



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:09 pm BST

PDB ID : 1DWP
Title : Crystal Structure of Hydroxynitrile Lyase from *Manihot esculenta* at 2.2 Angstrom Resolution
Authors : Lauble, H.; Wagner, U.; Kratky, C.; Mielich, B.; Wajant, H.; Forster, S.; Effenberger, F.
Deposited on : 1999-12-10
Resolution : 2.20 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

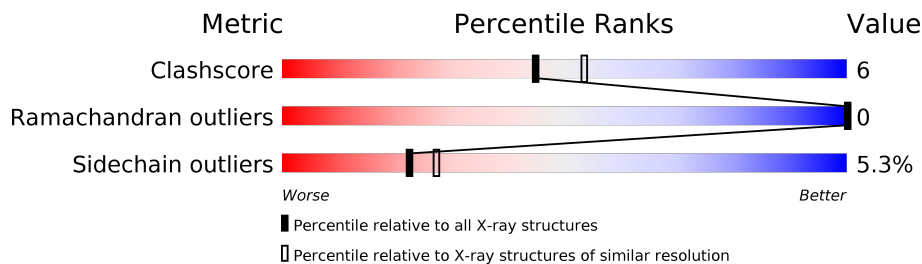
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	262	78% 18% ..
1	B	262	78% 18% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4498 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 HYDROXYNITRILE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	Total	C	N	O	S	0	0	0
			2104	1359	349	388	8			
1	B	258	Total	C	N	O	S	0	0	0
			2074	1339	344	383	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	cloning artifact	PDB 1DWP
A	-3	ILE	-	cloning artifact	PDB 1DWP
A	-2	SER	-	cloning artifact	PDB 1DWP
A	-1	LYS	-	cloning artifact	PDB 1DWP
A	1	MET	-	cloning artifact	PDB 1DWP
B	-4	PRO	-	cloning artifact	PDB 1DWP
B	-3	ILE	-	cloning artifact	PDB 1DWP
B	-2	SER	-	cloning artifact	PDB 1DWP
B	-1	LYS	-	cloning artifact	PDB 1DWP
B	1	MET	-	cloning artifact	PDB 1DWP

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

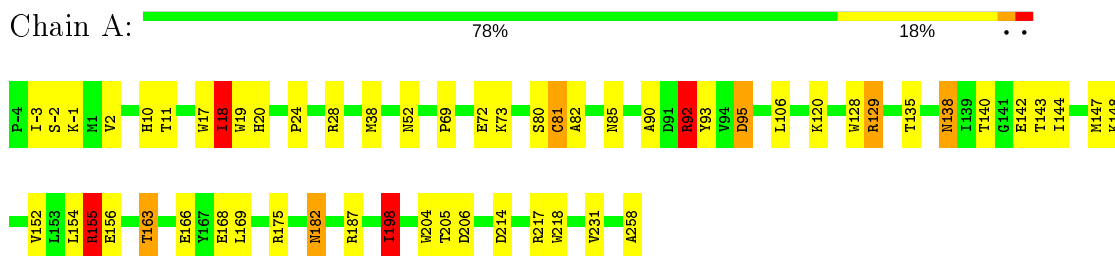
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	133	Total O 133 133	0	0
3	B	179	Total O 179 179	0	0

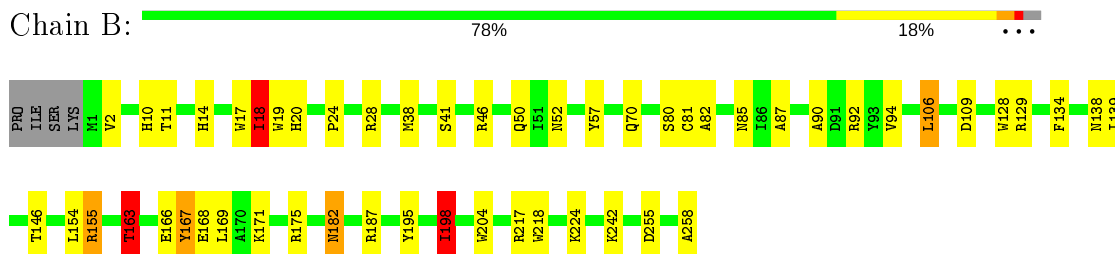
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: HYDROXYNITRILE LYASE



- Molecule 1: HYDROXYNITRILE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.60Å 106.60Å 189.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 15.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-2.20) 99.1 (15.08-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.91 (at 2.20Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.198 , 0.244 0.262 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtrriage
Anisotropy	0.496	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4498	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
ACT

