



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:41 PM GMT

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 : 2006-06-28
Resolution : 1.80 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

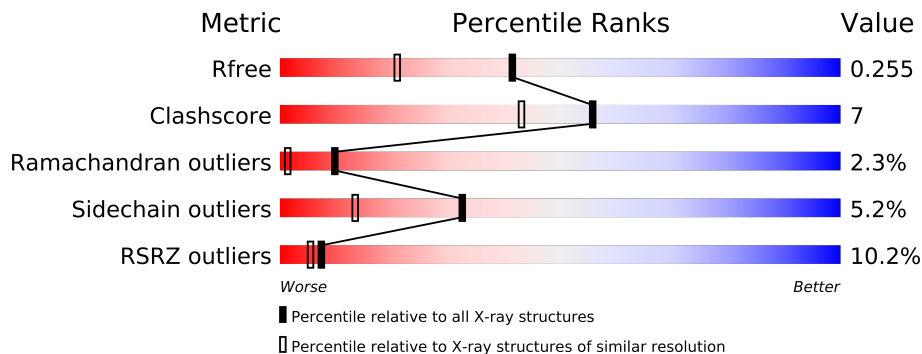
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
2	B	365	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5994 atoms, of which 0 are hydrogen and 0 are deuterium.

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-acidaminotransferase, mitochondrial.

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

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

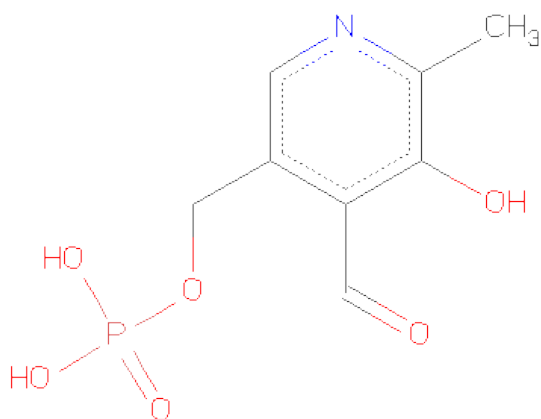
- Molecule 2 is a protein called Branched-chain-amino-acidaminotransferase, mitochondrial.

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

There are 2 discrepancies between the modelled and reference sequences:

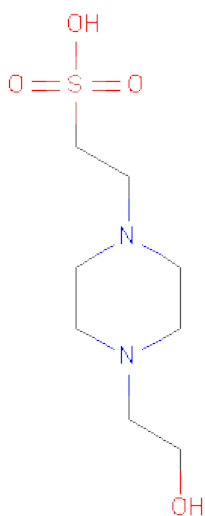
Chain	Residue	Modelled	Actual	Comment	Reference
B	608	OCS	CYS	MODIFIED RESIDUE	UNP O15382
B	659	ARG	THR	CONFLICT	UNP O15382

- 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-PIPERAZINEETHANESULFONIC 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.

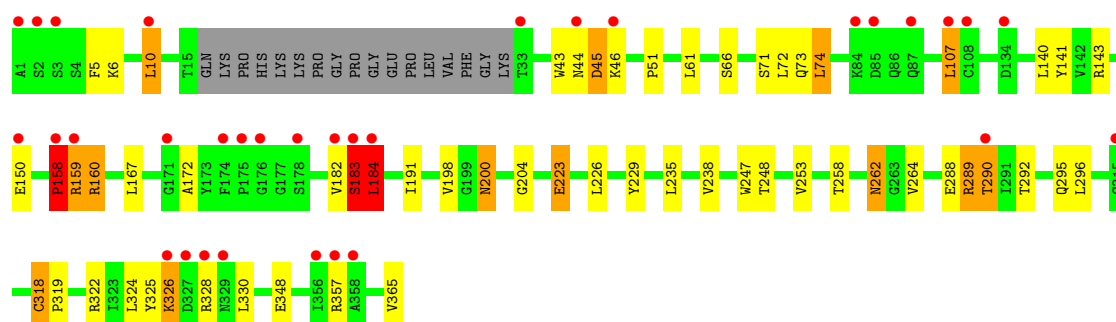
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total 97	O 97	0	0
5	B	109	Total 109	O 109	0	0

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 errors 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.

