Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:31 AM 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

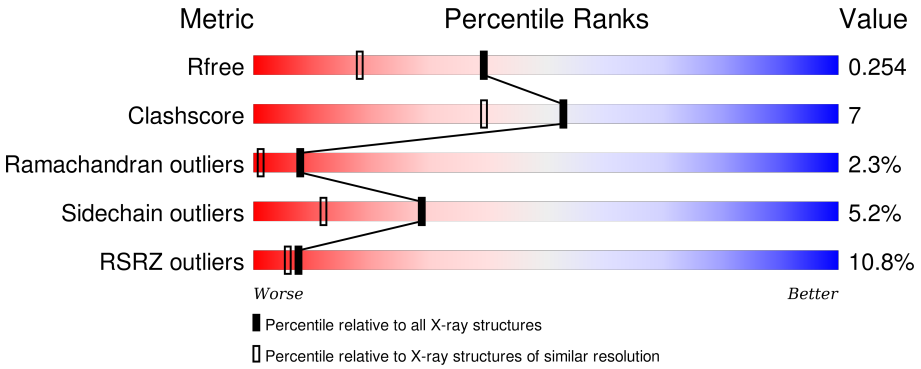
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 <=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	9% 79% 12% • • 5%
2	B	365	12% 87% 9% • •

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

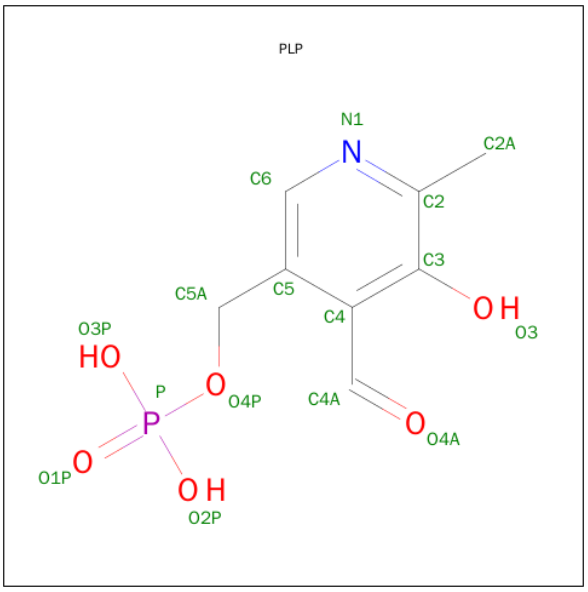
- Molecule 2 is a protein called Branched-chain-amino-acid aminotransferase, mitochondrial.

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:

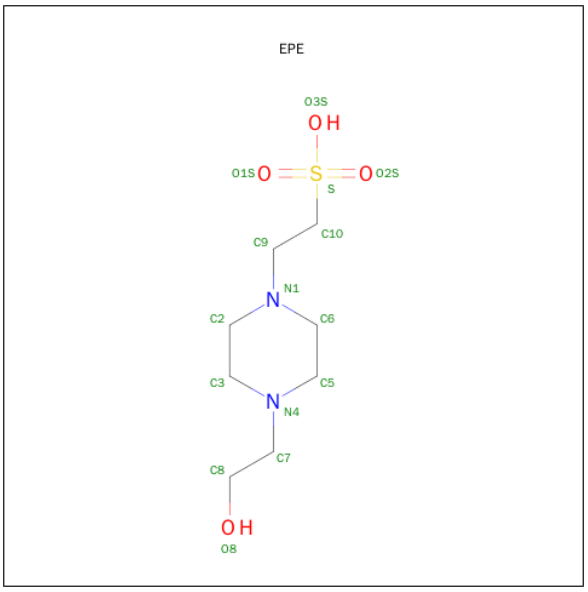
Chain	Residue	Modelled	Actual	Comment	Reference
B	608	OCS	CYS	MODIFIED RESIDUE	UNP O15382
B	659	ARG	THR	CONFLICT	UNP O15382

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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: $C_8H_{18}N_2O_4S$).



