



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:00 PM UTC

PDB ID : 1DWQ / pdb_00001dwq
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.; 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

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

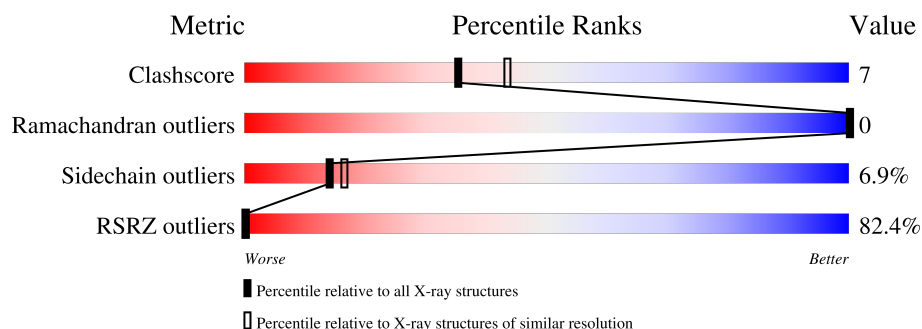
1 Overall quality at a glance

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	
1	B	262	

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.

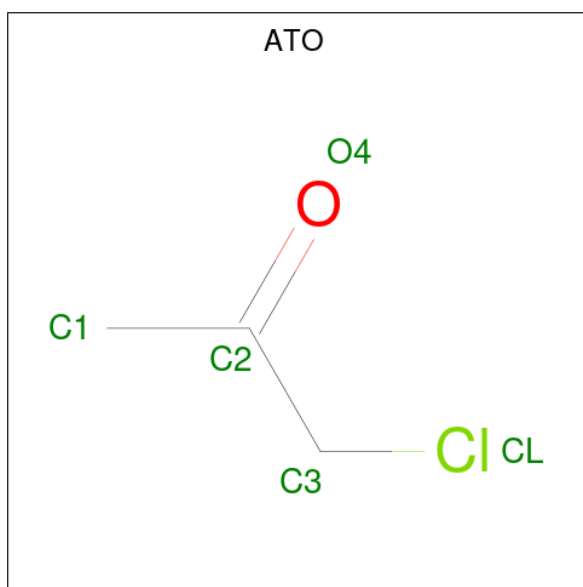
- Molecule 1 is a protein called HYDROXYNITRILE LYASE.

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 (CCD ID: ATO) (formula: C₃H₅ClO).



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

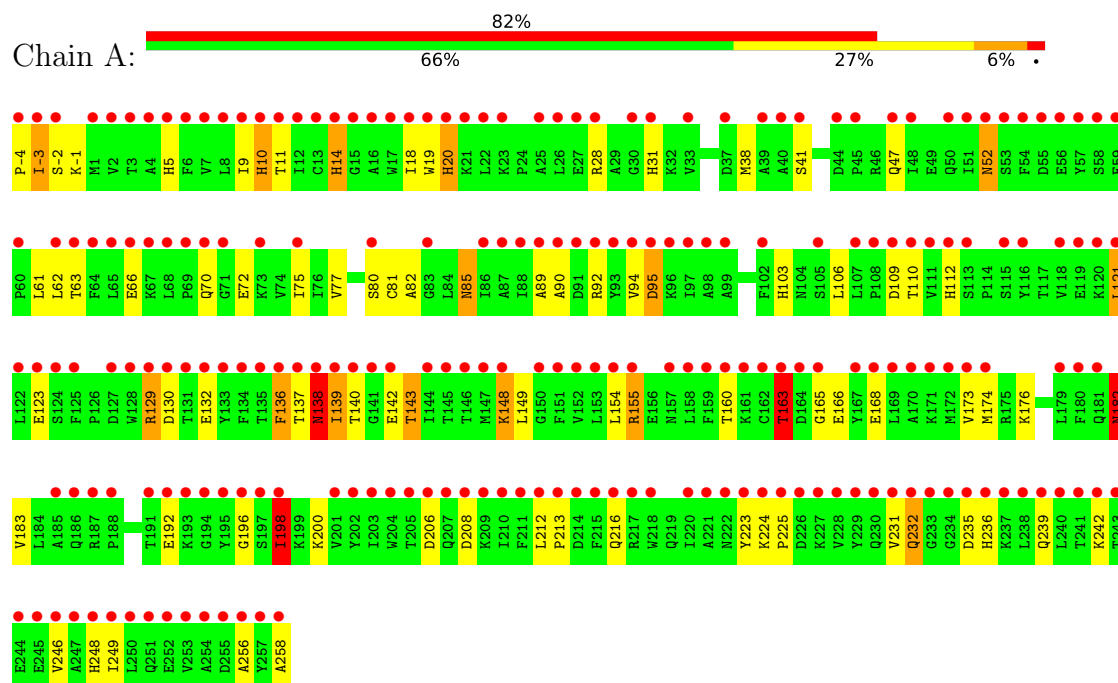
- Molecule 3 is water.