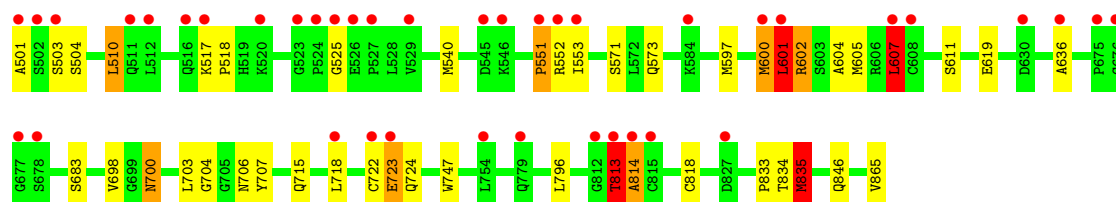
- Molecule 1: Branched-chain-amino-acidaminotransferase, mitochondrial

Chain A: 



- Molecule 2: Branched-chain-amino-acidaminotransferase, mitochondrial

Chain B: 



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 0.253 , 0.255	Depositor DCC
R_{free} test set	2945 reflections (5.35%)	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 , 29.0	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 58516 reflections	Xtriage
F_o, F_c correlation	0.91	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.

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
2	B	0	1

There are no bond length outliers.

All (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
1	A	184	LEU	N-CA-C	6.62	128.88	111.00
1	A	184	LEU	CA-CB-CG	6.12	129.37	115.30
2	B	551	PRO	CA-C-N	-5.56	104.97	117.20
1	A	107	LEU	CB-CA-C	-5.49	99.77	110.20
2	B	607	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	10	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	248	THR	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	707	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (76) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:159[B]:ARG:O	1:A:160:ARG:HB2	1.78	0.82
1:A:290[A]:THR:O	5:A:402:HOH:O	1.98	0.81
2:B:683:SER:H	2:B:723[A]:GLU:HB2	1.55	0.70
1:A:73:GLN:HE22	2:B:571:SER:H	1.41	0.68
1:A:253:VAL:N	5:A:472:HOH:O	2.27	0.67
1:A:183[A]:SER:HB3	1:A:223:GLU:N	2.07	0.67
2:B:540:MET:HB3	2:B:552[B]:ARG:HB2	1.77	0.65
1:A:183[B]:SER:O	1:A:322:ARG:O	2.14	0.64
1:A:71:SER:H	2:B:573:GLN:HE22	1.46	0.63
1:A:200:ASN:ND2	1:A:200:ASN:H	1.93	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:ASN:N	1:A:200:ASN:HD22	1.95	0.62
2:B:813[B]:THR:O	2:B:814:ALA:HB2	1.99	0.62
2:B:723[A]:GLU:O	2:B:724:GLN:HB2	2.02	0.60
2:B:501:ALA:N	2:B:611:SER:HG	2.01	0.56
2:B:601[A]:LEU:HD13	2:B:611:SER:HB2	1.88	0.56
2:B:834:THR:O	2:B:835:MET:HB2	2.07	0.55
1:A:150:GLU:HG3	1:A:159[B]:ARG:HB2	1.89	0.54
2:B:601[A]:LEU:HA	2:B:604:ALA:HB3	1.89	0.53
1:A:5:PHE:HB2	1:A:51:PRO:HD3	1.90	0.53
1:A:43:TRP:HZ3	1:A:159[A]:ARG:HA	1.75	0.52
1:A:73:GLN:NE2	2:B:571:SER:H	2.06	0.52
2:B:607:LEU:HD11	2:B:703:LEU:HD22	1.92	0.52
