



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2017 – 05:11 PM EDT

PDB ID : 2HHF
Title : X-ray crystal structure of oxidized human mitochondrial branched chain aminotransferase (hBCATm)
Authors : Yennawar, N.H.; Hutson, S.M.
Deposited on : unknown
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

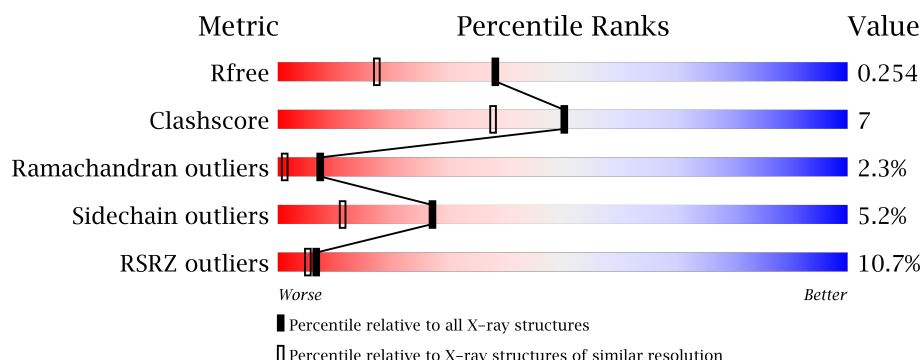
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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. 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	365	<div> <div>9%</div> <div>79%</div> <div>12%</div> <div>5%</div> </div>
2	B	365	<div> <div>12%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5994 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 Branched-chain-amino-acid aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	3	1
			2799	1795	488	498	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	OCS	CYS	MODIFIED RESIDUE	UNP O15382
A	141	TYO	TYR	MODIFIED RESIDUE	UNP O15382
A	159	ARG	THR	CONFLICT	UNP O15382

- Molecule 2 is a protein called Branched-chain-amino-acid aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	365	Total	C	N	O	S	0	4	0
			2944	1893	513	520	18			

There are 2 discrepancies between the modelled and reference sequences:

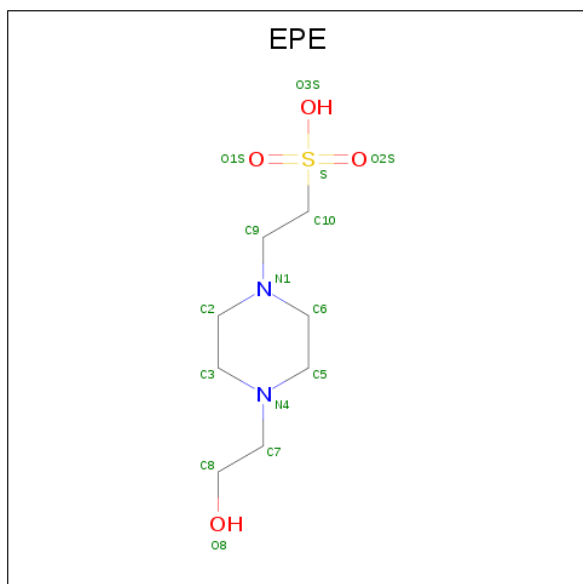
Chain	Residue	Modelled	Actual	Comment	Reference
B	608	OCS	CYS	MODIFIED RESIDUE	UNP O15382
B	659	ARG	THR	CONFLICT	UNP O15382

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

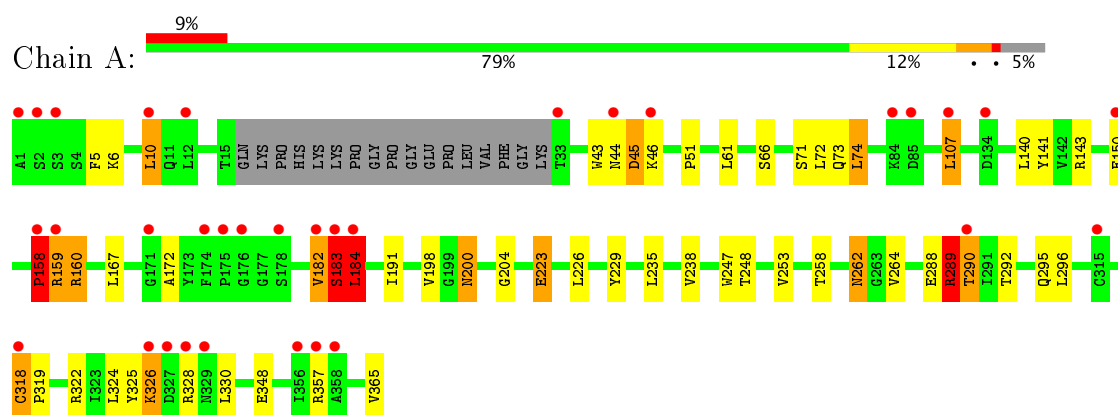
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total 97	O 97	0	0
5	B	109	Total 109	O 109	0	0