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

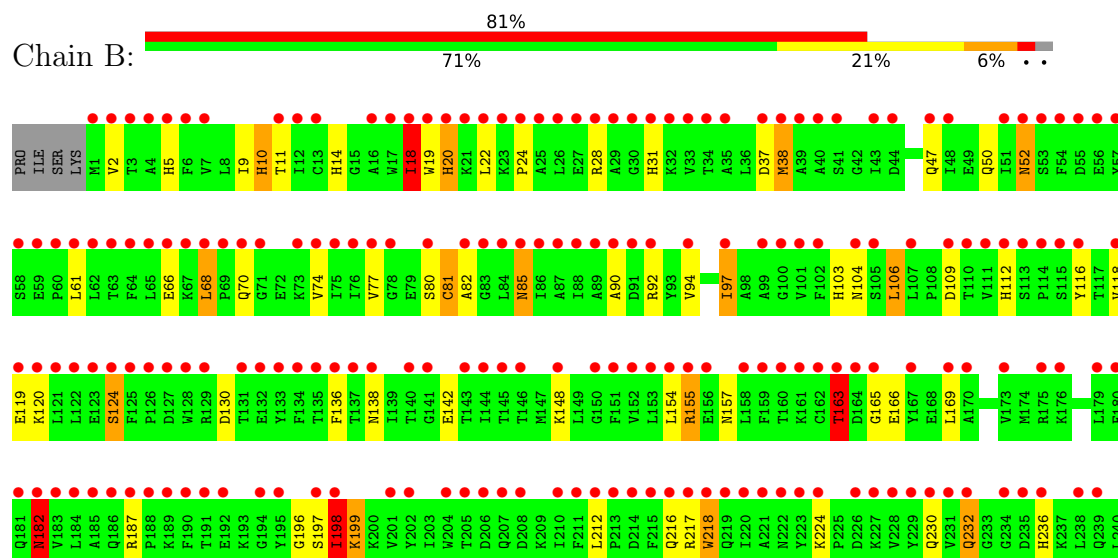
3 Residue-property plots [i](#)

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



T241	T242	T243	E244	E245	V246	A247	H248	I249	L250	Q251	E252	V253	A254	I255	A256	Y257	A258
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.50Å 104.50Å 189.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.4 (8.00-2.20) 96.1 (8.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.17Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.207 , 0.244 0.479 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	4402	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: CSA, ATO

