Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 02:48 PM EDT

PDB ID	:	2HGW
Title	:	Crystal structure of Cys318Ala mutant of human mitochondrial branched chain aminotransferase
Authors	:	Yennawar, N.H.; Hutson, S.M.
Deposited on	:	2006-06-27
Resolution	:	1.98 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

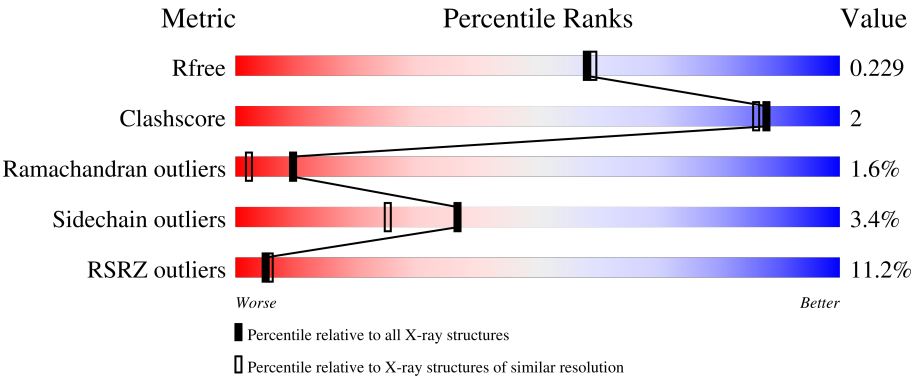
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.98 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	11% 90% 7%
1	B	365	11% 91% 7%

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	ACY	B	1005	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5983 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.

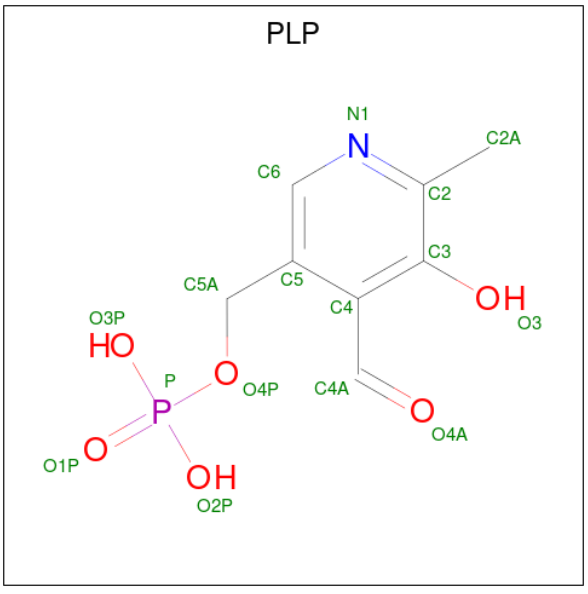
- Molecule 1 is a protein called Branched-chain-amino-acid aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2855	1839	499	500	17			
1	B	359	Total	C	N	O	S	0	0	0
			2860	1842	500	501	17			

There are 4 discrepancies between the modelled and reference sequences:

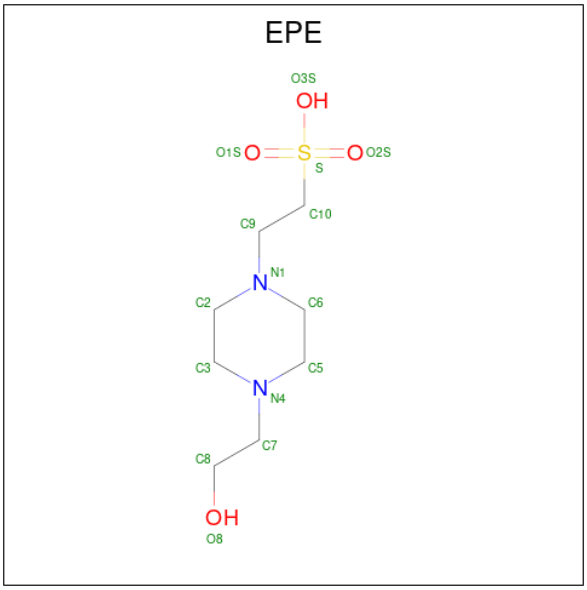
Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ARG	THR	conflict	UNP O15382
A	318	ALA	CYS	engineered mutation	UNP O15382
B	659	ARG	THR	conflict	UNP O15382
B	818	ALA	CYS	engineered mutation	UNP O15382

