



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:33 PM UTC

PDB ID : 1DWP / pdb\_00001dwp  
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](mailto: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>.

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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

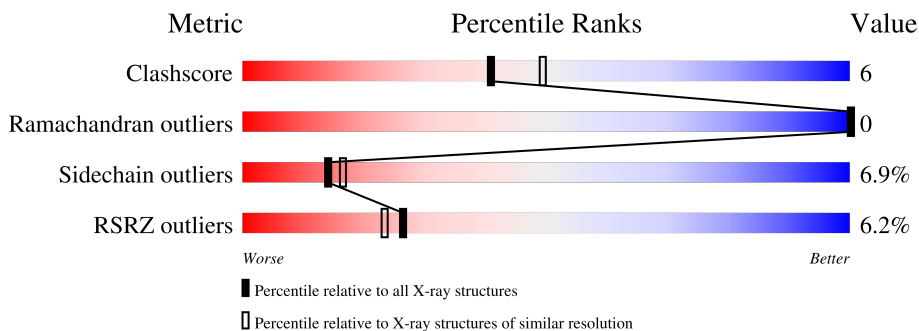
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

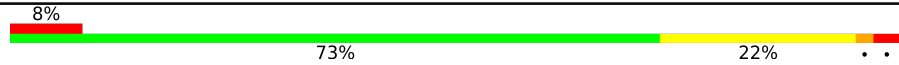

The reported resolution of this entry is 2.20 Å.

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  $\geq 3$ , 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	
1	B	262	

## 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	2104	1359	349	388	8	0	0	0
1	B	258	2074	1339	344	383	8	0	0	0

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 (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

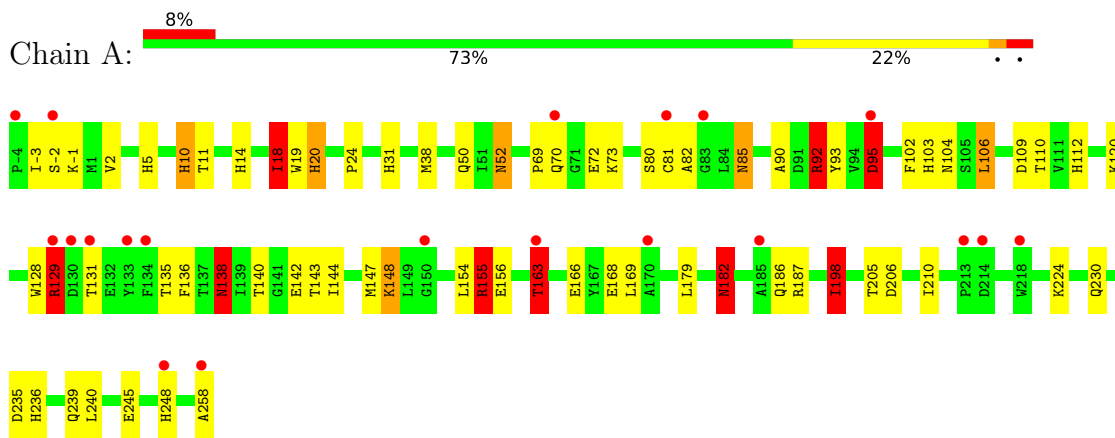
- Molecule 3 is water.

