



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:36 pm GMT

PDB ID : 1DWQ  
Title : CRYSTAL STRUCTURE OF HYDROXYNITRILE LYASE FROM MANI-HOT ESCULENTA IN COMPLEX WITH SUBSTRATES ACETONE AND CHLOROACETONE:IMPLICATIONS FOR THE MECHANISM OF CYANOGENESIS  
Authors : Lauble, H.; Forster, S.; Mielich, B.; Wajant, H.; 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](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

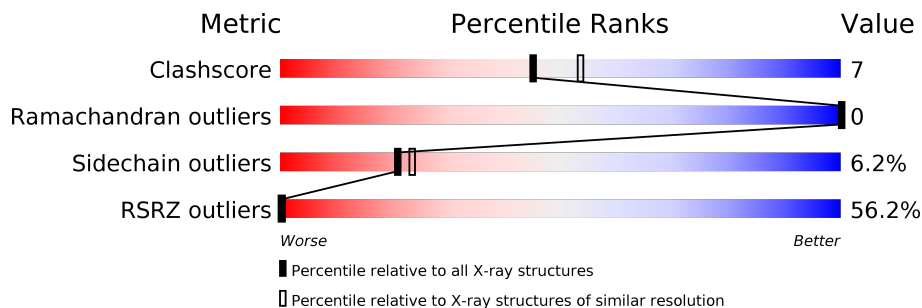
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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  $\geq 3$ , 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	262	<div> <div>59%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>
1	B	262	<div> <div>52%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>...</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4402 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.

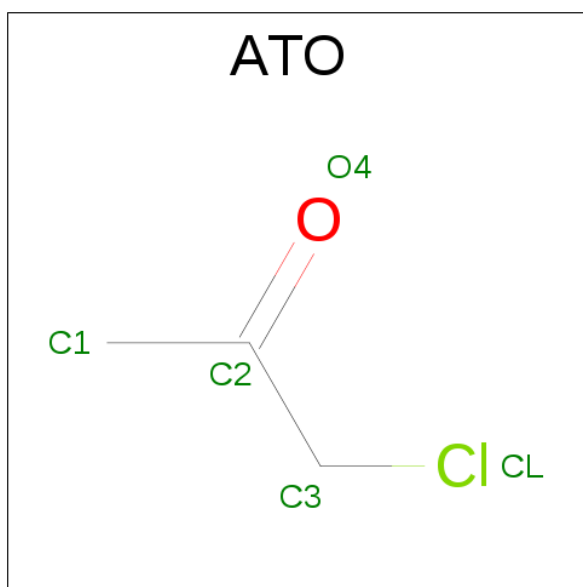
- Molecule 1 is a protein called HYDROXYNITRILE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2108	1362	349	389	8			
1	B	258	Total	C	N	O	S	0	0	0
			2078	1342	344	384	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	CLONING ARTIFACT	PDB 1DWQ
A	-3	ILE	-	CLONING ARTIFACT	PDB 1DWQ
A	-2	SER	-	CLONING ARTIFACT	PDB 1DWQ
A	-1	LYS	-	CLONING ARTIFACT	PDB 1DWQ
A	1	MET	-	CLONING ARTIFACT	PDB 1DWQ
B	-4	PRO	-	CLONING ARTIFACT	PDB 1DWQ
B	-3	ILE	-	CLONING ARTIFACT	PDB 1DWQ
B	-2	SER	-	CLONING ARTIFACT	PDB 1DWQ
B	-1	LYS	-	CLONING ARTIFACT	PDB 1DWQ
B	1	MET	-	CLONING ARTIFACT	PDB 1DWQ