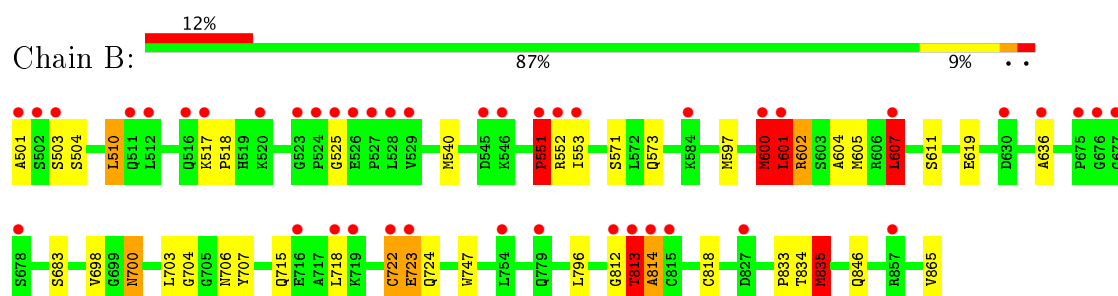
3 Residue-property plots

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: Branched-chain-amino-acid aminotransferase, mitochondrial



- Molecule 2: Branched-chain-amino-acid aminotransferase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.12Å 104.18Å 58.26Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (30.00-1.80) 91.9 (29.69-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.283 0.252 , 0.254	Depositor DCC
R_{free} test set	2949 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5994	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: OCS, EPE, TYO, PLP

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	0.69	0/2843	0.89	9/3855 (0.2%)
2	B	0.70	0/3011	0.87	3/4085 (0.1%)
All	All	0.69	0/5854	0.88	12/7940 (0.2%)

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	6
2	B	0	9
All	All	0	15

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	VAL	CA-C-N	-9.42	96.47	117.20
2	B	722	CYS	CA-C-N	-8.24	99.08	117.20
1	A	158	PRO	N-CA-C	7.68	132.06	112.10
1	A	107	LEU	CA-CB-CG	6.89	131.14	115.30
1	A	74	LEU	CA-CB-CG	6.86	131.09	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	A	182	VAL	Mainchain
1	A	289	ARG	Mainchain
2	B	551	PRO	Mainchain
2	B	600	MET	Mainchain

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	2799	0	2799	47	0
2	B	2944	0	2953	33	0
3	A	15	0	6	0	0
3	B	15	0	6	0	0
4	B	15	0	17	0	0
5	A	97	0	0	5	0
5	B	109	0	0	5	0
All	All	5994	0	5781	76	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 7.

The worst 5 of 76 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:200:ASN:HD22	1:A:200:ASN:H	1.15	0.94
1:A:183[A]:SER:HB3	1:A:223:GLU:H	1.35	0.91
1:A:184:LEU:HD21	1:A:238:VAL:HG13	1.60	0.83
1:A:289:ARG:HG2	1:A:290[B]:THR:H	1.40	0.83
2:B:700:ASN:HD22	2:B:700:ASN:H	1.26	0.82

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	345/365 (94%)	319 (92%)	16 (5%)	10 (3%)	5	1
2	B	366/365 (100%)	336 (92%)	18 (5%)	12 (3%)	4	0
All	All	711/730 (97%)	655 (92%)	34 (5%)	22 (3%)	7	0