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	0.88	0/2156	1.52	37/2921 (1.3%)
1	B	0.88	0/2125	1.51	35/2880 (1.2%)
All	All	0.88	0/4281	1.52	72/5801 (1.2%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	B	155	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	92	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	A	147	MET	CG-SD-CE	-8.67	86.32	100.20
1	B	204	TRP	CD1-CG-CD2	8.58	113.16	106.30
1	B	19	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	B	155	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	92	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	A	175	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	175	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	217	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	A	19	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	A	92	ARG	NE-CZ-NH2	7.71	124.15	120.30
1	A	218	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	A	19	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	B	204	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	B	57	TYR	CB-CG-CD2	-7.41	116.56	121.00
1	A	204	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	A	198	ILE	CA-CB-CG1	-7.10	97.51	111.00
1	A	129	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	128	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	A	198	ILE	CA-CB-CG2	7.07	125.04	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	B	198	ILE	CA-CB-CG1	-7.06	97.59	111.00
1	A	17	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	A	19	TRP	CG-CD2-CE3	6.96	140.17	133.90
1	B	92	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	A	204	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	A	218	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	B	198	ILE	CA-CB-CG2	6.77	124.43	110.90
1	A	19	TRP	CB-CG-CD1	-6.76	118.21	127.00
1	B	204	TRP	CG-CD2-CE3	6.74	139.97	133.90
1	A	17	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	A	128	TRP	CE2-CD2-CG	-6.57	102.04	107.30
1	B	187	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	17	TRP	CD1-CG-CD2	6.45	111.46	106.30
1	A	155	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	218	TRP	CE2-CD2-CG	-6.37	102.21	107.30
1	A	206	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	128	TRP	CD1-CG-CD2	6.26	111.31	106.30
1	B	187	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	218	TRP	CD1-CG-CD2	6.16	111.23	106.30
1	B	70	GLN	CA-CB-CG	6.14	126.90	113.40
1	A	152	VAL	CG1-CB-CG2	-6.05	101.22	110.90
1	B	167	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	B	175	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	231	VAL	CG1-CB-CG2	-5.92	101.43	110.90
1	B	163	THR	N-CA-CB	-5.92	99.06	110.30
1	A	18	ILE	CB-CA-C	-5.80	100.00	111.60
1	B	204	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	B	17	TRP	CE2-CD2-CG	-5.73	102.72	107.30
1	A	-3	ILE	N-CA-C	-5.72	95.56	111.00
1	A	163	THR	CA-CB-CG2	5.71	120.40	112.40
1	B	19	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	B	18	ILE	CB-CA-C	-5.54	100.52	111.60
1	A	163	THR	N-CA-CB	-5.54	99.78	110.30
1	B	28	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	B	204	TRP	CB-CG-CD1	-5.39	120.00	127.00
1	A	-1	LYS	CB-CG-CD	-5.35	97.68	111.60
1	A	28	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	129	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	128	TRP	CD1-CG-CD2	5.33	110.56	106.30
1	B	218	TRP	CB-CG-CD1	-5.32	120.09	127.00
1	A	81	CYS	CA-CB-SG	-5.29	104.47	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	A	217	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	218	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	214	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	19	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	A	218	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	B	46	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	18	ILE	N-CA-CB	5.02	122.35	110.80

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	2104	0	2101	30	0
1	B	2074	0	2065	26	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	133	0	0	2	0
3	B	179	0	0	1	0
All	All	4498	0	4172	54	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 6.