- Molecule 2 is CHLOROACETONE (three-letter code: ATO) (formula: C<sub>3</sub>H<sub>5</sub>ClO).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	114	Total	O	0	0
			114	114		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.50Å 104.50Å 189.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 19.77 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.4 (8.00-2.20) 96.6 (19.77-2.17)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.17Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.207 , 0.244 0.463 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.67	EDS
Total number of atoms	4402	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.93	0/2149	1.56	36/2910 (1.2%)
1	B	0.92	0/2118	1.58	36/2869 (1.3%)
All	All	0.92	0/4267	1.57	72/5779 (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	129	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	B	92	ARG	NE-CZ-NH2	9.91	125.26	120.30
1	A	155	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	B	198	ILE	CA-CB-CG1	-8.65	94.57	111.00
1	A	28	ARG	NE-CZ-NH2	8.55	124.58	120.30
1	B	218	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	A	198	ILE	CA-CB-CG1	-8.25	95.32	111.00
1	A	28	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	B	204	TRP	CD1-CG-CD2	7.91	112.62	106.30
1	A	19	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	218	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	B	198	ILE	CA-CB-CG2	7.73	126.37	110.90
1	B	92	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	B	19	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	A	46	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	B	204	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	B	217	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	A	19	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	B	218	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	204	TRP	CD1-CG-CD2	7.27	112.12	106.30
1	A	129	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	17	TRP	CD1-CG-CD2	7.23	112.08	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	B	19	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	A	198	ILE	CA-CB-CG2	7.21	125.32	110.90
1	A	218	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	A	155	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	19	TRP	CB-CG-CD1	-6.99	117.92	127.00
1	B	28	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	B	17	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	B	128	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	A	204	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	A	128	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	A	17	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	A	17	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	A	229	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	A	228	VAL	CG1-CB-CG2	-6.35	100.74	110.90
1	B	80	SER	N-CA-CB	-6.30	101.05	110.50
1	B	163	THR	CA-CB-CG2	6.21	121.09	112.40
1	B	128	TRP	CD1-CG-CD2	6.19	111.25	106.30
1	B	218	TRP	CG-CD2-CE3	6.02	139.32	133.90
1	A	19	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	B	116	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	217	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	B	155	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	19	TRP	CB-CG-CD1	-5.76	119.51	127.00
1	B	19	TRP	CG-CD2-CE3	5.75	139.07	133.90
1	B	218	TRP	CB-CG-CD1	-5.75	119.52	127.00
1	A	116	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	A	163	THR	CA-CB-CG2	5.61	120.25	112.40
1	B	163	THR	N-CA-CB	-5.60	99.65	110.30
1	A	121	LEU	CA-CB-CG	-5.56	102.52	115.30
1	B	218	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	B	1	MET	CA-C-N	5.46	129.21	117.20
1	B	133	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	95	ASP	CA-CB-CG	5.39	125.25	113.40
1	A	128	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	B	217	ARG	CB-CG-CD	-5.30	97.81	111.60
1	B	204	TRP	CG-CD2-CE3	5.29	138.67	133.90
1	B	187	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	218	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	A	128	TRP	CD1-CG-CD2	5.24	110.49	106.30
1	A	130	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	70	GLN	CA-C-N	-5.18	105.84	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	CB-CG-CD	-5.16	98.19	111.60
1	A	18	ILE	CB-CA-C	-5.15	101.30	111.60
1	B	163	THR	CA-CB-OG1	-5.11	98.28	109.00
1	A	18	ILE	N-CA-CB	5.05	122.42	110.80
1	A	214	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	204	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	A	178	SER	CA-C-N	-5.01	106.19	117.20
1	B	129	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2108	0	2105	39	3
1	B	2078	0	2069	26	3
2	A	5	0	3	0	0
3	A	97	0	0	5	0
3	B	114	0	0	0	0
All	All	4402	0	4177	62	3