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

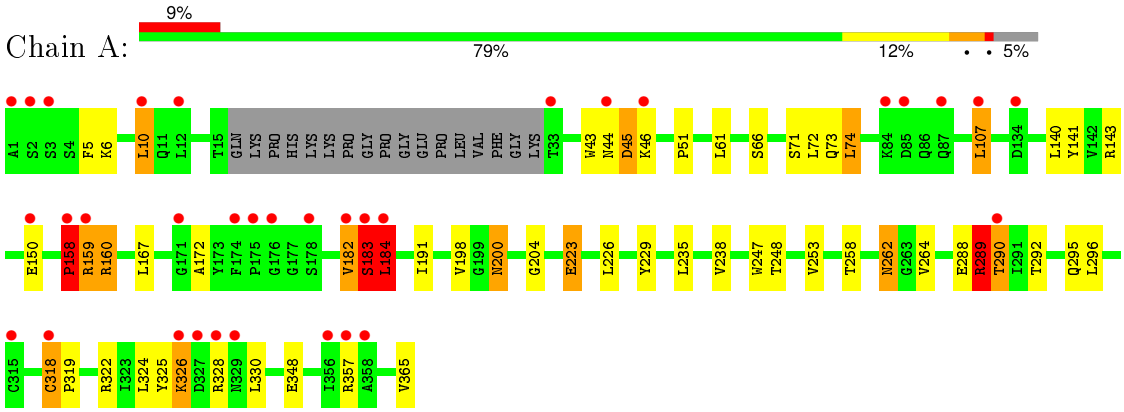
- Molecule 5 is water.

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

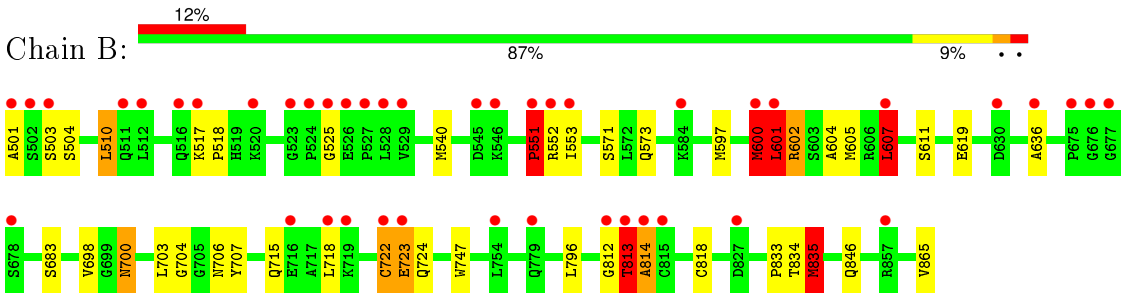
3 Residue-property plots (i)

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-acid aminotransferase, mitochondrial



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



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 58516 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PRO	Mainchain
1	A	182	VAL	Mainchain
1	A	289	ARG	Mainchain
2	B	551	PRO	Mainchain
2	B	600	MET	Mainchain
2	B	707	TYR	Sidechain
2	B	722	CYS	Mainchain
2	B	812	GLY	Mainchain

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	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.

All (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
1:A:159[B]:ARG:O	1:A:160:ARG:HB2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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%)	6 1
2	B	366/365 (100%)	336 (92%)	18 (5%)	12 (3%)	5 0
All	All	711/730 (97%)	655 (92%)	34 (5%)	22 (3%)	8 0

All (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
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 (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%)	22 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	318/315 (101%)	302 (95%)	16 (5%)	30 13
All	All	619/629 (98%)	584 (94%)	35 (6%)	29 10

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
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
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 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	7,8,9	1.16	1 (14%)	7,11,13	2.44	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TYO	A	141	1	10,13,14	2.72	4 (40%)	5,14,16	1.82	1 (20%)
2	OCS	B	608	2	7,8,9	1.31	1 (14%)	7,11,13	2.51	3 (42%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	OCS	OD3-SG	-2.54	1.37	1.45
1	A	108	OCS	OD3-SG	-2.04	1.39	1.45
1	A	141	TYO	OE1-CE1	2.29	1.43	1.33
1	A	141	TYO	OH-CZ	3.47	1.43	1.36
1	A	141	TYO	CE2-CD2	5.00	1.59	1.43
1	A	141	TYO	CD1-CG	5.42	1.56	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	608	OCS	OD3-SG-CB	-5.22	102.54	106.94
1	A	108	OCS	OD1-SG-CB	-5.09	102.65	106.94
2	B	608	OCS	OD1-SG-CB	-2.65	104.71	106.94
1	A	108	OCS	OD3-SG-CB	-2.42	104.90	106.94
1	A	108	OCS	OD2-SG-OD3	3.00	118.58	111.61
2	B	608	OCS	OD2-SG-OD3	3.00	118.59	111.61
1	A	141	TYO	CD1-CG-CD2	3.05	123.84	118.98

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1.56	4 (26%)	21,22,23	1.81	6 (28%)
3	PLP	B	401	2	15,15,16	1.67	4 (26%)	21,22,23	1.94	7 (33%)
4	EPE	B	430	-	14,15,15	1.25	2 (14%)	18,20,20	0.97	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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	PLP	P-O1P	-2.06	1.44	1.51
3	A	400	PLP	P-O1P	-2.03	1.44	1.51

