



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:49 am GMT

PDB ID : 5BWW  
Title : X-RAY CRYSTAL STRUCTURE AT 1.82Å RESOLUTION OF HUMAN MITOCHONDRIAL BRANCHED CHAIN AMINOTRANSFERASE (BCATM) COMPLEXED WITH A PYRROLIDINE AMIDE COMPOUND AND AN INTERNAL ALDIMINE LINKED PLP COFACTOR.  
Authors : SOMERS, D.O.  
Deposited on : 2015-06-08  
Resolution : 1.82 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](mailto: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.

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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	:	trunk28620
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)	:	recalc28949

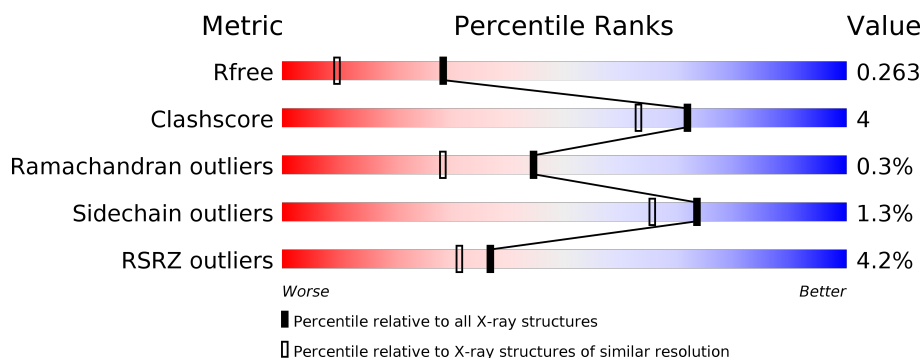
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

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  $\geq 3$ , 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	369	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	B	369	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div></div> </div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	407	-	-	-	X
4	EDO	A	408	-	-	-	X
4	EDO	B	405	-	-	-	X
4	EDO	B	409	-	-	-	X
6	GOL	A	411	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6572 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.

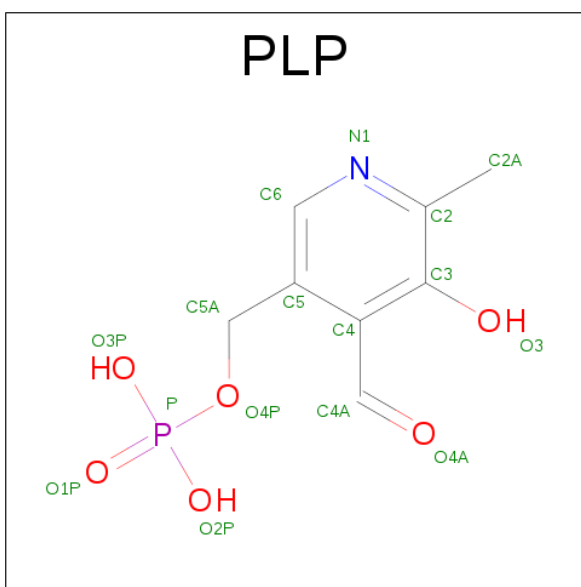
- Molecule 1 is a protein called Branched-chain-amino-acid aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	8	0
			2892	1862	507	503	20			
1	B	353	Total	C	N	O	S	0	2	0
			2838	1828	494	497	19			

There are 8 discrepancies between the modelled and reference sequences:

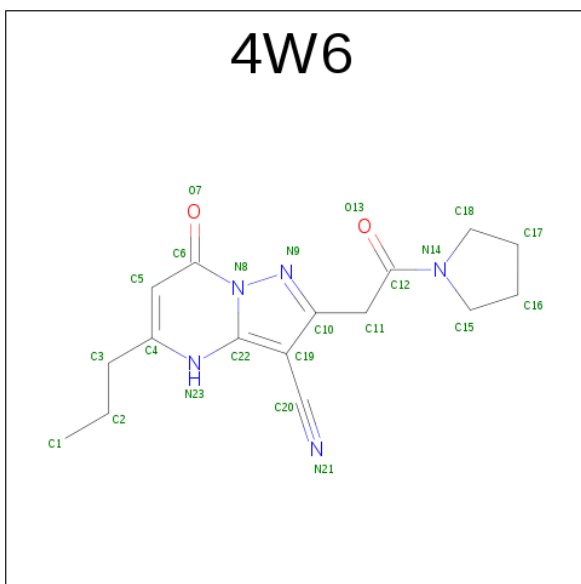
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O15382
A	-2	SER	-	expression tag	UNP O15382
A	-1	HIS	-	expression tag	UNP O15382
A	0	MET	-	expression tag	UNP O15382
B	-3	GLY	-	expression tag	UNP O15382
B	-2	SER	-	expression tag	UNP O15382
B	-1	HIS	-	expression tag	UNP O15382
B	0	MET	-	expression tag	UNP O15382