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



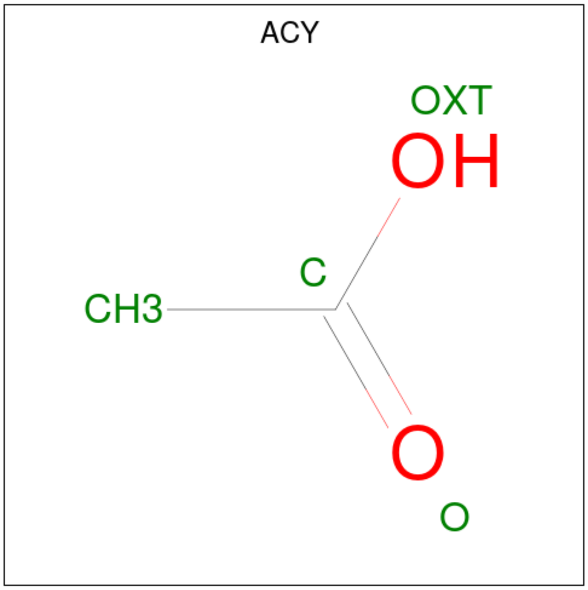
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



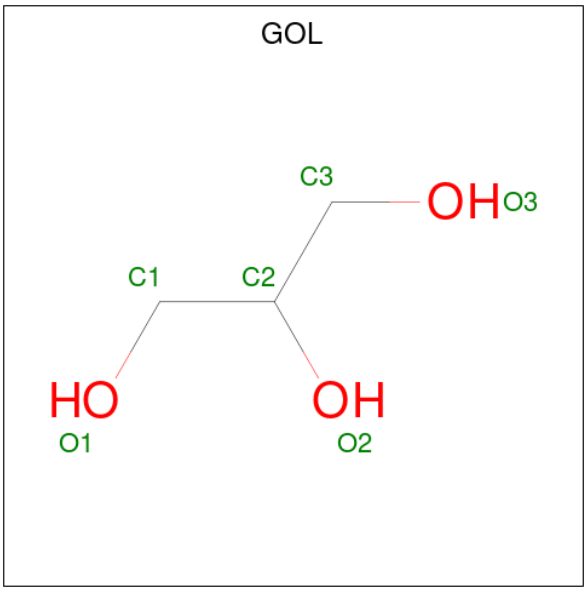
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



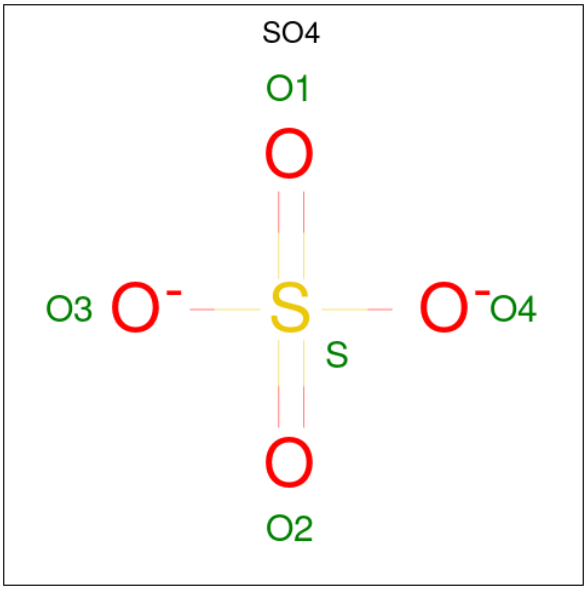
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