1:A:290[A]:THR:HG22	5:A:447:HOH:O	2.10	0.51
2:B:715:GLN:HA	2:B:718:LEU:HD12	1.94	0.50
1:A:159[B]:ARG:O	1:A:160:ARG:CB	2.57	0.50
2:B:700:ASN:ND2	2:B:700:ASN:H	2.02	0.50
1:A:73:GLN:HE21	1:A:204:GLY:HA3	1.76	0.50
1:A:290[B]:THR:O	1:A:295:GLN:NE2	2.27	0.49
1:A:141:TYO:CZ	1:A:141:TYO:HE1	2.42	0.49
1:A:328:ARG:HE	1:A:330:LEU:HD21	1.78	0.49
1:A:289:ARG:CG	1:A:290[B]:THR:H	2.10	0.49
1:A:158:PRO:O	1:A:160:ARG:N	2.46	0.49
2:B:813[B]:THR:HG23	5:B:69:HOH:O	2.12	0.49
2:B:600:MET:O	2:B:602:ARG:N	2.46	0.49
2:B:573:GLN:HE21	2:B:704:GLY:HA3	1.78	0.48
2:B:597:MET:O	2:B:601[B]:LEU:HB2	2.14	0.48
2:B:813[B]:THR:O	2:B:814:ALA:CB	2.63	0.47
1:A:43:TRP:CZ3	1:A:159[A]:ARG:HA	2.50	0.46
1:A:71:SER:H	2:B:573:GLN:NE2	2.12	0.46
1:A:191:ILE:HD11	1:A:229:TYR:HD1	1.80	0.46
2:B:700:ASN:N	2:B:700:ASN:HD22	2.04	0.45
2:B:683:SER:OG	2:B:723[A]:GLU:HG2	2.16	0.45
1:A:72:LEU:HD22	1:A:107:LEU:O	2.17	0.45
1:A:191:ILE:HD11	1:A:229:TYR:CD1	2.52	0.45
1:A:66:SER:HB2	1:A:72:LEU:HD12	1.99	0.45
2:B:552[A]:ARG:O	2:B:553:ILE:HB	2.17	0.45
2:B:706:ASN:ND2	5:B:112:HOH:O	2.51	0.44
1:A:292:THR:H	1:A:295:GLN:HE21	1.65	0.44
1:A:184:LEU:HD13	1:A:226:LEU:HB2	2.00	0.44
1:A:183[B]:SER:O	1:A:184:LEU:HB2	2.18	0.43
2:B:724:GLN:NE2	5:B:206:HOH:O	2.51	0.43
1:A:262:ASN:HD21	1:A:264:VAL:HG22	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:601[A]:LEU:O	2:B:605:MET:HB2	2.19	0.43
1:A:141:TYO:CZ	1:A:143:ARG:HH21	2.31	0.43
2:B:813[A]:THR:HG21	5:B:150:HOH:O	2.18	0.43
2:B:551:PRO:O	2:B:552[A]:ARG:HB3	2.18	0.43
1:A:290[B]:THR:O	5:A:464:HOH:O	2.21	0.42
2:B:517:LYS:HA	2:B:518:PRO:HD2	1.92	0.42
1:A:46:LYS:H	1:A:46:LYS:HD2	1.84	0.42
1:A:258:THR:O	1:A:288:GLU:HA	2.19	0.42
1:A:183[B]:SER:HB2	1:A:322:ARG:N	2.34	0.41
1:A:140:LEU:HD21	1:A:167:LEU:HD13	2.02	0.41
1:A:322:ARG:HA	1:A:330:LEU:O	2.21	0.41
2:B:510:LEU:HD12	2:B:551:PRO:HB2	2.02	0.41
1:A:325:TYR:O	1:A:326:LYS:HG3	2.21	0.41
1:A:66:SER:HB3	5:A:450:HOH:O	2.20	0.41
1:A:318:CYS:HA	1:A:319:PRO:HD2	1.92	0.41
1:A:235:LEU:HD21	1:A:296:LEU:HD22	2.02	0.40
2:B:503:SER:HB3	2:B:504:SER:H	1.75	0.40
1:A:348:GLU:HG3	1:A:357:ARG:HH22	1.86	0.40
2:B:601[B]:LEU:HD22	5:B:17:HOH:O	2.22	0.40