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

- Molecule 3 is 7-oxo-2-[2-oxo-2-(pyrrolidin-1-yl)ethyl]-5-propyl-4,7-dihydropyrazolo[1,5-a]pyrimidine-3-carbonitrile (three-letter code: 4W6) (formula: C<sub>16</sub>H<sub>19</sub>N<sub>5</sub>O<sub>2</sub>).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			23	16	5	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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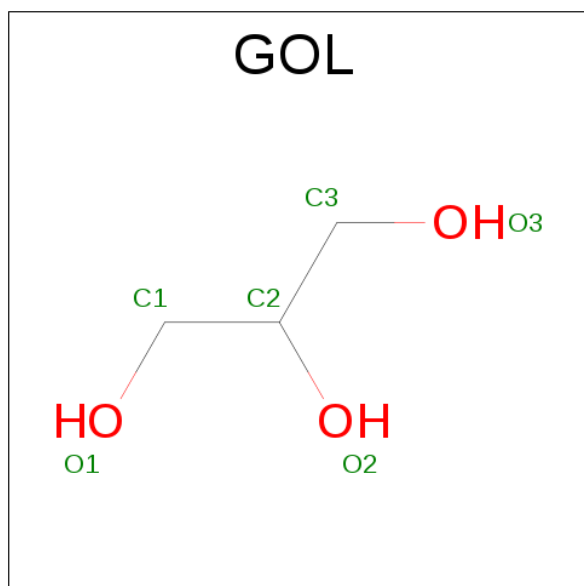
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

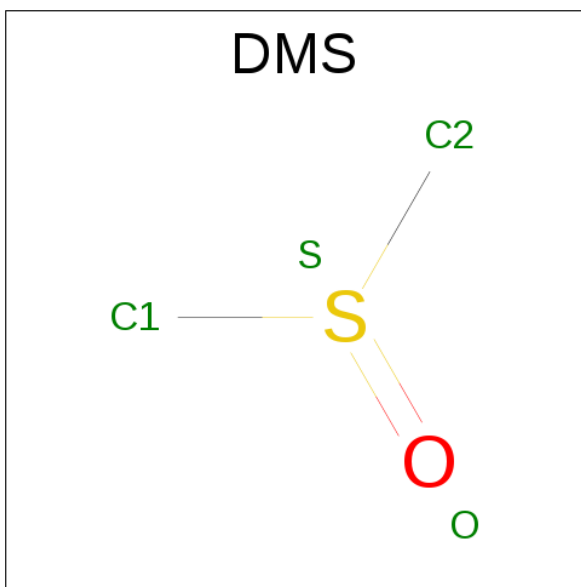
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			4	2	1	1		

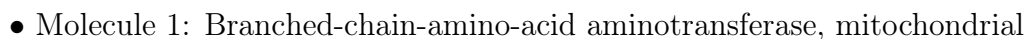
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	348	Total	O	0	0
			348	348		
8	B	344	Total	O	0	0
			344	344		





- Molecule 1: Branched-chain-amino-acid aminotransferase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.29Å 106.59Å 106.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.82 39.32 – 1.82	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-1.82) 95.0 (39.32-1.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 1.82Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.220 , 0.261 0.227 , 0.263	Depositor DCC
$R_{free}$ test set	3449 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PLP, CL, EDO, DMS, 4W6

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	0.47	0/2963	0.67	0/4017
1	B	0.46	0/2908	0.65	0/3943
All	All	0.47	0/5871	0.66	0/7960

There are no bond length outliers.

There are no bond angle outliers.

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	2892	0	2929	25	0
1	B	2838	0	2871	21	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
3	A	23	0	19	1	0
3	B	23	0	19	1	0
4	A	28	0	42	1	0
4	B	28	0	42	2	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	8	0	0
7	B	4	0	6	2	0
8	A	348	0	0	5	0
8	B	344	0	0	5	0
All	All	6572	0	5956	47	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 4.