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	1.21	15/2149 (0.7%)	1.86	52/2910 (1.8%)
1	B	1.19	13/2118 (0.6%)	1.85	58/2869 (2.0%)
All	All	1.20	28/4267 (0.7%)	1.86	110/5779 (1.9%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	HIS	CD2-NE2	-7.97	1.29	1.37
1	B	10	HIS	CD2-NE2	-7.85	1.29	1.37
1	A	20	HIS	CD2-NE2	-7.84	1.29	1.37
1	A	5	HIS	CD2-NE2	-7.83	1.29	1.37
1	A	-3	ILE	CA-CB	7.75	1.65	1.54
1	A	10	HIS	CD2-NE2	-7.67	1.29	1.37
1	B	236	HIS	CD2-NE2	-7.23	1.29	1.37
1	B	5	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	213	PRO	CA-CB	-6.83	1.44	1.53
1	B	198	ILE	CA-CB	6.74	1.61	1.54
1	A	14	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	248	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	20	HIS	CG-ND1	-6.55	1.31	1.38
1	A	112	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	103	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	5	HIS	CG-ND1	-6.06	1.31	1.38
1	B	18	ILE	CA-CB	5.98	1.62	1.54
1	B	31	HIS	CD2-NE2	-5.86	1.31	1.37
1	B	20	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	236	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	248	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	95	ASP	CA-CB	5.47	1.62	1.53
1	B	31	HIS	CG-ND1	-5.45	1.32	1.38
1	B	103	HIS	CD2-NE2	-5.18	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	HIS	CD2-NE2	-5.17	1.32	1.37
1	B	14	HIS	CD2-NE2	-5.16	1.32	1.37
1	B	77	VAL	CA-CB	-5.16	1.47	1.54
1	A	10	HIS	CG-ND1	-5.08	1.32	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ASP	CA-CB-CG	12.65	125.25	112.60
1	B	109	ASP	CA-CB-CG	10.51	123.11	112.60
1	B	198	ILE	CA-CB-CG2	9.34	126.37	110.50
1	B	198	ILE	CA-CB-CG1	-9.31	94.57	110.40
1	A	198	ILE	CA-CB-CG1	-8.87	95.32	110.40
1	A	198	ILE	CA-CB-CG2	8.72	125.32	110.50
1	B	85	ASN	OD1-CG-ND2	-7.75	114.85	122.60
1	B	216	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	B	47	GLN	CG-CD-NE2	7.66	127.89	116.40
1	B	163	THR	CA-CB-OG1	-7.55	98.28	109.60
1	B	47	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	A	138	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	A	70	GLN	OE1-CD-NE2	-7.36	115.25	122.60
1	A	138	ASN	CB-CG-ND2	7.10	127.05	116.40
1	B	236	HIS	CB-CG-CD2	-7.10	121.97	131.20
1	A	31	HIS	CB-CG-CD2	-6.95	122.16	131.20
1	B	157	ASN	CA-CB-CG	-6.94	105.66	112.60
1	B	230	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	182	ASN	CA-CB-CG	6.90	119.50	112.60
1	B	52	ASN	CB-CG-ND2	6.89	126.73	116.40
1	A	109	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	236	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	B	182	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	B	92	ARG	NE-CZ-NH2	6.73	125.26	119.20
1	B	37	ASP	CA-CB-CG	6.71	119.31	112.60
1	B	197	SER	N-CA-C	6.70	118.66	111.36
1	A	163	THR	CA-CB-OG1	-6.65	99.62	109.60
1	B	52	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	B	182	ASN	CA-CB-CG	6.60	119.20	112.60
1	B	124	SER	CA-CB-OG	6.50	124.10	111.10
1	A	121	LEU	N-CA-C	-6.48	104.15	111.14
1	B	163	THR	N-CA-CB	-6.42	99.65	109.92
1	A	85	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	130	ASP	CA-CB-CG	6.32	118.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	THR	CA-CB-CG2	6.23	121.09	110.50
1	A	103	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	B	97	ILE	N-CA-CB	-6.11	103.97	111.67
1	B	104	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	143	THR	CA-C-O	6.09	127.06	120.43
1	B	118	VAL	N-CA-C	-6.07	104.59	110.72
1	A	77	VAL	N-CA-C	-6.04	99.72	108.17
1	B	248	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	B	112	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	A	112	HIS	CB-CG-CD2	-6.00	123.39	131.20
1	A	19	TRP	CB-CG-CD1	-5.99	117.92	126.90
1	A	206	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	28	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A	110	THR	CA-C-O	5.96	125.69	119.14
1	A	256	ALA	N-CA-C	5.87	117.76	111.36
1	A	14	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	B	217	ARG	CB-CG-CD	-5.87	97.81	111.30
1	A	139	ILE	N-CA-C	5.81	118.32	111.05
1	A	235	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	183	VAL	N-CA-C	-5.80	104.67	111.00
1	A	216	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	14	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	A	163	THR	CA-CB-CG2	5.73	120.25	110.50
1	A	129	ARG	CB-CG-CD	-5.70	98.19	111.30
1	B	182	ASN	CB-CG-ND2	5.69	124.93	116.40
1	B	236	HIS	CB-CG-ND1	5.64	131.15	122.70
1	B	14	HIS	CB-CG-ND1	5.62	131.14	122.70
1	A	138	ASN	CA-CB-CG	5.59	118.19	112.60
1	B	80	SER	N-CA-CB	-5.56	101.05	110.50
1	A	236	HIS	CB-CG-ND1	5.55	131.03	122.70
1	A	163	THR	N-CA-CB	-5.55	101.04	109.92
1	A	173	VAL	N-CA-C	5.55	118.48	113.10
1	B	199	LYS	CA-CB-CG	-5.54	103.02	114.10
1	A	160	THR	N-CA-C	5.52	120.48	111.37
1	B	230	GLN	CG-CD-NE2	5.52	124.68	116.40
1	B	136	PHE	N-CA-C	-5.48	100.98	109.14
1	B	232	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	A	176	LYS	CB-CG-CD	-5.45	98.77	111.30
1	A	232	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	B	68	LEU	CB-CA-C	-5.43	101.10	109.62
1	B	218	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	A	70	GLN	CG-CD-NE2	5.42	124.53	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	B	22	LEU	CA-C-O	-5.39	114.71	120.42
1	B	18	ILE	N-CA-C	-5.35	106.05	113.00
1	B	130	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	239	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	A	208	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	112	HIS	CA-CB-CG	5.31	119.11	113.80
1	A	28	ARG	NE-CZ-NH1	-5.29	116.20	121.50
1	B	38	MET	N-CA-C	-5.29	102.16	110.36
1	A	249	ILE	N-CA-C	-5.28	105.23	110.62
1	B	212	LEU	CA-C-N	5.27	125.33	119.32
1	B	212	LEU	C-N-CA	5.27	125.33	119.32
1	A	92	ARG	N-CA-C	-5.26	106.18	113.18
1	B	251	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	B	187	ARG	CA-C-N	5.25	125.25	119.90
1	B	187	ARG	C-N-CA	5.25	125.25	119.90
1	B	28	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	136	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	52	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	B	19	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	A	123	GLU	CB-CA-C	-5.17	102.76	110.88
1	B	198	ILE	CB-CG1-CD1	-5.16	102.96	113.80
1	B	196	GLY	CA-C-N	5.12	127.56	120.29
1	B	196	GLY	C-N-CA	5.12	127.56	120.29
1	B	70	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	B	10	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	198	ILE	N-CA-CB	-5.10	101.92	110.14
1	A	-1	LYS	CB-CG-CD	-5.09	99.58	111.30
1	A	47	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	70	GLN	CG-CD-NE2	5.07	124.01	116.40
1	A	212	LEU	CA-C-N	5.07	124.86	119.28
1	A	212	LEU	C-N-CA	5.07	124.86	119.28
1	B	92	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	246	VAL	N-CA-C	-5.04	105.58	110.42

