



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 PM UTC

PDB ID : 1DWO / pdb_00001dwo
Title : Crystal Structure of Hydroxynitrile Lyase from Manihot esculenta in Complex with Substrates Acetone and Chloroacetone:Implications for the Mechanism of Cyanogenesis
Authors : Lauble, H.; Forster, S.; Miehlisch, 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

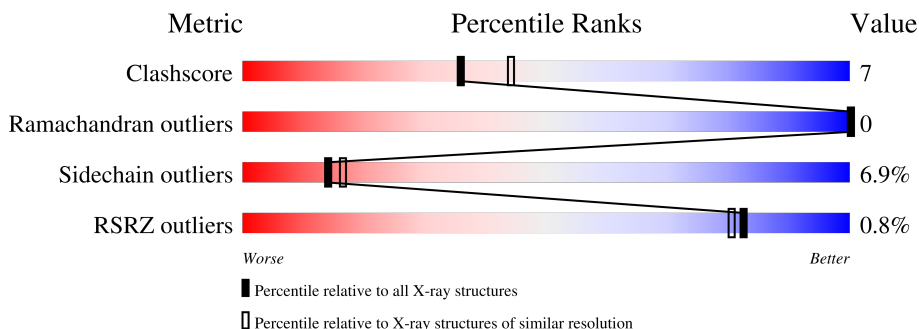
1 Overall quality at a glance

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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	% 72% 19% 6% .
1	B	262	% 71% 21% . . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4453 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.

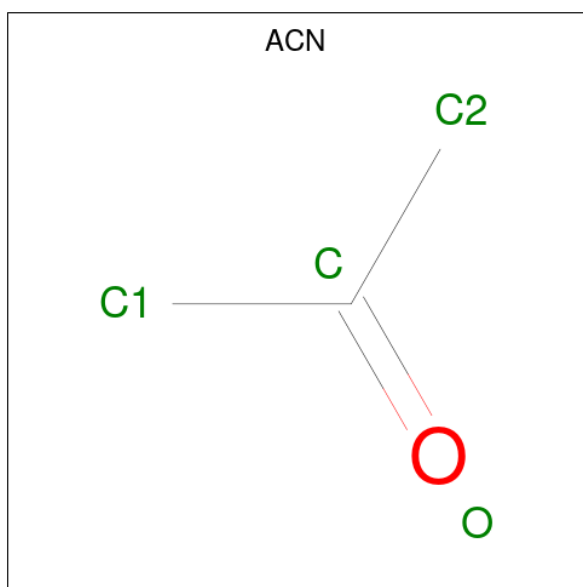
- Molecule 1 is a protein called HYDROXYNITRILE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			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 1DWO
A	-3	ILE	-	cloning artifact	PDB 1DWO
A	-2	SER	-	cloning artifact	PDB 1DWO
A	-1	LYS	-	cloning artifact	PDB 1DWO
A	1	MET	-	cloning artifact	PDB 1DWO
B	-4	PRO	-	cloning artifact	PDB 1DWO
B	-3	ILE	-	cloning artifact	PDB 1DWO
B	-2	SER	-	cloning artifact	PDB 1DWO
B	-1	LYS	-	cloning artifact	PDB 1DWO
B	1	MET	-	cloning artifact	PDB 1DWO

- Molecule 2 is ACETONE (CCD ID: ACN) (formula: C₃H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		

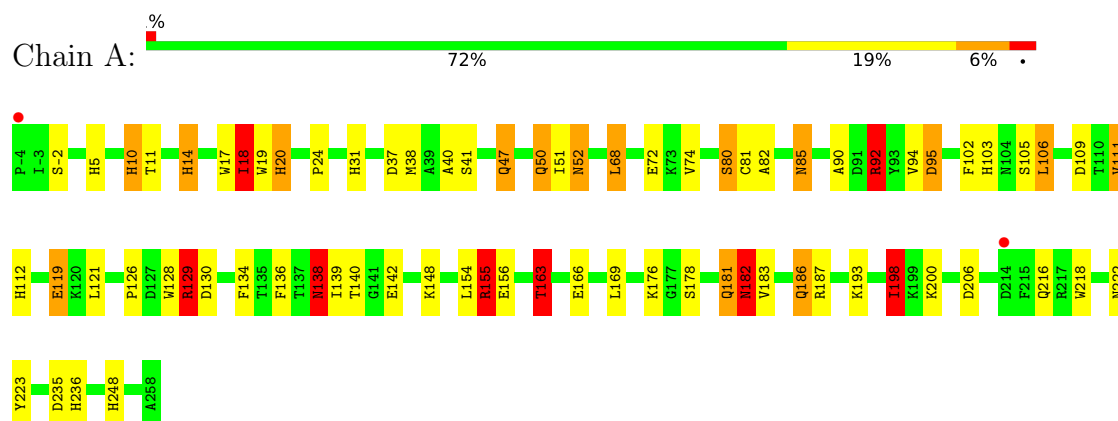
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	151	Total	O	0	0
			151	151		