All (47) 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:40:MET:SD	1:A:162[A]:LEU:HD11	1.93	1.08
5:B:411:CL:CL	8:B:729:HOH:O	2.41	0.76
1:A:315:CYS:SG	8:A:752:HOH:O	2.48	0.70
1:B:338:GLY:O	8:B:501:HOH:O	2.12	0.68
1:A:215[B]:GLN:OE1	8:A:501:HOH:O	2.16	0.62
1:A:215[B]:GLN:NE2	8:A:503:HOH:O	2.33	0.61
1:A:261:LEU:HB3	4:A:408:EDO:H21	1.86	0.57
1:A:237:GLU:OE1	2:A:401:PLP:N1	2.39	0.55
1:B:66:SER:HB2	1:B:72:LEU:HD12	1.89	0.53
1:A:12:LEU:HD11	1:A:14:MET:SD	2.49	0.53
1:B:318[A]:CYS:SG	3:B:402:4W6:H16	2.49	0.51
1:A:82:LYS:HD2	1:A:134:ASP:HB3	1.91	0.51
1:A:179:VAL:HG21	1:A:346:GLN:HE22	1.76	0.50
1:B:162:LEU:HD11	7:B:403:DMS:C2	2.42	0.49
1:B:237:GLU:OE1	2:B:401:PLP:N1	2.46	0.49
1:A:318[A]:CYS:SG	3:A:402:4W6:H16	2.53	0.48
1:B:34:PHE:CE1	1:B:168:CYS:SG	3.06	0.48
1:A:242:ASN:O	1:A:310:GLY:HA2	2.14	0.48
4:B:409:EDO:H21	8:B:604:HOH:O	2.13	0.48
1:A:238[B]:VAL:HG23	1:A:238[B]:VAL:O	2.15	0.47
5:A:410:CL:CL	8:A:791:HOH:O	2.58	0.46
1:B:67:SER:HB3	1:B:148:GLY:O	2.16	0.46
1:B:162:LEU:HD11	7:B:403:DMS:H21	1.97	0.45
1:A:56:PHE:CZ	1:B:63:PRO:HG2	2.52	0.45
1:A:238[B]:VAL:HG23	1:A:241:MET:HB2	1.99	0.44
1:B:179:VAL:HG13	1:B:346:GLN:HE22	1.82	0.44
1:B:124:LEU:HG	1:B:167:LEU:HD11	1.99	0.44
1:B:238[B]:VAL:HG13	1:B:238[B]:VAL:O	2.18	0.44
1:B:184:LEU:CD2	1:B:224:GLN:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:CYS:SG	8:B:815:HOH:O	2.62	0.43
1:B:132:VAL:HG22	1:B:140:LEU:HD22	2.00	0.42
1:A:150:GLU:HG3	1:A:152:SER:HB3	2.01	0.42
1:B:242:ASN:O	1:B:310:GLY:HA2	2.18	0.42
1:A:211:VAL:O	1:A:215[B]:GLN:HG2	2.20	0.42
1:A:124:LEU:HG	1:A:167:LEU:HD11	2.01	0.42
1:B:160:ARG:NH1	8:B:518:HOH:O	2.52	0.42
1:B:105:MET:HE2	1:B:105:MET:HA	2.02	0.41
1:A:260:PRO:HD3	1:A:289[A]:ARG:C	2.42	0.41
1:A:258:THR:O	1:A:288:GLU:HA	2.21	0.41
1:A:360:GLU:HB2	8:A:655:HOH:O	2.20	0.41
1:B:261:LEU:HB3	4:B:409:EDO:C2	2.51	0.41
1:A:184:LEU:CD2	1:A:224:GLN:HB2	2.51	0.40
1:A:109:LEU:HB3	1:A:110:PRO:HD2	2.03	0.40
1:A:135:ALA:HB3	1:A:138:THR:HG21	2.03	0.40
1:A:157:GLN:OE1	1:B:215:GLN:NE2	2.39	0.40
1:A:33:THR:O	1:A:169:PRO:HD2	2.21	0.40
1:B:309:PHE:HB3	1:B:342:ILE:HD11	2.04	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	355/369 (96%)	342 (96%)	12 (3%)	1 (0%)	44	28
1	B	349/369 (95%)	340 (97%)	8 (2%)	1 (0%)	44	28
All	All	704/738 (95%)	682 (97%)	20 (3%)	2 (0%)	44	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
1	B	316	GLN