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
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:HD22	1:A:182:ASN:H	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:O	1:A:121:LEU:HG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:ILE:HD11	1:B:61:LEU:HD13	1.95	0.47
1:B:246:VAL:HG12	1:B:250:LEU:HD22	1.96	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:HD3	1:A:155:ARG:O	2.17	0.45
1:A:94:VAL:HG23	1:A:198:ILE:HD12	1.98	0.44
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 [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	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 [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	226/226 (100%)	210 (93%)	16 (7%)	13	16
1	B	222/226 (98%)	207 (93%)	15 (7%)	14	17
All	All	448/452 (99%)	417 (93%)	31 (7%)	14	16

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

Mol	Chain	Res	Type
1	A	-3	ILE

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Mol	Chain	Res	Type
1	A	-2	SER
1	A	18	ILE
1	A	72	GLU
1	A	95	ASP
1	A	106	LEU
1	A	129	ARG
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	18	ILE
1	B	50	GLN
1	B	106	LEU
1	B	119	GLU
1	B	124	SER
1	B	142	GLU
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	199	LYS
1	B	224	LYS
1	B	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	232	GLN
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	181	GLN
1	B	182	ASN
1	B	216	GLN

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	8,9,10	1.07	0	7,10,12	1.63	3 (42%)
1	CSA	B	81	1	8,9,10	1.01	0	7,10,12	1.76	4 (57%)

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	-	3/6/8/10	-
1	CSA	B	81	1	-	4/6/8/10	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	CSA	C2-C3-SG	-2.50	104.31	113.75
1	A	81	CSA	C1-C2-C3	2.43	120.24	116.17
1	B	81	CSA	C1-C2-C3	2.40	120.18	116.17
1	A	81	CSA	O4-C2-C3	-2.25	118.31	121.24
1	B	81	CSA	O4-C2-C3	-2.22	118.34	121.24
1	B	81	CSA	CB-CA-C	-2.15	104.96	110.80
1	A	81	CSA	C2-C3-SG	-2.12	105.72	113.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	81	CSA	CA-CB-SG-C3
1	B	81	CSA	O4-C2-C3-SG
1	B	81	CSA	C1-C2-C3-SG
1	B	81	CSA	C2-C3-SG-CB
1	A	81	CSA	CA-CB-SG-C3
1	A	81	CSA	C2-C3-SG-CB
1	A	81	CSA	C1-C2-C3-SG