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	345/365 (94%)	319 (92%)	16 (5%)	10 (3%)	7	1
2	B	366/365 (100%)	336 (92%)	18 (5%)	12 (3%)	6	0
All	All	711/730 (97%)	655 (92%)	34 (5%)	22 (3%)	10	0

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASP

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Mol	Chain	Res	Type
1	A	159[A]	ARG
1	A	159[B]	ARG
1	A	160	ARG
1	A	172	ALA
1	A	183[A]	SER
1	A	183[B]	SER
1	A	290[A]	THR
1	A	290[B]	THR
2	B	601[A]	LEU
2	B	601[B]	LEU
2	B	602	ARG
2	B	723[A]	GLU
2	B	723[B]	GLU
2	B	813[A]	THR
2	B	813[B]	THR
2	B	636	ALA
2	B	814	ALA
2	B	835	MET
1	A	184	LEU
2	B	525	GLY
2	B	833	PRO

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	301/314 (96%)	282 (94%)	19 (6%)	25	9
2	B	318/315 (101%)	302 (95%)	16 (5%)	34	14
All	All	619/629 (98%)	584 (94%)	35 (6%)	32	11

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	10	LEU
1	A	44	ASN
1	A	45	ASP

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Mol	Chain	Res	Type
1	A	61	LEU
1	A	74	LEU
1	A	158	PRO
1	A	183[A]	SER
1	A	183[B]	SER
1	A	198	VAL
1	A	200	ASN
1	A	223	GLU
1	A	247	TRP
1	A	262	ASN
1	A	289	ARG
1	A	318	CYS
1	A	324	LEU
1	A	326	LYS
1	A	365	VAL
2	B	510	LEU
2	B	600	MET
2	B	601[A]	LEU
2	B	601[B]	LEU
2	B	607	LEU
2	B	619	GLU
2	B	698	VAL
2	B	700	ASN
2	B	747	TRP
2	B	796	LEU
2	B	813[A]	THR
2	B	813[B]	THR
2	B	818	CYS
2	B	835	MET
2	B	846	GLN
2	B	865	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	54	GLN
1	A	57	GLN
1	A	73	GLN
1	A	200	ASN
1	A	206	ASN
1	A	234	GLN

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Mol	Chain	Res	Type
1	A	242	ASN
1	A	249	HIS
1	A	262	ASN
2	B	550	GLN
2	B	554	GLN
2	B	573	GLN
2	B	586	GLN
2	B	587	GLN
2	B	657	GLN
2	B	700	ASN
2	B	706	ASN
2	B	724	GLN
2	B	795	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	6.67	3 (37%)	9,11,13	7.77	5 (55%)
1	TYO	A	141	1	13,13,14	5.54	6 (46%)	11,14,16	2.12	2 (18%)
2	OCS	B	608	2	8,8,9	6.81	4 (50%)	9,11,13	6.76	3 (33%)