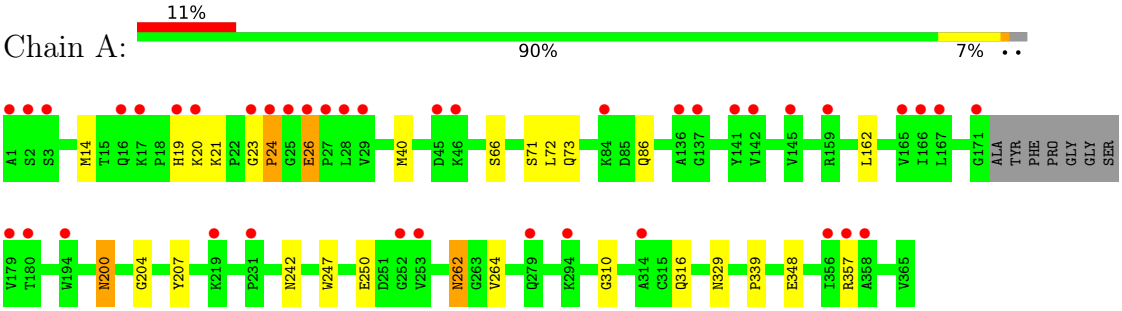
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	89	Total O 89 89	0	0
7	B	83	Total O 83 83	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

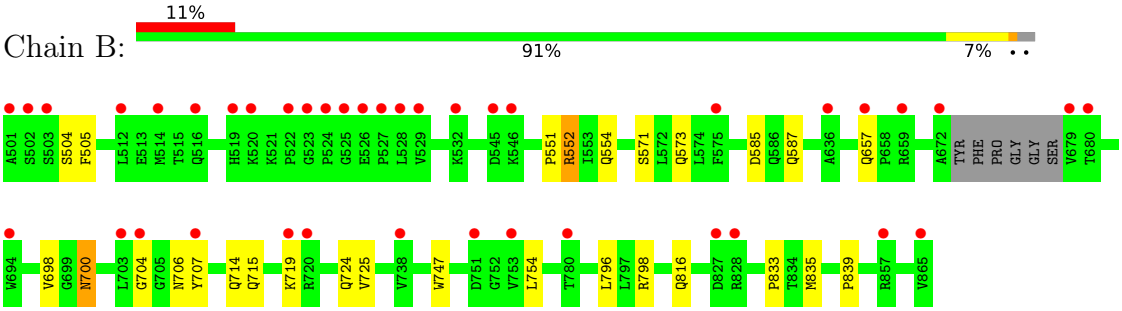
• Molecule 1: Branched-chain-amino-acid aminotransferase, mitochondrial

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.67Å 105.58Å 106.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.98 29.48 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.6 (25.00-1.98) 97.7 (29.48-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.254 0.223 , 0.229	Depositor DCC
R_{free} test set	2905 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5983	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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, 0.333 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: EPE, PLP, GOL, ACY, SO4

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	0.64	0/2928	0.76	1/3974 (0.0%)
1	B	0.63	0/2933	0.74	0/3981
All	All	0.64	0/5861	0.75	1/7955 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	GLY	C-N-CD	-5.90	107.62	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain
1	B	707	TYR	Sidechain

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	2855	0	2884	13	0
1	B	2860	0	2887	13	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
3	A	15	0	17	1	0
4	A	32	0	24	0	0
4	B	8	0	6	0	0
5	A	6	0	8	0	0
6	B	5	0	0	0	0
7	A	89	0	0	0	0
7	B	83	0	0	0	0
All	All	5983	0	5838	23	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 2.