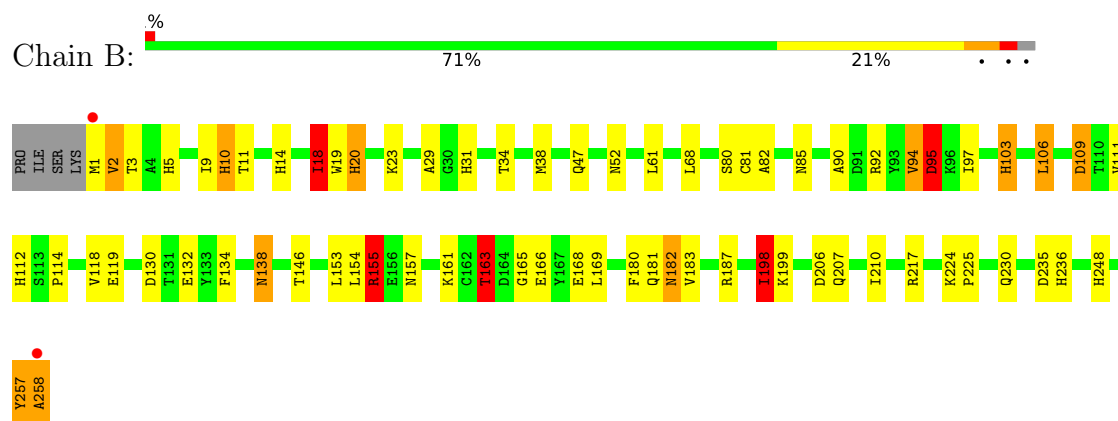
3 Residue-property plots [i](#)

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: 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	105.50Å 105.50Å 188.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (8.00-2.20) 94.8 (8.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.98 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.192 , 0.252 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 81.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4453	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: ACN

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	1.10	9/2156 (0.4%)	1.77	52/2921 (1.8%)
1	B	1.12	11/2125 (0.5%)	1.73	48/2880 (1.7%)
All	All	1.11	20/4281 (0.5%)	1.75	100/5801 (1.7%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	HIS	CD2-NE2	-8.06	1.28	1.37
1	A	111	VAL	CA-CB	7.41	1.64	1.54
1	A	10	HIS	CD2-NE2	-7.10	1.30	1.37
1	B	5	HIS	CD2-NE2	-6.95	1.30	1.37
1	B	112	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	5	HIS	CD2-NE2	-6.79	1.30	1.37
1	B	248	HIS	CD2-NE2	-6.44	1.30	1.37
1	B	10	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	14	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	20	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	31	HIS	CD2-NE2	-6.18	1.31	1.37
1	B	18	ILE	CA-CB	5.98	1.63	1.54
1	A	112	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	236	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	20	HIS	CD2-NE2	-5.56	1.31	1.37
1	A	236	HIS	CD2-NE2	-5.28	1.32	1.37
1	A	103	HIS	CD2-NE2	-5.21	1.32	1.37
1	B	14	HIS	CD2-NE2	-5.17	1.32	1.37
1	B	132	GLU	CA-CB	-5.15	1.45	1.53
1	B	31	HIS	CG-ND1	-5.07	1.32	1.38