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 (62) 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:139:ILE:O	3:A:2052:HOH:O	1.91	0.88
1:B:10:HIS:HE1	1:B:38:MET:H	1.22	0.83
1:A:10:HIS:HE1	1:A:38:MET:H	1.25	0.83
1:A:137:THR:N	3:A:2050:HOH:O	1.94	0.80
1:B:90:ALA:HB1	1:B:198:ILE:HD13	1.66	0.77
1:B:52:ASN:HD22	1:B:138:ASN:HB2	1.51	0.74
1:A:90:ALA:HB1	1:A:198:ILE:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASN:HD22	1:A:138:ASN:HB2	1.55	0.70
1:B:10:HIS:HD2	1:B:11:THR:O	1.78	0.67
1:B:163:THR:HG22	1:B:166:GLU:H	1.63	0.64
1:A:138:ASN:ND2	1:A:142:GLU:H	1.96	0.62
1:A:10:HIS:HD2	1:A:11:THR:O	1.82	0.62
1:B:82:ALA:HA	1:B:85:ASN:HD22	1.66	0.61
1:A:182:ASN:H	1:A:182:ASN:HD22	1.50	0.59
1:A:10:HIS:HE1	1:A:38:MET:N	2.00	0.58
1:A:163:THR:HG22	1:A:166:GLU:H	1.68	0.58
1:A:121:LEU:HG	1:A:121:LEU:O	2.01	0.57
1:B:20:HIS:HE1	1:B:166:GLU:OE1	1.87	0.57
1:A:75:ILE:HD11	1:A:258:ALA:HB2	1.85	0.57
1:A:136:PHE:HA	3:A:2050:HOH:O	2.05	0.56
1:A:136:PHE:CA	3:A:2050:HOH:O	2.54	0.56
1:A:14:HIS:O	1:A:41:SER:HB3	2.07	0.55
1:B:120:LYS:HG3	1:B:218:TRP:CH2	2.42	0.54
1:A:82:ALA:HA	1:A:85:ASN:HD22	1.74	0.53
1:B:81:CSA:HA	1:B:106:LEU:HD22	1.89	0.53
1:B:94:VAL:HG23	1:B:198:ILE:CD1	2.39	0.52
1:A:200:LYS:HE2	1:A:223:TYR:HE2	1.75	0.52
1:B:94:VAL:HG23	1:B:198:ILE:HD11	1.92	0.52
1:A:148:LYS:HE2	1:A:149:LEU:H	1.75	0.51
1:A:20:HIS:HD2	1:B:165:GLY:O	1.95	0.50
1:A:148:LYS:HE2	1:A:149:LEU:N	2.27	0.50
1:B:116:TYR:O	1:B:120:LYS:HG2	2.12	0.50
1:A:231:VAL:HG11	1:A:242:LYS:HG3	1.94	0.49
1:A:139:ILE:HG23	1:A:140:THR:HG23	1.95	0.48
1:A:192:GLU:HA	1:A:196:GLY:HA3	1.94	0.48
1:B:68:LEU:HD11	1:B:74:VAL:HG13	1.96	0.47
1:A:132:GLU:HB3	3:A:2046:HOH:O	2.13	0.47
1:A:168:GLU:HG2	1:B:24:PRO:HD3	1.96	0.47
1:B:246:VAL:HG12	1:B:250:LEU:HD22	1.96	0.47
1:B:9:ILE:HD11	1:B:61:LEU:HD13	1.95	0.47
1:B:182:ASN:H	1:B:182:ASN:HD22	1.61	0.47
1:B:2:VAL:HG11	1:B:258:ALA:HA	1.97	0.47
1:A:10:HIS:CE1	1:A:38:MET:H	2.16	0.46
1:B:10:HIS:CB	1:B:18:ILE:HD11	2.46	0.46
1:B:10:HIS:CE1	1:B:38:MET:H	2.15	0.46
1:A:20:HIS:HE1	1:A:166:GLU:OE1	1.98	0.45
1:A:155:ARG:O	1:A:155:ARG:HD3	2.17	0.45
1:A:94:VAL:HG23	1:A:198:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HB	1:A:80:SER:HB3	2.00	0.44
1:A:90:ALA:CB	1:A:198:ILE:HD13	2.44	0.43
1:A:9:ILE:HD11	1:A:61:LEU:HD13	2.00	0.43
1:B:90:ALA:HA	1:B:97:ILE:HD12	2.01	0.43
1:A:94:VAL:HG23	1:A:198:ILE:CD1	2.49	0.42
1:A:63:THR:O	1:A:66:GLU:HB3	2.20	0.42
1:B:155:ARG:HD3	1:B:155:ARG:HA	1.65	0.42
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.90	0.42
1:A:138:ASN:ND2	1:A:140:THR:H	2.17	0.41
1:A:165:GLY:O	1:B:20:HIS:HD2	2.03	0.41
1:A:148:LYS:HE3	1:A:174:MET:HG3	2.01	0.41
1:B:148:LYS:HB2	1:B:148:LYS:HE3	1.86	0.41
1:A:224:LYS:HA	1:A:225:PRO:HD2	1.97	0.41
1:A:62:LEU:HD21	1:A:89:ALA:HA	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-4:PRO:N	1:B:232:GLN:OE1[3_545]	1.85	0.35
1:A:137:THR:OG1	1:B:66:GLU:OE1[7_556]	1.93	0.27
1:A:-4:PRO:O	1:B:232:GLN:N[3_545]	2.03	0.17