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	-	0/5/7/9	0/0/0/0
1	TYO	A	141	1	-	0/10/14/16	0/0/0/0
2	OCS	B	608	2	-	0/5/7/9	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	OCS	O-C	18.48	1.24	1.11
1	A	108	OCS	O-C	18.08	1.23	1.11
1	A	141	TYO	O-C	17.83	1.23	1.11
1	A	141	TYO	CE2-CD2	5.21	1.59	1.43
1	A	141	TYO	CD1-CG	4.98	1.56	1.44
1	A	108	OCS	CB-CA	-3.36	1.49	1.53
2	B	608	OCS	CB-CA	-3.30	1.49	1.53
2	B	608	OCS	CA-C	3.02	1.54	1.48
1	A	108	OCS	CA-C	3.01	1.54	1.48
1	A	141	TYO	OH-CZ	2.97	1.43	1.36
1	A	141	TYO	OE1-CE1	2.74	1.43	1.33
1	A	141	TYO	CA-C	2.67	1.53	1.48
2	B	608	OCS	OD3-SG	-2.45	1.37	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	OCS	C-CA-N	-22.37	91.49	113.83
2	B	608	OCS	C-CA-N	-19.70	94.15	113.83
1	A	141	TYO	C-CA-N	-5.47	108.36	113.83
1	A	108	OCS	CB-CA-N	-3.96	103.81	110.16
2	B	608	OCS	OD2-SG-OD3	3.15	118.59	111.78
1	A	108	OCS	OD2-SG-OD3	3.14	118.58	111.78
1	A	141	TYO	CD1-CG-CD2	3.00	123.84	119.02
2	B	608	OCS	OD3-SG-CB	-2.56	102.54	107.03
1	A	108	OCS	OD1-SG-CB	-2.50	102.65	107.03
1	A	108	OCS	CA-CB-SG	2.39	119.70	114.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	14,15,16	1.43	3 (21%)	20,22,23	1.63	5 (25%)
3	PLP	B	401	2	14,15,16	1.56	3 (21%)	20,22,23	1.74	6 (30%)
4	EPE	B	430	-	15,15,15	1.39	3 (20%)	20,20,20	0.92	2 (10%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	PLP	C2A-C2	3.32	1.57	1.50
3	A	400	PLP	C2A-C2	2.91	1.56	1.50
4	B	430	EPE	C10-S	2.84	1.81	1.77
4	B	430	EPE	C2-N1	2.53	1.53	1.47
4	B	430	EPE	C6-N1	2.49	1.53	1.47
3	A	400	PLP	C4-C5	2.21	1.43	1.39
3	B	401	PLP	C4-C5	2.18	1.42	1.39
3	B	401	PLP	P-O1P	-2.03	1.44	1.51
3	A	400	PLP	P-O1P	-2.01	1.44	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	PLP	O4P-C5A-C5	3.44	116.25	109.26
3	B	401	PLP	O4P-C5A-C5	3.26	115.89	109.26
3	B	401	PLP	O3P-P-O1P	3.20	120.90	110.44
3	B	401	PLP	O2P-P-O4P	-3.00	98.36	106.65
3	A	400	PLP	O3P-P-O1P	3.00	120.25	110.44
3	A	400	PLP	O2P-P-O4P	-2.64	99.36	106.65
4	B	430	EPE	C9-N1-C6	-2.34	105.28	111.32
3	B	401	PLP	O4P-P-O1P	2.34	113.56	106.71
4	B	430	EPE	C7-N4-C3	2.25	117.13	111.32
3	B	401	PLP	C5A-C5-C6	-2.21	115.10	119.28
3	B	401	PLP	C3-C4-C5	-2.07	117.38	121.29
3	A	400	PLP	C5A-C5-C6	-2.05	115.41	119.28
3	A	400	PLP	C3-C4-C5	-2.04	117.43	121.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	347/365 (95%)	0.64	33 (9%) 8 6	13, 22, 37, 47	0
2	B	365/365 (100%)	0.74	40 (10%) 6 5	13, 22, 40, 48	0
All	All	712/730 (97%)	0.69	73 (10%) 7 5	13, 22, 39, 48	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	601[A]	LEU	13.7
1	A	290[A]	THR	11.4
1	A	159[A]	ARG	11.3
2	B	813[A]	THR	10.7
1	A	175	PRO	9.7
2	B	552[A]	ARG	9.4
2	B	525	GLY	9.3
2	B	501	ALA	9.1
2	B	502	SER	7.0
1	A	183[A]	SER	6.9
1	A	1	ALA	6.9
2	B	524	PRO	6.6
2	B	676	GLY	6.5
2	B	607	LEU	6.3
2	B	723[A]	GLU	6.2
2	B	526	GLU	6.0
2	B	523	GLY	5.4
2	B	511	GLN	5.3
1	A	2	SER	5.2
2	B	512	LEU	5.2
1	A	356	ILE	5.2
1	A	327	ASP	5.0
1	A	171	GLY	4.9
2	B	677	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	84	LYS	4.6
1	A	182	VAL	4.3
1	A	108	OCS	4.3
2	B	503	SER	4.1
1	A	3	SER	4.1
2	B	517	LYS	4.0
2	B	546	LYS	3.9
1	A	328	ARG	3.8
1	A	33	THR	3.8
2	B	520	LYS	3.7
2	B	527	PRO	3.6
1	A	326	LYS	3.6
2	B	516	GLN	3.4
2	B	545	ASP	3.3
2	B	754	LEU	3.3
1	A	358	ALA	3.2
2	B	551	PRO	3.2
1	A	329	ASN	3.2
1	A	357	ARG	3.1
2	B	722	CYS	3.1
2	B	636	ALA	3.1
1	A	178	SER	3.0
2	B	529	VAL	2.9
2	B	812	GLY	2.9
1	A	184	LEU	2.9
1	A	10	LEU	2.6
2	B	718	LEU	2.6
1	A	46	LYS	2.6
2	B	779	GLN	2.6
2	B	584	LYS	2.5
2	B	553	ILE	2.5
1	A	107	LEU	2.5
1	A	85	ASP	2.5
1	A	174	PHE	2.4
1	A	134	ASP	2.4
1	A	158	PRO	2.4
1	A	44	ASN	2.4
2	B	600	MET	2.3
2	B	814	ALA	2.3
2	B	675	PRO	2.3
2	B	678	SER	2.3
1	A	87	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	315	CYS	2.1
2	B	815	CYS	2.1
2	B	827	ASP	2.1
1	A	176	GLY	2.1
1	A	150	GLU	2.1
2	B	630	ASP	2.0
2	B	608	OCS	2.0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OCS	A	108	9/10	0.33	3.81	29,33,39,39	0
1	TYO	A	141	14/15	0.19	3.51	19,25,34,37	0
2	OCS	B	608	9/10	0.22	0.65	28,32,38,38	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EPE	B	430	15/15	0.20	0.11	37,40,46,46	0
3	PLP	A	400	15/16	0.12	-0.03	17,19,20,23	0
3	PLP	B	401	15/16	0.10	-0.48	15,19,22,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.