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	159[A]	ARG
1	A	159[B]	ARG
1	A	160	ARG
1	A	172	ALA

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	301/314 (96%)	282 (94%)	19 (6%)	21	7
2	B	318/315 (101%)	302 (95%)	16 (5%)	28	12
All	All	619/629 (98%)	584 (94%)	35 (6%)	27	9

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	318	CYS

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Mol	Chain	Res	Type
2	B	510	LEU
2	B	835	MET
1	A	324	LEU
1	A	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
2	B	550	GLN
2	B	700	ASN
1	A	242	ASN
1	A	249	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	A	108	1	8,8,9	1.45	2 (25%)	7,11,13	2.52	4 (57%)
1	TYO	A	141	1	12,13,14	2.66	5 (41%)	7,14,16	1.49	1 (14%)
2	OCS	B	608	2	8,8,9	1.59	2 (25%)	7,11,13	2.58	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	A	108	1	-	1/4/7/9	0/0/0/0
1	TYO	A	141	1	-	0/9/14/16	0/0/0/0
2	OCS	B	608	2	-	1/4/7/9	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	OCS	OD3-SG	-2.62	1.37	1.45
1	A	108	OCS	OD3-SG	-2.09	1.39	1.45
1	A	141	TYO	OE1-CE1	2.27	1.43	1.33
1	A	141	TYO	CA-C	2.31	1.53	1.50
1	A	108	OCS	CA-C	2.83	1.54	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	608	OCS	OD3-SG-CB	-5.01	102.54	106.83
1	A	108	OCS	OD1-SG-CB	-4.89	102.65	106.83
2	B	608	OCS	OD1-SG-CB	-2.48	104.71	106.83
2	B	608	OCS	OD2-SG-CB	-2.27	103.23	106.01
1	A	108	OCS	OD3-SG-CB	-2.26	104.90	106.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	608	OCS	SG-CB-CA-N
1	A	108	OCS	SG-CB-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	141	TYO	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	A	400	1	15,15,16	1.59	3 (20%)	20,22,23	1.67	6 (30%)
3	PLP	B	401	2	15,15,16	1.70	3 (20%)	20,22,23	1.81	6 (30%)
4	EPE	B	430	-	15,15,15	1.44	3 (20%)	18,20,20	0.96	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	400	1	-	0/6/6/8	0/1/1/1
3	PLP	B	401	2	-	0/6/6/8	0/1/1/1
4	EPE	B	430	-	-	0/9/19/19	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	PLP	C5-C4	2.07	1.42	1.40
3	A	400	PLP	C5-C4	2.11	1.43	1.40
4	B	430	EPE	C6-N1	2.53	1.53	1.47
4	B	430	EPE	C2-N1	2.57	1.53	1.47
3	B	401	PLP	C4A-C4	2.66	1.57	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	PLP	O2P-P-O4P	-3.15	98.36	106.73
3	A	400	PLP	O2P-P-O4P	-2.77	99.36	106.73
3	B	401	PLP	C5A-C5-C6	-2.46	115.10	119.33
4	B	430	EPE	C9-N1-C6	-2.33	105.28	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	400	PLP	C5A-C5-C6	-2.28	115.41	119.33

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 [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	346/365 (94%)	0.65	33 (9%) 9 7	13, 22, 37, 47	0
2	B	364/365 (99%)	0.77	43 (11%) 5 4	13, 22, 40, 48	0
All	All	710/730 (97%)	0.71	76 (10%) 7 5	13, 22, 39, 48	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	601[A]	LEU	15.2
2	B	813[A]	THR	12.0
1	A	290[A]	THR	11.9
1	A	159[A]	ARG	10.4
2	B	501	ALA	9.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	OCS	A	108	9/10	0.71	0.32	-	29,33,39,39	0
2	OCS	B	608	9/10	0.75	0.21	-	28,32,38,38	0
1	TYO	A	141	14/15	0.78	0.20	-	19,25,34,37	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PLP	A	400	15/16	0.96	0.13	0.37	17,19,20,23	0
4	EPE	B	430	15/15	0.74	0.21	0.15	37,40,46,46	0
3	PLP	B	401	15/16	0.96	0.10	-0.46	15,19,22,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.