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ASP	CA-CB-CG	8.69	121.29	112.60
1	A	109	ASP	CA-CB-CG	8.63	121.23	112.60
1	A	198	ILE	CA-CB-CG2	8.45	124.86	110.50
1	B	109	ASP	CA-CB-CG	8.37	120.97	112.60
1	A	129	ARG	NE-CZ-NH2	-8.30	111.73	119.20
1	A	52	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	B	198	ILE	CA-CB-CG1	-8.11	96.62	110.40
1	A	138	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	A	198	ILE	CA-CB-CG1	-7.74	97.24	110.40
1	B	258	ALA	N-CA-C	7.69	132.53	111.00
1	B	97	ILE	N-CA-CB	-7.58	102.11	111.67
1	A	47	GLN	OE1-CD-NE2	-7.40	115.20	122.60
1	B	198	ILE	CA-CB-CG2	7.15	122.65	110.50
1	A	95	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	31	HIS	CB-CG-CD2	-7.03	122.06	131.20
1	B	182	ASN	CA-CB-CG	6.92	119.52	112.60
1	A	47	GLN	CG-CD-NE2	6.90	126.75	116.40
1	A	222	ASN	OD1-CG-ND2	-6.86	115.74	122.60
1	B	118	VAL	N-CA-C	-6.78	103.87	110.72
1	A	92	ARG	NE-CZ-NH1	-6.72	114.78	121.50
1	B	257	TYR	CA-C-O	-6.67	111.02	118.69
1	A	19	TRP	CG-CD2-CE3	6.66	140.56	133.90
1	A	52	ASN	CB-CG-ND2	6.66	126.38	116.40
1	B	2	VAL	N-CA-C	-6.60	98.96	108.53
1	B	182	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	103	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	B	248	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	B	112	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	A	85	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	A	14	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	B	157	ASN	CA-CB-CG	-6.26	106.34	112.60
1	B	163	THR	N-CA-CB	-6.26	99.91	109.92
1	A	218	TRP	N-CA-C	-6.24	104.39	111.07
1	A	163	THR	N-CA-CB	-6.19	100.94	110.04
1	A	181	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	B	257	TYR	N-CA-C	6.16	123.32	114.39
1	B	92	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	A	206	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	103	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	A	148	LYS	N-CA-C	-6.03	97.48	108.02
1	B	80	SER	N-CA-CB	-6.00	100.36	110.49
1	A	236	HIS	CB-CG-CD2	-5.98	123.42	131.20
1	B	47	GLN	OE1-CD-NE2	-5.89	116.71	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	163	THR	CA-CB-OG1	-5.82	100.86	109.60
1	B	111	VAL	N-CA-C	5.82	116.60	110.72
1	B	153	LEU	N-CA-C	-5.82	105.02	111.36
1	B	183	VAL	N-CA-C	-5.81	104.67	111.00
1	B	31	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	A	248	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	198	ILE	CB-CG1-CD1	-5.75	101.72	113.80
1	B	230	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	B	207	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	235	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	163	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	218	TRP	CG-CD2-CE3	5.67	139.57	133.90
1	B	95	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	138	ASN	CB-CG-ND2	5.58	124.77	116.40
1	A	18	ILE	N-CA-CB	5.54	122.69	111.05
1	A	17	TRP	CA-C-O	-5.54	114.00	120.20
1	A	121	LEU	N-CA-C	-5.53	105.15	111.07
1	A	126	PRO	CA-C-N	-5.50	115.35	123.05
1	A	126	PRO	C-N-CA	-5.50	115.35	123.05
1	A	155	ARG	NE-CZ-NH2	-5.46	114.28	119.20
1	B	92	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	A	19	TRP	CB-CG-CD1	-5.46	118.72	126.90
1	B	94	VAL	CA-C-N	5.45	128.34	120.38
1	B	94	VAL	C-N-CA	5.45	128.34	120.38
1	B	155	ARG	NE-CZ-NH2	-5.42	114.33	119.20
1	A	80	SER	N-CA-CB	-5.40	101.36	110.49
1	A	31	HIS	CB-CG-ND1	5.39	130.78	122.70
1	B	138	ASN	CA-CB-CG	5.38	117.97	112.60
1	B	80	SER	O-C-N	-5.34	115.49	122.59
1	B	235	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	236	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	178	SER	CA-C-O	5.31	127.07	120.54
1	A	50	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	B	10	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	B	217	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	10	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	A	103	HIS	CA-CB-CG	5.25	119.05	113.80
1	A	51	ILE	O-C-N	-5.24	117.80	123.14
1	A	182	ASN	CB-CG-ND2	5.24	124.26	116.40
1	B	3	THR	N-CA-C	-5.24	101.74	110.17
1	B	18	ILE	N-CA-CB	5.22	122.02	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	29	ALA	CA-C-O	5.16	125.60	119.56
1	B	19	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	B	18	ILE	CB-CG1-CD1	-5.14	103.01	113.80
1	A	136	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	37	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	23	LYS	CA-C-N	5.12	124.73	119.05
1	B	23	LYS	C-N-CA	5.12	124.73	119.05
1	A	40	ALA	N-CA-C	5.10	118.64	111.90
1	B	47	GLN	CG-CD-NE2	5.10	124.05	116.40
1	B	34	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	138	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	130	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	186	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	A	50	GLN	CA-CB-CG	5.01	124.11	114.10