All (23) 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:B:700:ASN:HD22	1:B:700:ASN:H	1.13	0.96
1:A:200:ASN:H	1:A:200:ASN:HD22	1.17	0.90
1:B:724:GLN:HE21	1:B:725:VAL:H	1.30	0.80
1:B:700:ASN:HD22	1:B:700:ASN:N	1.93	0.65
1:A:200:ASN:H	1:A:200:ASN:ND2	1.95	0.63
1:B:700:ASN:H	1:B:700:ASN:ND2	1.93	0.62
1:A:71:SER:H	1:B:573:GLN:HE22	1.47	0.61
1:A:73:GLN:HE22	1:B:571:SER:H	1.50	0.59
1:A:66:SER:HB2	1:A:72:LEU:HD12	1.86	0.57
1:B:552:ARG:HD2	1:B:554:GLN:HE21	1.73	0.53
1:A:73:GLN:HE21	1:A:204:GLY:HA3	1.79	0.47
1:B:573:GLN:HE21	1:B:704:GLY:HA3	1.77	0.47
1:B:505:PHE:HB2	1:B:551:PRO:HD3	1.98	0.46
1:B:724:GLN:HE21	1:B:725:VAL:N	2.08	0.45
1:A:71:SER:H	1:B:573:GLN:NE2	2.15	0.44
1:A:200:ASN:HD22	1:A:200:ASN:N	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HB2	3:A:1011:EPE:O3S	2.19	0.42
1:B:698:VAL:HG23	1:B:706:ASN:HD21	1.84	0.42
1:A:262:ASN:HD21	1:A:264:VAL:HG22	1.84	0.42
1:B:715:GLN:O	1:B:719:LYS:HG2	2.20	0.41
1:A:242:ASN:O	1:A:310:GLY:HA2	2.19	0.41
1:A:40:MET:HG2	1:A:162:LEU:HD11	2.02	0.41
1:A:262:ASN:HD22	1:A:262:ASN:H	1.69	0.41

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	354/365 (97%)	337 (95%)	11 (3%)	6 (2%)	9 2
1	B	355/365 (97%)	343 (97%)	7 (2%)	5 (1%)	11 3
All	All	709/730 (97%)	680 (96%)	18 (2%)	11 (2%)	9 2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	24	PRO
1	A	26	GLU
1	B	835	MET
1	A	316	GLN
1	A	21	LYS
1	B	816	GLN
1	B	504	SER
1	B	833	PRO
1	B	839	PRO
1	A	339	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	310/315 (98%)	299 (96%)	11 (4%)	36	24
1	B	310/315 (98%)	300 (97%)	10 (3%)	39	28
All	All	620/630 (98%)	599 (97%)	21 (3%)	37	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	19	HIS
1	A	24	PRO
1	A	26	GLU
1	A	86	GLN
1	A	200	ASN
1	A	247	TRP
1	A	250	GLU
1	A	262	ASN
1	A	348	GLU
1	A	357	ARG
1	B	552	ARG
1	B	585	ASP
1	B	587	GLN
1	B	657	GLN
1	B	700	ASN
1	B	714	GLN
1	B	747	TRP
1	B	754	LEU
1	B	796	LEU
1	B	798	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	73	GLN
1	A	86	GLN
1	A	200	ASN
1	A	206	ASN
1	A	215	GLN
1	A	262	ASN
1	A	272	GLN
1	A	295	GLN
1	B	554	GLN
1	B	573	GLN
1	B	657	GLN
1	B	700	ASN
1	B	706	ASN
1	B	714	GLN
1	B	724	GLN
1	B	742	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

