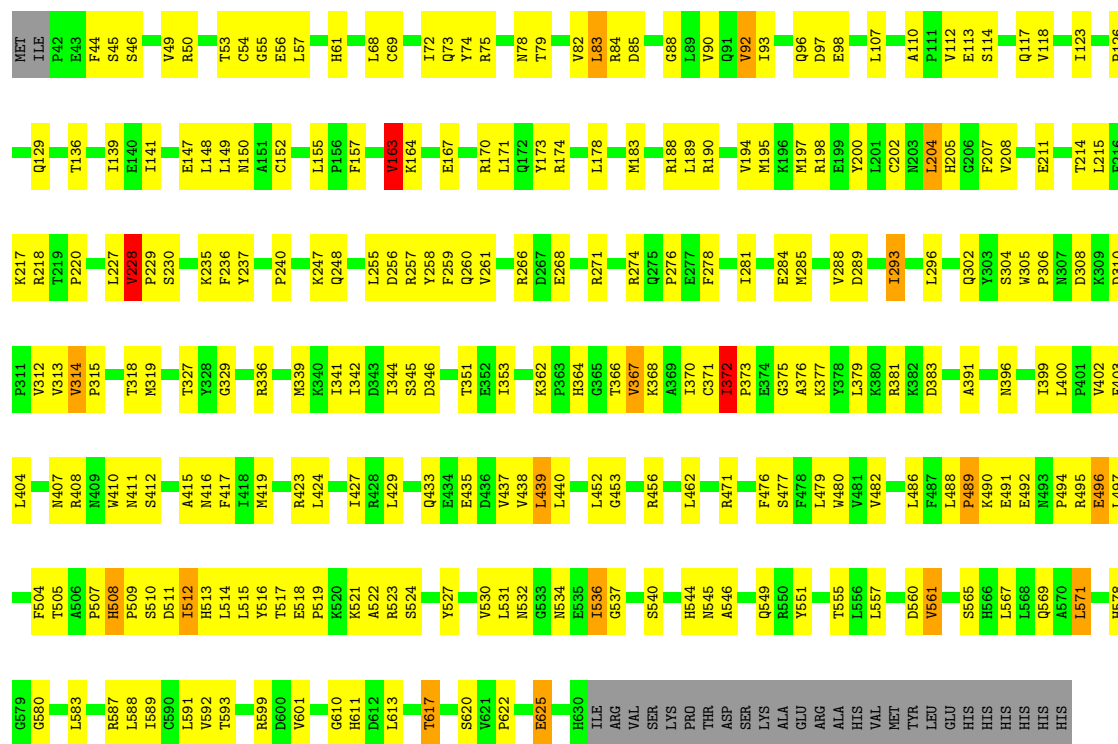
• Molecule 1: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL





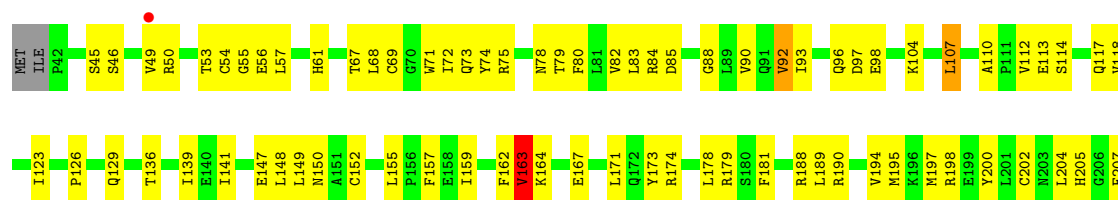
• Molecule 1: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL

Chain C: 55% 37% 5%



• Molecule 1: ASPARTATE-TRNA LIGASE, MITOCHONDRIAL

Chain D: 55% 38% 5%



L571	R495	N396	Q302	V208
H578	E496	I399	Y303	E211
L583	F504	L400	S304	T214
L585	T505	P401	W305	L215
	A506	V402	N307	F216
	P507	F403	D308	K217
L588	H508	L404	K309	R218
I589	S509		D310	T219
C590	S510	M407	P311	P220
L591	D511	R408	V312	
V592	H512	M409	V313	L227
T593	E513	W410	V314	V228
	L514	M411	P315	P229
R599	L515	S412		S230
D600	Y516	P413	T318	E231
V601	T517	V414	M319	E232
I602	E518	A415		P233
		M416	D334	G234
H611	A522	F417	T335	K235
D612	R523	I418	R336	F236
L613	S524	M419		Y237
			M339	S238
T617	Y527	R423		L239
		L424	I342	P240
P622	V530	I427	D343	
E625	L531		S345	K247
	N534	Q433	D346	Q248
H630	E535	E434		L255
ILE	I536	D435	T351	D256
ARG	G537	E436	F352	R257
VAL		V437	I353	Y258
	S540	V438		F259
SER	I541	L439	K362	Q260
LYS	R542	L440	P363	V261
PRO	I543		H364	
THR	H544		G365	Y265
ASP	N545	L452	T366	R266
SER	A546		V367	
ALA	E547	R456	K368	S270
GLU	L548	L462	A369	R271
ARG	Q549		I370	P272
ALA	R550	F476	C371	
HIS	V551		I372	Q275
VAL		L479	P373	P276
MET	T555	W480	E374	E277
TYR	L556	V481	G375	F278
LEU	L557	V482	A376	
GLU			K377	I281
HIS	D560	L486	Y378	
HIS	V561	F487	L379	E284
HIS		L488	K380	M285
HIS	S565	P489	R381	
HIS	H566	K490	K382	V288
HIS	L567	E491	D383	
	L568	E492		I293
	Q569	M493	A391	
	A570	P494	A392	L296

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.40Å 82.60Å 146.30Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	29.92 – 3.70 29.92 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.92-3.70) 98.6 (29.92-3.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.75Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.280 0.222 , 0.281	Depositor DCC
R_{free} test set	1782 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18840	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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	0.38	0/4819	0.90	14/6529 (0.2%)
1	B	0.39	0/4819	0.89	16/6529 (0.2%)
1	C	0.39	0/4819	0.90	17/6529 (0.3%)
1	D	0.39	0/4819	0.89	16/6529 (0.2%)
All	All	0.39	0/19276	0.90	63/26116 (0.2%)

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	372	ILE	CA-C-N	7.55	127.31	119.76
1	D	372	ILE	C-N-CA	7.55	127.31	119.76
1	C	488	LEU	CA-C-N	7.29	126.80	118.85
1	C	488	LEU	C-N-CA	7.29	126.80	118.85
1	A	488	LEU	CA-C-N	7.16	126.65	118.85

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	4710	0	4729	195	0
1	B	4710	0	4729	213	0
1	C	4710	0	4729	205	1
1	D	4710	0	4729	211	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18840	0	18916	754	1

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 20.

The worst 5 of 754 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:195:MET:CE	1:B:198:ARG:HG3	1.46	1.43
1:A:195:MET:HE1	1:B:198:ARG:CG	1.52	1.38
1:C:198:ARG:HG3	1:D:195:MET:CE	1.52	1.37
1:C:198:ARG:CG	1:D:195:MET:HE1	1.58	1.30
1:D:162:PHE:CE1	1:D:181:PHE:HB3	1.91	1.05

All (1) 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:C:517:THR:OG1	1:D:547:GLU:OE2[1_545]	2.18	0.02

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	587/617 (95%)	512 (87%)	71 (12%)	4 (1%)	18	50
1	B	587/617 (95%)	510 (87%)	73 (12%)	4 (1%)	18	50
1	C	587/617 (95%)	512 (87%)	71 (12%)	4 (1%)	18	50
1	D	587/617 (95%)	511 (87%)	72 (12%)	4 (1%)	18	50
All	All	2348/2468 (95%)	2045 (87%)	287 (12%)	16 (1%)	18	50

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	ILE
1	B	512	ILE
1	C	512	ILE
1	D	512	ILE
1	A	163	VAL

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	525/551 (95%)	501 (95%)	24 (5%)	24	49
1	B	525/551 (95%)	505 (96%)	20 (4%)	29	53
1	C	525/551 (95%)	502 (96%)	23 (4%)	25	50
1	D	525/551 (95%)	503 (96%)	22 (4%)	26	51
All	All	2100/2204 (95%)	2011 (96%)	89 (4%)	26	51

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	372	ILE
1	D	155	LEU
1	C	439	LEU
1	C	617	THR
1	D	228	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	GLN
1	D	78	ASN
1	C	422	GLN
1	C	544	HIS
1	D	205	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 oligosaccharides 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	589/617 (95%)	-0.13	1 (0%) 91 80	55, 102, 161, 211	0
1	B	589/617 (95%)	-0.12	3 (0%) 87 69	54, 104, 163, 205	0
1	C	589/617 (95%)	-0.08	0 100 100	53, 104, 162, 204	0
1	D	589/617 (95%)	-0.13	2 (0%) 90 76	53, 101, 160, 198	0
All	All	2356/2468 (95%)	-0.12	6 (0%) 90 76	53, 103, 162, 211	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	VAL	3.3
1	B	409	ASN	2.7
1	B	359	ALA	2.3
1	B	414	VAL	2.1
1	D	630	HIS	2.1

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 oligosaccharides 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.