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	35	0
1	B	2074	0	2065	28	0
2	A	4	0	6	0	0
3	A	120	0	0	0	0
3	B	151	0	0	3	0
All	All	4453	0	4172	61	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 (61) 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:10:HIS:HE1	1:B:38:MET:H	1.14	0.90
1:A:10:HIS:HE1	1:A:38:MET:H	1.20	0.89
1:A:52:ASN:HD22	1:A:138:ASN:HB2	1.45	0.81
1:A:81:CYS:HA	1:A:106:LEU:HD22	1.72	0.70
1:B:10:HIS:CE1	1:B:38:MET:H	2.06	0.66
1:A:10:HIS:CE1	1:A:38:MET:H	2.09	0.66
1:A:182:ASN:HD22	1:A:182:ASN:H	1.46	0.64
1:B:52:ASN:HD22	1:B:138:ASN:HB2	1.60	0.64
1:A:10:HIS:HD2	1:A:11:THR:O	1.81	0.63
1:A:138:ASN:ND2	1:A:142:GLU:H	1.98	0.62
1:B:95:ASP:HB3	3:B:423:HOH:O	2.00	0.61
1:B:163:THR:HG22	1:B:166:GLU:H	1.66	0.60
1:B:10:HIS:HD2	1:B:11:THR:O	1.85	0.60
1:A:11:THR:HB	1:A:80:SER:HB3	1.84	0.60
1:A:10:HIS:HE1	1:A:38:MET:N	1.96	0.58
1:B:94:VAL:HG23	1:B:198:ILE:CD1	2.34	0.58
1:B:82:ALA:HA	1:B:85:ASN:HD22	1.68	0.58
1:A:82:ALA:HA	1:A:85:ASN:HD22	1.69	0.57
1:B:81:CYS:HA	1:B:106:LEU:HD22	1.86	0.57
1:A:10:HIS:HB3	1:A:18:ILE:HD11	1.86	0.56
1:A:163:THR:HG22	1:A:166:GLU:H	1.71	0.55
1:B:94:VAL:HG23	1:B:198:ILE:HD12	1.89	0.54
1:A:14:HIS:O	1:A:41:SER:HB3	2.08	0.54
1:A:20:HIS:HE1	1:A:166:GLU:OE1	1.91	0.54
1:A:129:ARG:NH2	1:A:156:GLU:HB2	2.22	0.54
1:A:182:ASN:HD22	1:A:182:ASN:N	2.07	0.53
1:A:24:PRO:HD3	1:B:168:GLU:HG2	1.90	0.52
1:A:183:VAL:HA	1:A:186:GLN:HE21	1.75	0.52
1:B:10:HIS:HE1	1:B:38:MET:N	1.95	0.52
1:A:119:GLU:HG3	1:A:181:GLN:NE2	2.25	0.52
1:A:10:HIS:CB	1:A:18:ILE:HD11	2.40	0.51
1:A:200:LYS:HE2	1:A:223:TYR:HE2	1.76	0.50
1:B:20:HIS:HE1	1:B:166:GLU:OE1	1.95	0.50
1:B:90:ALA:HB1	1:B:198:ILE:HD13	1.94	0.49
1:A:47:GLN:H	1:A:50:GLN:NE2	2.12	0.47
1:A:90:ALA:HB1	1:A:198:ILE:HD13	1.96	0.47
1:A:94:VAL:HG23	1:A:198:ILE:HD12	1.97	0.47
1:B:180:PHE:HE1	3:B:311:HOH:O	1.98	0.46
1:B:2:VAL:HG11	1:B:258:ALA:HB2	1.98	0.46
1:B:155:ARG:HD3	1:B:155:ARG:HA	1.66	0.46
1:A:92:ARG:HH12	1:A:187:ARG:NH2	2.13	0.46
1:B:10:HIS:CB	1:B:18:ILE:HD11	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:HD3	1:A:155:ARG:O	2.17	0.45
1:B:119:GLU:HG3	1:B:181:GLN:NE2	2.31	0.45
1:B:134:PHE:HB2	1:B:146:THR:OG1	2.17	0.45
1:A:11:THR:CB	1:A:80:SER:HB3	2.47	0.45
1:A:102:PHE:HB3	1:A:105:SER:HB3	1.98	0.44
1:B:114:PRO:HG2	1:B:187:ARG:HD3	1.98	0.44
1:A:68:LEU:HD11	1:A:74:VAL:HG13	1.98	0.44
1:A:155:ARG:HD3	1:A:155:ARG:C	2.43	0.44
1:A:20:HIS:HD2	1:B:165:GLY:O	2.01	0.43
1:B:199:LYS:HD2	1:B:257:TYR:CE2	2.54	0.43
1:B:119:GLU:HG3	1:B:181:GLN:HE21	1.84	0.42
1:B:109:ASP:HB2	3:B:365:HOH:O	2.19	0.42
1:B:161:LYS:HD3	1:B:161:LYS:HA	1.90	0.42
1:A:134:PHE:CD1	1:A:176:LYS:HE3	2.55	0.42
1:A:139:ILE:HG23	1:A:140:THR:HG23	2.01	0.42
1:A:128:TRP:N	1:A:128:TRP:CD1	2.89	0.41
1:B:9:ILE:HD11	1:B:61:LEU:HD13	2.02	0.41
1:B:224:LYS:HA	1:B:225:PRO:HD3	1.86	0.41
1:A:182:ASN:H	1:A:182:ASN:ND2	2.12	0.40