## 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	259/262 (99%)	245 (95%)	14 (5%)	0	100	100
1	B	255/262 (97%)	246 (96%)	9 (4%)	0	100	100
All	All	514/524 (98%)	491 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	226/226 (100%)	211 (93%)	15 (7%)	19	21
1	B	222/226 (98%)	209 (94%)	13 (6%)	23	26
All	All	448/452 (99%)	420 (94%)	28 (6%)	21	23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ILE
1	A	-2	SER
1	A	18	ILE
1	A	72	GLU
1	A	95	ASP
1	A	106	LEU
1	A	138	ASN
1	A	143	THR
1	A	148	LYS
1	A	154	LEU
1	A	155	ARG
1	A	163	THR
1	A	182	ASN
1	A	198	ILE
1	A	232	GLN
1	B	1	MET
1	B	18	ILE
1	B	50	GLN
1	B	106	LEU
1	B	124	SER
1	B	155	ARG
1	B	163	THR
1	B	169	LEU
1	B	182	ASN
1	B	198	ILE

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Mol	Chain	Res	Type
1	B	199	LYS
1	B	224	LYS
1	B	250	LEU

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	47	GLN
1	A	52	ASN
1	A	85	ASN
1	A	138	ASN
1	A	181	GLN
1	A	182	ASN
1	B	10	HIS
1	B	20	HIS
1	B	47	GLN
1	B	52	ASN
1	B	85	ASN
1	B	182	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	CSA	A	81	1	9,9,10	1.15	0	4,10,12	2.01	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSA	B	81	1	9,9,10	0.96	0	4,10,12	1.76	2 (50%)

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	CSA	A	81	1	-	0/6/8/10	0/0/0/0
1	CSA	B	81	1	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	CSA	O-C-CA	-3.42	115.58	125.02
1	B	81	CSA	C2-C3-SG	-2.50	104.31	113.75
1	B	81	CSA	O-C-CA	-2.44	118.29	125.02
1	A	81	CSA	C2-C3-SG	-2.12	105.72	113.75

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
1	B	81	CSA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	ATO	A	1259	-	4,4,4	0.84	0	4,4,4	1.60	1 (25%)

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	ATO	A	1259	-	-	0/1/2/2	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1259	ATO	C2-C3-CL	-3.14	108.13	112.58