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 oligosaccharides 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	0.80	0	4,4,4	1.54	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1259	ATO	C2-C3-CL	-3.00	108.13	112.43

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, 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	261/262 (99%)	3.15	215 (82%) 0 0	18, 28, 47, 62	0
1	B	257/262 (98%)	3.00	212 (82%) 0 0	17, 26, 42, 74	0
All	All	518/524 (98%)	3.07	427 (82%) 0 0	17, 27, 46, 74	0

All (427) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	SER	9.5
1	B	170	ALA	7.6
1	A	214	ASP	7.6
1	A	165	GLY	7.1
1	A	223	TYR	6.8
1	B	185	ALA	6.8
1	B	1	MET	6.5
1	A	25	ALA	6.4
1	B	90	ALA	6.2
1	A	163	THR	6.1
1	B	2	VAL	6.1
1	B	24	PRO	6.0
1	B	41	SER	6.0
1	A	124	SER	6.0
1	B	165	GLY	6.0
1	A	135	THR	5.9
1	A	4	ALA	5.8
1	A	220	ILE	5.8
1	A	95	ASP	5.7
1	A	256	ALA	5.7
1	A	258	ALA	5.6
1	A	241	THR	5.6
1	B	105	SER	5.5
1	A	150	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	127	ASP	5.4
1	A	207	GLN	5.4
1	B	30	GLY	5.3
1	A	110	THR	5.3
1	A	205	THR	5.2
1	B	27	GLU	5.2
1	B	150	GLY	5.1
1	B	191	THR	5.1
1	A	193	LYS	5.1
1	A	-2	SER	5.1
1	A	71	GLY	5.1
1	A	18	ILE	5.1
1	B	97	ILE	5.0
1	B	63	THR	5.0
1	B	241	THR	5.0
1	B	213	PRO	4.9
1	A	109	ASP	4.9
1	B	214	ASP	4.9
1	A	247	ALA	4.9
1	B	256	ALA	4.8
1	B	161	LYS	4.8
1	A	7	VAL	4.7
1	A	-4	PRO	4.7
1	B	83	GLY	4.7
1	A	3	THR	4.7
1	B	206	ASP	4.7
1	B	4	ALA	4.6
1	A	111	VAL	4.6
1	B	205	THR	4.6
1	B	18	ILE	4.6
1	B	252	GLU	4.5
1	B	234	GLY	4.5
1	A	239	GLN	4.5
1	A	93	TYR	4.5
1	A	121	LEU	4.5
1	B	245	GLU	4.5
1	A	194	GLY	4.4
1	A	162	CYS	4.4
1	A	221	ALA	4.4
1	B	29	ALA	4.4
1	B	54	PHE	4.4
1	A	139	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	228	VAL	4.3
1	A	204	TRP	4.3
1	A	215	PHE	4.3
1	A	63	THR	4.3
1	B	132	GLU	4.2
1	A	54	PHE	4.2
1	A	233	GLY	4.2
1	A	224	LYS	4.2
1	A	99	ALA	4.2
1	B	254	ALA	4.2
1	A	211	PHE	4.2
1	A	217	ARG	4.2
1	A	226	ASP	4.2
1	B	3	THR	4.2
1	A	208	ASP	4.2
1	B	219	GLN	4.2
1	A	133	TYR	4.2
1	A	188	PRO	4.2
1	B	23	LYS	4.2
1	B	11	THR	4.2
1	B	64	PHE	4.1
1	A	56	GLU	4.1
1	A	252	GLU	4.1
1	B	75	ILE	4.1
1	B	221	ALA	4.1
1	B	121	LEU	4.1
1	B	218	TRP	4.1
1	A	19	TRP	4.0
1	A	146	THR	4.0
1	A	201	VAL	4.0
1	A	148	LYS	4.0