There are no symmetry-related clashes.

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	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
1	B	256/262 (98%)	244 (95%)	12 (5%)	0	100	100
All	All	516/524 (98%)	494 (96%)	22 (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	227/227 (100%)	209 (92%)	18 (8%)	11	13
1	B	223/227 (98%)	210 (94%)	13 (6%)	18	22
All	All	450/454 (99%)	419 (93%)	31 (7%)	14	16

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	18	ILE
1	A	68	LEU
1	A	72	GLU
1	A	92	ARG
1	A	95	ASP
1	A	106	LEU
1	A	111	VAL
1	A	119	GLU
1	A	129	ARG
1	A	138	ASN
1	A	154	LEU
1	A	155	ARG
1	A	163	THR
1	A	169	LEU
1	A	182	ASN
1	A	193	LYS
1	A	198	ILE
1	B	1	MET
1	B	18	ILE
1	B	68	LEU
1	B	95	ASP
1	B	103	HIS
1	B	106	LEU
1	B	154	LEU
1	B	155	ARG
1	B	163	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	LEU
1	B	182	ASN
1	B	198	ILE
1	B	210	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) 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	181	GLN
1	A	182	ASN
1	A	186	GLN
1	A	248	HIS
1	A	251	GLN
1	B	10	HIS
1	B	20	HIS
1	B	47	GLN
1	B	50	GLN
1	B	52	ASN
1	B	85	ASN
1	B	181	GLN
1	B	182	ASN
1	B	248	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	ACN	A	301	-	3,3,3	0.78	0	3,3,3	0.34	0

There are no bond length outliers.

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	262/262 (100%)	-0.77	2 (0%) 82 80	10, 18, 36, 50	0
1	B	258/262 (98%)	-0.88	2 (0%) 82 80	9, 17, 31, 58	0
All	All	520/524 (99%)	-0.83	4 (0%) 82 80	9, 18, 34, 58	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	ALA	6.1
1	A	214	ASP	2.6
1	B	1	MET	2.5
1	A	-4	PRO	2.5

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 oligosaccharides 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, 95th 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
2	ACN	A	301	4/4	0.90	0.06	20,27,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.