15 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	$\#\|Z\|>2$
2	PLP	A	400	1	15,15,16	1.42	3 (20%)	20,22,23	1.73	6 (30%)
4	ACY	B	1005	-	1,3,3	2.93	1 (100%)	0,3,3	-	-
4	ACY	B	1010	-	1,3,3	2.81	1 (100%)	0,3,3	-	-
4	ACY	A	1002	-	1,3,3	2.56	1 (100%)	0,3,3	-	-
4	ACY	A	1007	-	1,3,3	3.03	1 (100%)	0,3,3	-	-
4	ACY	A	1008	-	1,3,3	3.10	1 (100%)	0,3,3	-	-
3	EPE	A	1011	-	15,15,15	1.52	5 (33%)	18,20,20	1.33	4 (22%)
4	ACY	A	1004	-	1,3,3	2.78	1 (100%)	0,3,3	-	-
4	ACY	A	1003	-	1,3,3	2.23	1 (100%)	0,3,3	-	-
6	SO4	B	1012	-	4,4,4	0.26	0	6,6,6	0.06	0
4	ACY	A	1001	-	1,3,3	2.94	1 (100%)	0,3,3	-	-
5	GOL	A	2001	-	5,5,5	0.91	0	5,5,5	0.35	0
2	PLP	B	401	1	15,15,16	1.47	2 (13%)	20,22,23	1.69	5 (25%)
4	ACY	A	1009	-	1,3,3	2.90	1 (100%)	0,3,3	-	-
4	ACY	A	1006	-	1,3,3	2.91	1 (100%)	0,3,3	-	-