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

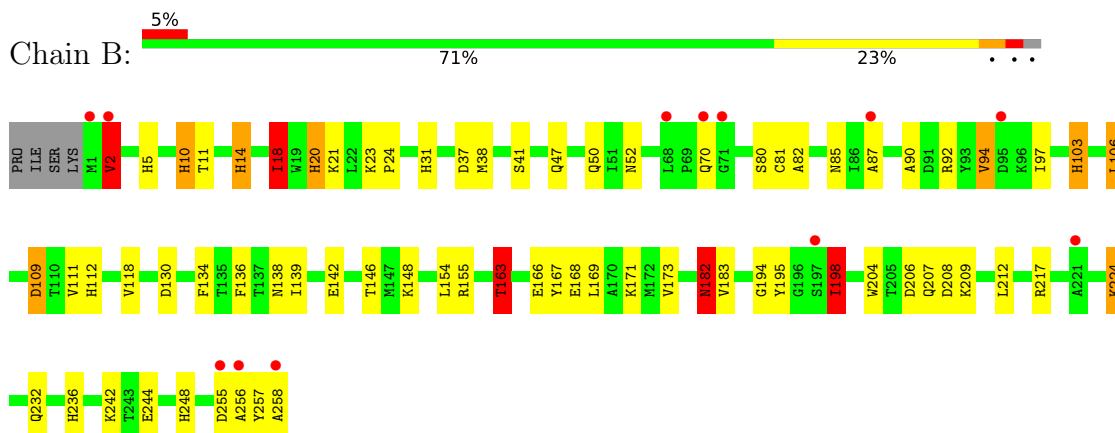
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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, $\alpha$ , $\beta$ , $\gamma$	106.60Å 106.60Å 189.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-2.20) 96.7 (8.00-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	25.4	Xtrriage
Anisotropy	0.496	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 95.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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: 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	1.11	9/2156 (0.4%)	1.77	57/2921 (2.0%)
1	B	1.12	11/2125 (0.5%)	1.77	47/2880 (1.6%)
All	All	1.11	20/4281 (0.5%)	1.77	104/5801 (1.8%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	HIS	CD2-NE2	-7.27	1.29	1.37
1	A	112	HIS	CD2-NE2	-7.18	1.29	1.37
1	B	10	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	10	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	31	HIS	CD2-NE2	-6.96	1.30	1.37
1	B	5	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	14	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	20	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	248	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	103	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	236	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	236	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	31	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	14	HIS	CD2-NE2	-5.83	1.31	1.37
1	B	20	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	129	ARG	NE-CZ	5.59	1.39	1.33
1	A	103	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	198	ILE	CA-CB	5.36	1.59	1.54
1	B	112	HIS	CD2-NE2	-5.29	1.32	1.37
1	B	18	ILE	CB-CG1	-5.17	1.43	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLN	OE1-CD-NE2	-8.95	113.65	122.60
1	A	-3	ILE	N-CA-C	-8.63	95.56	108.17
1	A	198	ILE	CA-CB-CG2	8.55	125.04	110.50
1	B	182	ASN	OD1-CG-ND2	-8.50	114.10	122.60
1	B	198	ILE	CA-CB-CG2	8.20	124.43	110.50
1	B	109	ASP	CA-CB-CG	8.18	120.78	112.60
1	A	198	ILE	CA-CB-CG1	-7.58	97.51	110.40
1	B	198	ILE	CA-CB-CG1	-7.53	97.59	110.40
1	A	186	GLN	OE1-CD-NE2	-7.13	115.47	122.60
1	A	50	GLN	OE1-CD-NE2	-7.06	115.54	122.60
1	A	31	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	B	212	LEU	CA-C-N	6.89	126.41	119.24
1	B	212	LEU	C-N-CA	6.89	126.41	119.24
1	A	109	ASP	CA-CB-CG	6.88	119.48	112.60
1	B	21	LYS	N-CA-C	-6.88	104.52	113.12
1	A	235	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	163	THR	N-CA-CB	-6.79	99.06	109.92
1	A	138	ASN	CA-CB-CG	6.75	119.34	112.60
1	B	257	TYR	O-C-N	6.74	130.34	122.19
1	A	147	MET	CG-SD-CE	-6.63	86.32	100.90
1	A	148	LYS	N-CA-C	-6.61	97.64	108.41
1	A	112	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	A	236	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	A	206	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	118	VAL	N-CA-C	-6.45	104.47	110.53
1	B	70	GLN	CA-CB-CG	6.40	126.90	114.10
1	B	248	HIS	CB-CG-CD2	-6.37	122.91	131.20
1	B	232	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	A	163	THR	N-CA-CB	-6.34	99.78	109.92
1	B	47	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	A	138	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	A	19	TRP	CG-CD2-CE3	6.27	140.17	133.90
1	A	179	LEU	N-CA-C	-6.24	105.50	113.23
1	A	163	THR	CA-CB-OG1	-6.20	100.31	109.60
1	A	138	ASN	CB-CG-ND2	6.12	125.58	116.40
1	A	210	ILE	O-C-N	-6.11	114.94	122.57
1	B	204	TRP	CG-CD2-CE3	6.07	139.97	133.90
1	A	85	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	B	94	VAL	N-CA-C	6.00	117.46	110.62
1	B	182	ASN	CB-CG-ND2	5.94	125.31	116.40
1	A	182	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	-1	LYS	CB-CG-CD	-5.92	97.68	111.30
1	A	104	ASN	CA-CB-CG	5.92	118.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ILE	N-CA-CB	-5.89	104.25	111.67
1	A	92	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	A	163	THR	CA-CB-CG2	5.82	120.40	110.50
1	B	37	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	19	TRP	CB-CG-CD1	-5.79	118.21	126.90
1	A	224	LYS	CA-C-N	5.79	125.75	119.78
1	A	224	LYS	C-N-CA	5.79	125.75	119.78
1	B	208	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	155	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	B	10	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	95	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	230	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	B	92	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	A	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	128	TRP	CA-C-O	5.64	127.42	120.15
1	B	31	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	B	183	VAL	N-CA-C	-5.60	104.90	111.00
1	A	70	GLN	CG-CD-NE2	5.59	124.78	116.40
1	B	232	GLN	CB-CG-CD	5.58	122.08	112.60
1	A	92	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	136	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	248	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	B	173	VAL	N-CA-C	5.48	118.46	113.20
1	B	182	ASN	CA-CB-CG	5.45	118.05	112.60
1	B	136	PHE	N-CA-C	-5.45	100.84	108.96
1	B	130	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	182	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	18	ILE	N-CA-CB	5.38	122.35	111.05
1	A	102	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	112	HIS	CB-CG-ND1	5.37	130.75	122.70
1	B	18	ILE	CB-CG1-CD1	-5.37	102.53	113.80
1	A	182	ASN	CB-CG-ND2	5.36	124.44	116.40
1	B	194	GLY	N-CA-C	-5.33	105.36	110.21
1	B	206	ASP	CA-CB-CG	5.30	117.91	112.60
1	A	248	HIS	CB-CG-ND1	5.30	130.66	122.70
1	A	245	GLU	CB-CA-C	-5.28	102.59	110.88
1	B	244	GLU	CB-CG-CD	5.27	121.56	112.60
1	B	14	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	A	240	LEU	N-CA-C	-5.26	105.93	112.93
1	B	2	VAL	N-CA-C	-5.26	100.89	108.89
1	A	198	ILE	N-CA-CB	-5.24	101.95	110.13
1	B	23	LYS	CA-C-N	5.24	124.87	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	LYS	C-N-CA	5.24	124.87	119.05
1	A	52	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	18	ILE	CB-CA-C	-5.18	100.00	111.77
1	B	256	ALA	N-CA-C	5.17	117.00	111.36
1	B	20	HIS	CA-CB-CG	5.16	118.96	113.80
1	B	207	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	31	HIS	CB-CG-ND1	5.13	130.40	122.70
1	A	104	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	217	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	110	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	236	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	209	LYS	N-CA-C	5.08	118.62	112.93
1	A	131	THR	CA-CB-OG1	-5.07	101.99	109.60
1	B	111	VAL	N-CA-C	5.05	117.40	111.09
1	A	236	HIS	CB-CG-ND1	5.04	130.27	122.70
1	B	257	TYR	CA-C-N	5.03	130.76	121.70
1	B	257	TYR	C-N-CA	5.03	130.76	121.70
1	A	239	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	B	224	LYS	CG-CD-CE	5.00	122.81	111.30