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

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	261/262 (99%)	2.44	155 (59%) <b>0</b> <b>0</b>	18, 28, 47, 62	0
1	B	257/262 (98%)	2.22	136 (52%) <b>0</b> <b>0</b>	17, 26, 42, 74	0
All	All	518/524 (98%)	2.33	291 (56%) <b>0</b> <b>0</b>	17, 27, 46, 74	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	VAL	7.7
1	B	197	SER	7.5
1	B	170	ALA	7.4
1	A	233	GLY	6.1
1	B	30	GLY	6.0
1	A	151	PHE	5.6
1	A	162	CYS	5.5
1	A	218	TRP	5.2
1	A	240	LEU	5.2
1	A	231	VAL	5.2
1	B	3	THR	5.2
1	A	111	VAL	5.0
1	A	258	ALA	4.8
1	A	215	PHE	4.8
1	A	160	THR	4.7
1	A	135	THR	4.7
1	B	97	ILE	4.6
1	A	211	PHE	4.6
1	A	4	ALA	4.5
1	A	109	ASP	4.5
1	B	258	ALA	4.5
1	A	223	TYR	4.5
1	B	90	ALA	4.4
1	B	105	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	26	LEU	4.4
1	A	141	GLY	4.4
1	A	234	GLY	4.4
1	A	116	TYR	4.4
1	B	63	THR	4.3
1	B	36	LEU	4.3
1	B	107	LEU	4.3
1	A	165	GLY	4.3
1	A	205	THR	4.2
1	A	152	VAL	4.2
1	B	88	ILE	4.2
1	A	125	PHE	4.2
1	B	159	PHE	4.1
1	A	25	ALA	4.1
1	B	1	MET	4.1
1	A	213	PRO	4.1
1	A	133	TYR	4.1
1	B	167	TYR	4.0
1	B	231	VAL	4.0
1	A	237	LYS	4.0
1	A	257	TYR	3.9
1	A	110	THR	3.9
1	B	191	THR	3.9
1	A	145	THR	3.9
1	A	54	PHE	3.9
1	A	169	LEU	3.9
1	B	238	LEU	3.9
1	A	204	TRP	3.9
1	B	213	PRO	3.9
1	A	241	THR	3.8
1	B	29	ALA	3.8
1	B	64	PHE	3.8
1	A	40	ALA	3.8
1	A	7	VAL	3.8
1	A	39	ALA	3.7
1	A	134	PHE	3.7
1	A	209	LYS	3.7
1	A	130	ASP	3.7
1	A	3	THR	3.7
1	A	239	GLN	3.6
1	B	161	LYS	3.6
1	A	214	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	75	ILE	3.6
1	A	18	ILE	3.6
1	A	107	LEU	3.6
1	A	253	VAL	3.6
1	B	111	VAL	3.6
1	B	255	ASP	3.6
1	A	117	THR	3.6
1	A	225	PRO	3.6
1	B	6	PHE	3.5
1	B	27	GLU	3.5
1	B	184	LEU	3.5
1	A	195	TYR	3.5
1	B	202	TYR	3.5
1	A	12	ILE	3.5
1	A	179	LEU	3.5
1	B	4	ALA	3.5
1	A	167	TYR	3.5
1	A	172	MET	3.5
1	A	93	TYR	3.5
1	B	24	PRO	3.4
1	A	121	LEU	3.4
1	A	250	LEU	3.4
1	A	71	GLY	3.4
1	A	153	LEU	3.4
1	A	198	ILE	3.4
1	B	247	ALA	3.4
1	A	51	ILE	3.4
1	B	248	HIS	3.4
1	A	127	ASP	3.3
1	B	23	LYS	3.3
1	A	147	MET	3.3
1	A	33	VAL	3.3
1	B	17	TRP	3.3
1	B	169	LEU	3.3
1	B	232	GLN	3.3
1	B	48	ILE	3.3
1	A	108	PRO	3.3
1	A	157	ASN	3.3
1	B	54	PHE	3.3
1	A	57	TYR	3.2
1	A	238	LEU	3.2
1	A	139	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	112	HIS	3.2
1	A	84	LEU	3.2
1	B	76	ILE	3.2
1	B	153	LEU	3.2
1	B	43	ILE	3.2
1	A	207	GLN	3.1
1	A	190	PHE	3.1
1	B	16	ALA	3.1
1	A	155	ARG	3.1
1	B	250	LEU	3.1
1	A	163	THR	3.1
1	A	210	ILE	3.1
1	A	64	PHE	3.1
1	B	185	ALA	3.1
1	B	223	TYR	3.1
1	B	228	VAL	3.1
1	A	67	LYS	3.1
1	A	171	LYS	3.1
1	B	158	LEU	3.1
1	A	146	THR	3.1
1	A	144	ILE	3.1
1	A	128	TRP	3.1
1	A	20	HIS	3.0
1	B	150	GLY	3.0
1	A	13	CYS	3.0
1	A	45	PRO	3.0
1	A	154	LEU	3.0
1	B	256	ALA	3.0
1	A	224	LYS	3.0
1	A	148	LYS	3.0
1	A	62	LEU	2.9
1	A	19	TRP	2.9
1	B	162	CYS	2.9
1	A	6	PHE	2.9
1	A	22	LEU	2.9
1	A	41	SER	2.9
1	B	18	ILE	2.9
1	A	2	VAL	2.9
1	A	201	VAL	2.9
1	B	165	GLY	2.9