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	400	1	-	0/6/6/8	0/1/1/1
5	GOL	A	2001	-	-	0/4/4/4	-
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
3	EPE	A	1011	-	-	0/9/19/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1008	ACY	CH3-C	3.10	1.52	1.48
4	A	1007	ACY	CH3-C	3.03	1.52	1.48
3	A	1011	EPE	C7-N4	2.99	1.54	1.47
4	A	1001	ACY	CH3-C	2.94	1.52	1.48
4	B	1005	ACY	CH3-C	2.93	1.52	1.48
4	A	1006	ACY	CH3-C	2.91	1.52	1.48
4	A	1009	ACY	CH3-C	2.90	1.52	1.48
4	B	1010	ACY	CH3-C	2.81	1.52	1.48
4	A	1004	ACY	CH3-C	2.78	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C4A-C4	2.62	1.57	1.51
4	A	1002	ACY	CH3-C	2.56	1.52	1.48
2	A	400	PLP	C5-C4	2.35	1.43	1.40
3	A	1011	EPE	C2-N1	2.31	1.53	1.46
2	A	400	PLP	P-O1P	-2.30	1.43	1.50
3	A	1011	EPE	C6-N1	2.26	1.53	1.46
3	A	1011	EPE	C10-S	2.25	1.80	1.77
2	B	401	PLP	P-O1P	-2.25	1.43	1.50
4	A	1003	ACY	CH3-C	2.23	1.51	1.48
2	A	400	PLP	C4A-C4	2.15	1.56	1.51
3	A	1011	EPE	C9-N1	2.08	1.52	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	PLP	O4P-C5A-C5	3.78	116.56	109.35
2	B	401	PLP	O4P-C5A-C5	3.75	116.50	109.35
2	B	401	PLP	O2P-P-O4P	-2.69	99.58	106.73
2	A	400	PLP	O3P-P-O1P	2.46	120.32	110.68
2	B	401	PLP	O3P-P-O1P	2.44	120.22	110.68
2	A	400	PLP	C5A-C5-C6	-2.42	115.39	119.37
2	A	400	PLP	O2P-P-O4P	-2.42	100.28	106.73
3	A	1011	EPE	C3-C2-N1	-2.35	105.82	110.64
3	A	1011	EPE	C7-N4-C5	-2.32	105.31	111.23
3	A	1011	EPE	C9-N1-C6	-2.24	105.51	111.23
2	B	401	PLP	C5A-C5-C6	-2.16	115.82	119.37
2	A	400	PLP	C4A-C4-C5	2.09	123.08	120.94
2	B	401	PLP	O4P-P-O1P	2.06	112.27	106.47
2	A	400	PLP	O4P-P-O1P	2.03	112.17	106.47
3	A	1011	EPE	C6-C5-N4	2.02	114.79	110.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1011	EPE	1	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^{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	358/365 (98%)	0.83	40 (11%)	5	6	21, 30, 50, 69	0
1	B	359/365 (98%)	0.91	40 (11%)	5	6	22, 31, 49, 65	0
All	All	717/730 (98%)	0.87	80 (11%)	5	6	21, 31, 50, 69	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	ALA	10.4
1	B	503	SER	10.2
1	A	2	SER	8.9
1	A	27	PRO	8.8
1	A	24	PRO	8.6
1	A	23	GLY	8.0
1	A	1	ALA	7.8
1	B	527	PRO	7.2
1	B	502	SER	7.0
1	A	26	GLU	6.8
1	B	672	ALA	6.4
1	A	20	LYS	6.1
1	B	523	GLY	5.8
1	B	524	PRO	5.8
1	A	25	GLY	5.7
1	A	358	ALA	5.3
1	B	516	GLN	5.2
1	B	520	LYS	5.1
1	A	19	HIS	4.6
1	A	357	ARG	4.6
1	B	526	GLU	4.5
1	B	528	LEU	4.5
1	B	827	ASP	4.5
1	A	84	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	525	GLY	4.3
1	A	3	SER	4.3
1	B	546	LYS	4.3
1	B	636	ALA	4.2
1	B	514	MET	4.1
1	B	680	THR	4.0
1	A	136	ALA	3.7
1	B	679	VAL	3.7
1	A	252	GLY	3.5
1	A	28	LEU	3.5
1	B	519	HIS	3.3
1	A	159	ARG	3.2
1	B	545	ASP	3.2
1	B	659	ARG	3.2
1	B	529	VAL	3.1
1	B	828	ARG	3.1
1	A	17	LYS	3.1
1	A	165	VAL	3.0
1	A	46	LYS	3.0
1	B	575	PHE	3.0
1	A	145	VAL	3.0
1	B	751	ASP	3.0
1	A	137	GLY	3.0
1	A	45	ASP	2.9
1	B	720	ARG	2.9
1	B	512	LEU	2.9
1	A	29	VAL	2.8
1	B	753	VAL	2.8
1	B	719	LYS	2.7
1	A	179	VAL	2.7
1	A	171	GLY	2.6
1	A	142	VAL	2.5
1	B	857	ARG	2.5
1	A	166	ILE	2.5
1	B	738	VAL	2.5
1	B	865	VAL	2.5
1	A	16	GLN	2.4
1	B	694	TRP	2.4
1	A	180	THR	2.4
1	A	314	ALA	2.4
1	A	356	ILE	2.4
1	B	657	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	LEU	2.3
1	B	532	LYS	2.3
1	A	194	TRP	2.2
1	A	253	VAL	2.2
1	B	522	PRO	2.1
1	B	780	THR	2.1
1	B	704	GLY	2.1
1	A	219	LYS	2.1
1	B	707	TYR	2.1
1	A	279	GLN	2.1
1	A	231	PRO	2.1
1	B	703	LEU	2.1
1	A	294	LYS	2.1
1	A	141	TYR	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	ACY	A	1009	4/4	0.66	0.26	45,47,47,47	0
4	ACY	A	1001	4/4	0.69	0.24	48,50,50,51	0
4	ACY	A	1004	4/4	0.71	0.28	49,49,49,50	0
4	ACY	B	1005	4/4	0.76	0.42	46,48,48,49	0
3	EPE	A	1011	15/15	0.77	0.26	40,45,49,49	0
5	GOL	A	2001	6/6	0.79	0.19	44,44,46,47	0
4	ACY	A	1007	4/4	0.83	0.19	42,43,43,43	0
4	ACY	B	1010	4/4	0.84	0.20	46,46,47,47	0
4	ACY	A	1008	4/4	0.84	0.17	44,44,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACY	A	1002	4/4	0.86	0.17	41,43,44,44	0
4	ACY	A	1006	4/4	0.86	0.15	49,49,49,49	0
4	ACY	A	1003	4/4	0.87	0.33	46,46,47,47	0
6	SO4	B	1012	5/5	0.94	0.14	49,49,49,51	0
2	PLP	A	400	15/16	0.96	0.15	27,28,30,33	0
2	PLP	B	401	15/16	0.97	0.20	24,25,26,28	0

6.5 Other polymers (i)

There are no such residues in this entry.