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
1:A:90:ALA:HB1	1:A:198:ILE:HD13	1.77	0.65
1:A:129:ARG:NH2	1:A:156:GLU:HB2	2.11	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:HD22	1:A:182:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASP:HB2	3:B:2089:HOH:O	2.19	0.43
1:A:148:LYS:HD2	1:A:148:LYS:HA	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
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:HA	1:A:155:ARG:HD3	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%)	211 (93%)	16 (7%)	14	16
1	B	223/227 (98%)	208 (93%)	15 (7%)	15	17
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	92	ARG
1	A	95	ASP
1	A	106	LEU
1	A	120	LYS
1	A	129	ARG
1	A	138	ASN
1	A	143	THR
1	A	154	LEU
1	A	155	ARG
1	A	163	THR
1	A	169	LEU
1	A	182	ASN
1	A	198	ILE
1	A	205	THR
1	B	2	VAL
1	B	18	ILE
1	B	50	GLN
1	B	80	SER
1	B	103	HIS
1	B	106	LEU
1	B	142	GLU
1	B	148	LYS
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

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	10	HIS
1	A	20	HIS
1	A	47	GLN
1	A	50	GLN
1	A	52	ASN
1	A	85	ASN
1	A	138	ASN
1	A	182	ASN
1	A	248	HIS
1	A	251	GLN
1	B	10	HIS
1	B	20	HIS
1	B	47	GLN
1	B	52	ASN
1	B	85	ASN
1	B	182	ASN
1	B	216	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 oligosaccharides 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	B	1259	-	3,3,3	2.09	1 (33%)	3,3,3	1.11	0
2	ACT	A	1259	-	3,3,3	2.28	1 (33%)	3,3,3	1.06	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1259	ACT	O-C	3.37	1.36	1.22
2	B	1259	ACT	O-C	3.19	1.36	1.22

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

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	262/262 (100%)	0.70	20 (7%) 20 17	12, 22, 41, 64	0
1	B	258/262 (98%)	0.49	12 (4%) 36 33	13, 20, 34, 69	0
All	All	520/524 (99%)	0.60	32 (6%) 26 23	12, 21, 38, 69	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	ALA	5.4
1	A	-4	PRO	4.7
1	B	2	VAL	3.6
1	A	-2	SER	3.5
1	B	258	ALA	3.4
1	B	1	MET	3.2
1	A	95	ASP	3.0
1	A	81	CYS	3.0
1	A	70	GLN	2.7
1	B	71	GLY	2.7
1	B	256	ALA	2.7
1	A	163	THR	2.6
1	A	131	THR	2.5
1	A	248	HIS	2.5
1	A	213	PRO	2.4
1	A	130	ASP	2.4
1	A	214	ASP	2.3
1	A	129	ARG	2.3
1	A	170	ALA	2.3
1	B	197	SER	2.3
1	A	185	ALA	2.2
1	A	134	PHE	2.2
1	A	83	GLY	2.2
1	A	218	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	255	ASP	2.1
1	B	87	ALA	2.1
1	B	70	GLN	2.1
1	A	150	GLY	2.1
1	B	221	ALA	2.1
1	B	68	LEU	2.1
1	B	95	ASP	2.1
1	A	133	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 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	A	1259	4/4	0.71	0.12	41,44,46,47	0
2	ACT	B	1259	4/4	0.86	0.10	47,49,49,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.