### 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	317/319 (99%)	313 (99%)	4 (1%)	73	65
1	B	311/319 (98%)	307 (99%)	4 (1%)	73	65
All	All	628/638 (98%)	620 (99%)	8 (1%)	73	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	247	TRP
1	A	328	ARG
1	A	357	ARG
1	B	45	ASP
1	B	179	VAL
1	B	219	LYS
1	B	247	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN
1	B	11	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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$
2	PLP	A	401	1	15,15,16	3.97	3 (20%)	20,22,23	1.88	5 (25%)
3	4W6	A	402	-	20,25,25	1.48	4 (20%)	17,35,35	1.05	1 (5%)
4	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.26	0
4	EDO	A	404	-	3,3,3	0.35	0	2,2,2	0.56	0
4	EDO	A	405	-	3,3,3	0.31	0	2,2,2	0.51	0
4	EDO	A	406	-	3,3,3	0.38	0	2,2,2	0.36	0
4	EDO	A	407	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	A	408	-	3,3,3	0.33	0	2,2,2	0.86	0
4	EDO	A	409	-	3,3,3	0.38	0	2,2,2	0.54	0
6	GOL	A	411	-	5,5,5	0.45	0	5,5,5	0.56	0
2	PLP	B	401	1	15,15,16	3.79	3 (20%)	20,22,23	2.09	6 (30%)
3	4W6	B	402	-	20,25,25	1.58	4 (20%)	17,35,35	1.33	3 (17%)
7	DMS	B	403	-	3,3,3	0.60	0	3,3,3	0.76	0
4	EDO	B	404	-	3,3,3	0.41	0	2,2,2	0.52	0
4	EDO	B	405	-	3,3,3	0.33	0	2,2,2	0.60	0
4	EDO	B	406	-	3,3,3	0.38	0	2,2,2	0.48	0
4	EDO	B	407	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	B	408	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	409	-	3,3,3	0.09	0	2,2,2	0.56	0
4	EDO	B	410	-	3,3,3	0.44	0	2,2,2	0.40	0
6	GOL	B	412	-	5,5,5	0.27	0	5,5,5	0.20	0

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
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
3	4W6	A	402	-	-	0/10/20/20	0/3/3/3
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
4	EDO	A	405	-	-	0/1/1/1	0/0/0/0
4	EDO	A	406	-	-	0/1/1/1	0/0/0/0
4	EDO	A	407	-	-	0/1/1/1	0/0/0/0
4	EDO	A	408	-	-	0/1/1/1	0/0/0/0
4	EDO	A	409	-	-	0/1/1/1	0/0/0/0
6	GOL	A	411	-	-	0/4/4/4	0/0/0/0
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
3	4W6	B	402	-	-	0/10/20/20	0/3/3/3
7	DMS	B	403	-	-	0/0/0/0	0/0/0/0
4	EDO	B	404	-	-	0/1/1/1	0/0/0/0
4	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	EDO	B	406	-	-	0/1/1/1	0/0/0/0
4	EDO	B	407	-	-	0/1/1/1	0/0/0/0
4	EDO	B	408	-	-	0/1/1/1	0/0/0/0
4	EDO	B	409	-	-	0/1/1/1	0/0/0/0
4	EDO	B	410	-	-	0/1/1/1	0/0/0/0
6	GOL	B	412	-	-	0/4/4/4	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	4W6	C11-C10	-3.89	1.47	1.51
3	B	402	4W6	C5-C4	-3.07	1.34	1.39
3	A	402	4W6	C5-C4	-2.94	1.34	1.39
3	A	402	4W6	C11-C10	-2.61	1.48	1.51
3	B	402	4W6	C19-C22	-2.54	1.37	1.45
3	A	402	4W6	C19-C22	-2.44	1.37	1.45
3	B	402	4W6	C4-N23	3.29	1.39	1.32
2	A	401	PLP	C3-C4	3.47	1.47	1.40
2	B	401	PLP	C3-C4	3.62	1.47	1.40
3	A	402	4W6	C4-N23	3.74	1.40	1.32
2	A	401	PLP	C5-C4	8.74	1.50	1.40
2	B	401	PLP	C5-C4	8.80	1.50	1.40
2	B	401	PLP	C3-C2	10.70	1.48	1.40
2	A	401	PLP	C3-C2	11.60	1.48	1.40