All (54) 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:10:HIS:HE1	1:A:38:MET:H	1.22	0.86
1:B:10:HIS:HE1	1:B:38:MET:H	1.27	0.81
1:B:2:VAL:HG13	1:B:255:ASP:HA	1.72	0.71
1:B:52:ASN:HD22	1:B:138:ASN:HB2	1.54	0.71
1:A:168:GLU:HG3	1:B:24:PRO:HD3	1.76	0.66
1:A:10:HIS:HD2	1:A:11:THR:O	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	1:A:156:GLU:HB2	2.11	0.65
1:A:90:ALA:HB1	1:A:198:ILE:HD13	1.77	0.65
1:B:10:HIS:HD2	1:B:11:THR:O	1.80	0.64
1:B:90:ALA:HB1	1:B:198:ILE:HD13	1.78	0.64
1:B:81:CYS:HA	1:B:106:LEU:HD22	1.81	0.60
1:B:163:THR:HG22	1:B:166:GLU:H	1.66	0.60
1:A:24:PRO:HD3	1:B:168:GLU:HG2	1.84	0.60
1:B:2:VAL:HG21	1:B:258:ALA:HA	1.83	0.60
1:A:10:HIS:HE1	1:A:38:MET:N	1.97	0.59
1:A:10:HIS:CE1	1:A:38:MET:H	2.12	0.59
1:B:20:HIS:HE1	1:B:166:GLU:OE1	1.86	0.59
1:A:52:ASN:HD22	1:A:138:ASN:HB2	1.68	0.58
1:A:163:THR:HG22	1:A:166:GLU:H	1.68	0.57
1:A:95:ASP:HB3	3:A:2053:HOH:O	2.07	0.55
1:A:163:THR:HG23	3:A:2086:HOH:O	2.06	0.54
1:B:2:VAL:CG1	1:B:255:ASP:HA	2.36	0.54
1:A:129:ARG:HH22	1:A:156:GLU:HB2	1.72	0.54
1:A:138:ASN:ND2	1:A:142:GLU:H	2.05	0.54
1:B:82:ALA:HA	1:B:85:ASN:HD22	1.73	0.54
1:A:182:ASN:H	1:A:182:ASN:HD22	1.56	0.53
1:B:94:VAL:HG23	1:B:198:ILE:CD1	2.39	0.52
1:A:20:HIS:HE1	1:A:166:GLU:OE1	1.94	0.51
1:A:82:ALA:HA	1:A:85:ASN:HD22	1.76	0.50
1:B:182:ASN:H	1:B:182:ASN:HD22	1.57	0.50
1:B:10:HIS:CB	1:B:18:ILE:HD11	2.44	0.48
1:A:69:PRO:HB2	1:A:72:GLU:HG2	1.96	0.47
1:B:10:HIS:HB3	1:B:18:ILE:HD11	1.95	0.47
1:A:81:CYS:HA	1:A:106:LEU:HD22	1.96	0.46
1:B:10:HIS:CE1	1:B:38:MET:H	2.19	0.45
1:A:18:ILE:H	1:A:18:ILE:HG13	1.58	0.45
1:A:11:THR:HB	1:A:80:SER:HB3	1.99	0.44
1:A:138:ASN:ND2	1:A:140:THR:H	2.15	0.44
1:B:87:ALA:HA	1:B:195:TYR:CD1	2.52	0.44
1:B:167:TYR:CZ	1:B:171:LYS:HD2	2.53	0.43
1:B:109:ASP:HB2	3:B:2089:HOH:O	2.19	0.43
1:A:148:LYS:HA	1:A:148:LYS:HD2	1.94	0.42
1:A:135:THR:HA	1:A:144:ILE:O	2.20	0.42
1:B:14:HIS:O	1:B:41:SER:HB3	2.20	0.42
1:B:94:VAL:HG23	1:B:198:ILE:HD12	2.00	0.42
1:A:2:VAL:HG11	1:A:258:ALA:HA	2.01	0.42
1:B:134:PHE:HB2	1:B:146:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HE2	1:A:95:ASP:O	2.20	0.41
1:B:242:LYS:HD3	1:B:242:LYS:HA	1.85	0.41
1:A:155:ARG:HD3	1:A:155:ARG:HA	1.87	0.41
1:A:92:ARG:HH12	1:A:187:ARG:NH2	2.17	0.41
1:A:11:THR:CB	1:A:80:SER:HB3	2.50	0.41
1:B:52:ASN:ND2	1:B:139:ILE:H	2.19	0.40
1:A:92:ARG:HB3	1:A:93:TYR:CD1	2.56	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	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
1	B	256/262 (98%)	247 (96%)	9 (4%)	0	100	100
All	All	516/524 (98%)	498 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	227/227 (100%)	214 (94%)	13 (6%)	20	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	223/227 (98%)	212 (95%)	11 (5%)	25	31
All	All	450/454 (99%)	426 (95%)	24 (5%)	22	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	18	ILE
1	A	92	ARG
1	A	95	ASP
1	A	120	LYS
1	A	138	ASN
1	A	143	THR
1	A	154	LEU
1	A	155	ARG
1	A	169	LEU
1	A	182	ASN
1	A	198	ILE
1	A	205	THR
1	B	18	ILE
1	B	50	GLN
1	B	80	SER
1	B	106	LEU
1	B	154	LEU
1	B	155	ARG
1	B	163	THR
1	B	169	LEU
1	B	182	ASN
1	B	198	ILE
1	B	224	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	20	HIS
1	A	50	GLN
1	A	52	ASN
1	A	85	ASN
1	A	138	ASN
1	A	182	ASN

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Mol	Chain	Res	Type
1	A	251	GLN
1	B	10	HIS
1	B	20	HIS
1	B	52	ASN
1	B	85	ASN
1	B	182	ASN
1	B	230	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](#)

2 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	ACT	A	1259	-	1,3,3	5.01	1 (100%)	0,3,3	0.00	-
2	ACT	B	1259	-	1,3,3	4.03	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1259	ACT	CH3-C	5.01	1.55	1.48
2	B	1259	ACT	CH3-C	4.03	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.