1	A	61	LEU	2.9
1	B	39	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	116	TYR	2.9
1	A	95	ASP	2.9
1	B	210	ILE	2.9
1	A	138	ASN	2.9
1	B	254	ALA	2.9
1	B	34	THR	2.8
1	B	86	ILE	2.8
1	A	118	VAL	2.8
1	A	247	ALA	2.8
1	B	31	HIS	2.8
1	B	221	ALA	2.8
1	B	181	GLN	2.8
1	A	222	ASN	2.8
1	A	220	ILE	2.8
1	B	125	PHE	2.8
1	B	215	PHE	2.8
1	B	94	VAL	2.8
1	B	55	ASP	2.8
1	B	114	PRO	2.7
1	B	205	THR	2.7
1	A	188	PRO	2.7
1	A	212	LEU	2.7
1	A	92	ARG	2.7
1	B	229	TYR	2.7
1	B	102	PHE	2.7
1	A	202	TYR	2.7
1	B	89	ALA	2.7
1	B	179	LEU	2.7
1	A	136	PHE	2.7
1	B	38	MET	2.7
1	B	257	TYR	2.7
1	A	77	VAL	2.7
1	B	19	TRP	2.6
1	B	204	TRP	2.6
1	B	57	TYR	2.6
1	A	21	LYS	2.6
1	A	180	PHE	2.6
1	B	87	ALA	2.6
1	B	241	THR	2.6
1	B	41	SER	2.6
1	B	195	TYR	2.6
1	B	74	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	144	ILE	2.6
1	A	17	TRP	2.5
1	A	14	HIS	2.5
1	A	91	ASP	2.5
1	A	105	SER	2.5
1	A	203	ILE	2.5
1	B	219	GLN	2.5
1	A	236	HIS	2.5
1	B	7	VAL	2.5
1	A	217	ARG	2.5
1	A	137	THR	2.5
1	A	193	LYS	2.5
1	B	28	ARG	2.5
1	A	158	LEU	2.5
1	B	201	VAL	2.5
1	B	98	ALA	2.5
1	A	131	THR	2.5
1	A	221	ALA	2.5
1	B	51	ILE	2.5
1	B	33	VAL	2.4
1	B	211	PHE	2.4
1	B	128	TRP	2.4
1	B	218	TRP	2.4
1	A	86	ILE	2.4
1	B	139	ILE	2.4
1	A	159	PHE	2.4
1	B	198	ILE	2.4
1	B	234	GLY	2.4
1	A	242	LYS	2.4
1	A	8	LEU	2.4
1	A	35	ALA	2.4
1	A	129	ARG	2.4
1	B	252	GLU	2.4
1	A	75	ILE	2.4
1	B	12	ILE	2.4
1	B	61	LEU	2.4
1	B	173	VAL	2.4
1	B	67	LYS	2.3
1	B	14	HIS	2.3
1	A	106	LEU	2.3
1	A	161	LYS	2.3
1	B	32	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	108	PRO	2.3
1	A	56	GLU	2.3
1	B	151	PHE	2.3
1	B	176	LYS	2.3
1	B	154	LEU	2.3
1	A	48	ILE	2.3
1	A	124	SER	2.3
1	B	160	THR	2.3
1	A	31	HIS	2.3
1	A	52	ASN	2.3
1	A	174	MET	2.2
1	A	9	ILE	2.2
1	A	72	GLU	2.2
1	B	112	HIS	2.2
1	B	214	ASP	2.2
1	A	-2	SER	2.2
1	A	76	ILE	2.2
1	B	11	THR	2.2
1	B	110	THR	2.2
1	A	164	ASP	2.2
1	A	232	GLN	2.2
1	B	65	LEU	2.2
1	B	70	GLN	2.2
1	B	121	LEU	2.2
1	A	99	ALA	2.2
1	A	254	ALA	2.2
1	B	163	THR	2.2
1	B	22	LEU	2.2
1	B	84	LEU	2.2
1	B	175	ARG	2.2
1	A	83	GLY	2.2
1	A	98	ALA	2.2
1	B	135	THR	2.2
1	A	-4	PRO	2.2
1	A	69	PRO	2.2
1	A	235	ASP	2.2
1	B	91	ASP	2.2
1	B	239	GLN	2.2
1	A	228	VAL	2.1
1	B	220	ILE	2.1
1	A	26	LEU	2.1
1	A	122	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	62	LEU	2.1
1	B	206	ASP	2.1
1	A	123	GLU	2.1
1	B	253	VAL	2.1
1	B	71	GLY	2.1
1	A	181	GLN	2.1
1	B	5	HIS	2.1
1	B	120	LYS	2.1
1	B	93	TYR	2.1
1	A	103	HIS	2.0
1	B	25	ALA	2.0
1	A	256	ALA	2.0
1	B	92	ARG	2.0
1	B	145	THR	2.0
1	B	148	LYS	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<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
1	CSA	A	81	10/11	0.75	0.30	-	23,26,35,35	0
1	CSA	B	81	10/11	0.83	0.20	-	23,25,36,38	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<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( $\text{\AA}^2$ )	Q<0.9
2	ATO	A	1259	5/5	0.69	0.40	1.36	39,39,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.