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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	2.52	1.53	1.46
4	B	430	EPE	C2-N1	2.56	1.53	1.46
3	B	401	PLP	C4A-C4	2.62	1.57	1.51
3	A	400	PLP	C4A-C4	2.66	1.57	1.51
3	A	400	PLP	C2A-C2	2.92	1.56	1.50
3	B	401	PLP	C2A-C2	3.33	1.57	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	PLP	O2P-P-O4P	-2.85	98.36	106.56
3	A	400	PLP	O2P-P-O4P	-2.50	99.36	106.56
4	B	430	EPE	C9-N1-C6	-2.34	105.28	111.27
3	B	401	PLP	C5A-C5-C6	-2.21	115.10	119.28
3	A	400	PLP	C5A-C5-C6	-2.05	115.41	119.28
3	A	400	PLP	C4A-C4-C5	2.21	123.18	120.88
4	B	430	EPE	C7-N4-C3	2.29	117.13	111.27
3	A	400	PLP	C5A-C5-C4	2.43	124.86	121.65
3	B	401	PLP	C4A-C4-C5	2.49	123.48	120.88
3	B	401	PLP	O4P-P-O1P	2.52	113.56	107.14
3	B	401	PLP	C5A-C5-C4	2.54	125.01	121.65
3	A	400	PLP	O3P-P-O1P	3.00	120.25	110.58
3	B	401	PLP	O3P-P-O1P	3.21	120.90	110.58
3	B	401	PLP	O4P-C5A-C5	4.17	115.89	108.99
3	A	400	PLP	O4P-C5A-C5	4.39	116.25	108.99

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

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, 95^{th} 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%)	0.69	34 (9%)	10	7	13, 22, 37, 47	0
2	B	364/365 (99%)	0.82	43 (11%)	6	4	13, 22, 40, 48	0
All	All	710/730 (97%)	0.75	77 (10%)	8	6	13, 22, 39, 48	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	601[A]	LEU	15.5
2	B	813[A]	THR	12.1
1	A	290[A]	THR	12.0
1	A	159[A]	ARG	10.4
2	B	501	ALA	10.1
2	B	552[A]	ARG	9.8
2	B	525	GLY	9.8
1	A	175	PRO	9.5
2	B	502	SER	8.4
1	A	183[A]	SER	7.6
1	A	1	ALA	7.2
2	B	607	LEU	7.0
2	B	676	GLY	6.9
2	B	524	PRO	6.4
2	B	723[A]	GLU	6.4
1	A	2	SER	6.4
2	B	526	GLU	6.0
2	B	523	GLY	5.9
2	B	511	GLN	5.8
2	B	512	LEU	5.7
1	A	327	ASP	5.5
1	A	171	GLY	5.5
1	A	84	LYS	4.9
1	A	356	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	3	SER	4.7
2	B	677	GLY	4.4
2	B	503	SER	4.4
1	A	182	VAL	4.4
2	B	754	LEU	4.2
2	B	546	LYS	4.2
2	B	722	CYS	4.1
1	A	328	ARG	4.1
2	B	520	LYS	3.9
2	B	517	LYS	3.9
1	A	329	ASN	3.9
2	B	545	ASP	3.9
1	A	33	THR	3.6
1	A	184	LEU	3.6
2	B	516	GLN	3.4
1	A	357	ARG	3.4
1	A	326	LYS	3.4
1	A	178	SER	3.4
2	B	527	PRO	3.2
1	A	358	ALA	3.2
2	B	636	ALA	3.2
2	B	551	PRO	3.2
2	B	815	CYS	3.2
1	A	10	LEU	3.2
2	B	553	ILE	3.1
2	B	529	VAL	3.1
2	B	812	GLY	3.0
1	A	85	ASP	2.9
2	B	718	LEU	2.9
2	B	600	MET	2.8
1	A	46	LYS	2.8
1	A	107	LEU	2.8
1	A	134	ASP	2.8
2	B	675	PRO	2.7
2	B	584	LYS	2.7
1	A	315	CYS	2.5
2	B	779	GLN	2.5
1	A	158	PRO	2.5
2	B	827	ASP	2.5
2	B	814	ALA	2.5
1	A	150	GLU	2.4
1	A	12	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	44	ASN	2.3
1	A	318	CYS	2.2
1	A	176	GLY	2.2
2	B	528	LEU	2.2
2	B	630	ASP	2.2
2	B	678	SER	2.2
1	A	174	PHE	2.1
2	B	716	GLU	2.1
2	B	719	LYS	2.0
2	B	857	ARG	2.0
1	A	87	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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 (i)

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, 95^{th} 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
3	PLP	A	400	15/16	0.96	0.13	0.37	17,19,20,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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.