All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	PLP	O2P-P-O4P	-3.47	97.49	106.73
3	B	402	4W6	C5-C4-N23	-2.56	120.14	122.91
2	B	401	PLP	C4A-C4-C3	-2.50	116.23	120.54
2	A	401	PLP	O2P-P-O4P	-2.35	100.48	106.73
2	A	401	PLP	C3-C4-C5	-2.04	116.32	118.63
2	A	401	PLP	O3P-P-O2P	2.16	116.31	107.61
2	B	401	PLP	O2P-P-O1P	2.26	119.32	110.50
2	A	401	PLP	O3-C3-C2	2.29	122.57	117.78
3	B	402	4W6	C6-C5-C4	2.32	123.98	117.22
2	B	401	PLP	O3-C3-C2	2.36	122.72	117.78
3	A	402	4W6	C6-C5-C4	2.39	124.17	117.22
2	B	401	PLP	C6-N1-C2	2.42	123.92	119.26
3	B	402	4W6	C10-C19-C20	2.64	131.11	127.33
2	A	401	PLP	C4A-C4-C5	5.38	126.29	120.86
2	B	401	PLP	C4A-C4-C5	5.99	126.90	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	1	0
3	A	402	4W6	1	0
4	A	408	EDO	1	0
2	B	401	PLP	1	0
3	B	402	4W6	1	0
7	B	403	DMS	2	0
4	B	409	EDO	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	353/369 (95%)	0.32	17 (4%) 31 26	17, 30, 55, 85	0
1	B	353/369 (95%)	0.20	13 (3%) 42 37	18, 32, 60, 89	0
All	All	706/738 (95%)	0.26	30 (4%) 37 31	17, 31, 57, 89	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	8.6
1	B	3	SER	5.2
1	A	356	ILE	4.2
1	A	3	SER	4.2
1	B	16	GLN	3.9
1	B	28	LEU	3.9
1	B	179	VAL	3.8
1	A	19	HIS	3.4
1	A	357	ARG	3.3
1	A	84	LYS	3.3
1	A	358	ALA	3.1
1	A	179	VAL	3.1
1	A	27	PRO	3.0
1	B	23	GLY	3.0
1	B	8	ALA	2.9
1	A	20	LYS	2.9
1	B	12	LEU	2.8
1	B	10	LEU	2.7
1	B	14	MET	2.6
1	A	355	GLY	2.6
1	B	18	PRO	2.6
1	A	22	PRO	2.4
1	A	83	GLY	2.4
1	A	28	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	20	LYS	2.2
1	A	235	LEU	2.2
1	A	46	LYS	2.1
1	A	243	ILE	2.1
1	A	238[A]	VAL	2.1
1	B	19	HIS	2.0

## 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	B	405	4/4	0.87	0.18	9.66	41,43,44,47	0
4	EDO	B	409	4/4	0.88	0.25	9.16	28,31,40,41	0
6	GOL	A	411	6/6	0.81	0.21	2.83	51,52,56,56	0
4	EDO	A	407	4/4	0.80	0.23	2.71	52,55,56,60	0
4	EDO	A	408	4/4	0.85	0.21	2.59	27,28,31,35	0
4	EDO	A	406	4/4	0.93	0.15	1.76	46,49,51,58	0
4	EDO	A	405	4/4	0.91	0.12	1.07	35,37,37,39	0
4	EDO	B	410	4/4	0.89	0.21	0.71	55,57,57,59	0
4	EDO	A	404	4/4	0.68	0.22	0.70	54,57,57,60	0
7	DMS	B	403	4/4	0.97	0.12	0.49	45,51,52,52	0
4	EDO	B	406	4/4	0.93	0.11	0.06	39,40,41,42	0
3	4W6	B	402	23/23	0.93	0.10	-0.51	22,25,32,33	0
2	PLP	B	401	15/16	0.97	0.09	-0.77	20,27,36,36	0
3	4W6	A	402	23/23	0.94	0.10	-0.84	22,24,28,28	0
2	PLP	A	401	15/16	0.97	0.10	-1.29	18,23,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	404	4/4	0.70	0.22	-	53,55,58,59	0
4	EDO	A	409	4/4	0.69	0.28	-	63,65,66,70	0
5	CL	A	410	1/1	0.94	0.05	-	50,50,50,50	0
4	EDO	B	407	4/4	0.76	0.21	-	58,59,60,67	0
5	CL	B	411	1/1	0.82	0.09	-	43,43,43,43	0
6	GOL	B	412	6/6	0.82	0.13	-	65,68,71,75	0
4	EDO	A	403	4/4	0.82	0.21	-	51,53,53,55	0
4	EDO	B	408	4/4	0.80	0.22	-	61,62,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.