1	A	69	PRO	4.0
1	A	169	LEU	4.0
1	B	82	ALA	4.0
1	B	247	ALA	4.0
1	A	44	ASP	4.0
1	A	138	ASN	4.0
1	B	226	ASP	4.0
1	A	197	SER	4.0
1	B	88	ILE	4.0
1	A	186	GLN	3.9
1	B	6	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	152	VAL	3.9
1	B	55	ASP	3.9
1	A	105	SER	3.9
1	A	192	GLU	3.9
1	B	69	PRO	3.9
1	A	167	TYR	3.9
1	A	234	GLY	3.9
1	B	163	THR	3.9
1	A	13	CYS	3.8
1	B	198	ILE	3.8
1	A	83	GLY	3.8
1	A	179	LEU	3.8
1	B	141	GLY	3.8
1	B	162	CYS	3.8
1	B	26	LEU	3.8
1	A	27	GLU	3.8
1	A	73	LYS	3.8
1	B	125	PHE	3.8
1	A	45	PRO	3.8
1	B	60	PRO	3.8
1	B	223	TYR	3.7
1	A	213	PRO	3.7
1	A	116	TYR	3.7
1	A	70	GLN	3.7
1	B	94	VAL	3.7
1	A	147	MET	3.7
1	A	40	ALA	3.7
1	A	112	HIS	3.7
1	A	159	PHE	3.7
1	A	90	ALA	3.7
1	A	238	LEU	3.6
1	A	130	ASP	3.6
1	A	31	HIS	3.6
1	A	67	LYS	3.6
1	A	66	GLU	3.6
1	A	134	PHE	3.6
1	A	249	ILE	3.6
1	A	160	THR	3.6
1	A	253	VAL	3.6
1	A	210	ILE	3.6
1	B	43	ILE	3.6
1	B	74	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	257	TYR	3.6
1	A	231	VAL	3.6
1	A	230	GLN	3.5
1	B	116	TYR	3.5
1	A	125	PHE	3.5
1	B	134	PHE	3.5
1	B	32	LYS	3.5
1	B	44	ASP	3.5
1	A	145	THR	3.5
1	A	123	GLU	3.5
1	B	7	VAL	3.5
1	B	66	GLU	3.5
1	A	151	PHE	3.5
1	A	92	ARG	3.5
1	B	31	HIS	3.5
1	B	153	LEU	3.5
1	A	225	PRO	3.5
1	A	237	LYS	3.5
1	A	14	HIS	3.5
1	B	202	TYR	3.5
1	A	235	ASP	3.5
1	B	151	PHE	3.5
1	B	39	ALA	3.4
1	A	-3	ILE	3.4
1	A	55	ASP	3.4
1	A	229	TYR	3.4
1	A	232	GLN	3.4
1	B	251	GLN	3.4
1	B	248	HIS	3.4
1	B	181	GLN	3.4
1	B	232	GLN	3.4
1	A	206	ASP	3.4
1	B	25	ALA	3.4
1	B	204	TRP	3.3
1	B	119	GLU	3.3
1	B	175	ARG	3.3
1	B	115	SER	3.3
1	B	62	LEU	3.3
1	A	98	ALA	3.3
1	B	183	VAL	3.3
1	B	52	ASN	3.3
1	B	114	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	20	HIS	3.3
1	A	136	PHE	3.3
1	A	62	LEU	3.3
1	B	57	TYR	3.3
1	A	39	ALA	3.2
1	A	173	VAL	3.3
1	B	87	ALA	3.2
1	A	196	GLY	3.2
1	B	208	ASP	3.2
1	A	250	LEU	3.2
1	B	48	ILE	3.2
1	B	102	PHE	3.2
1	B	167	TYR	3.2
1	B	217	ARG	3.2
1	B	160	THR	3.2
1	A	2	VAL	3.2
1	B	78	GLY	3.2
1	B	235	ASP	3.2
1	A	107	LEU	3.2
1	B	230	GLN	3.2
1	B	16	ALA	3.2
1	B	91	ASP	3.2
1	A	10	HIS	3.2
1	A	128	TRP	3.2
1	A	22	LEU	3.2
1	A	154	LEU	3.2
1	B	249	ILE	3.2
1	B	80	SER	3.1
1	B	255	ASP	3.1
1	A	218	TRP	3.1
1	B	128	TRP	3.1
1	B	51	ILE	3.1
1	A	41	SER	3.1
1	A	113	SER	3.1
1	A	141	GLY	3.1
1	B	186	GLN	3.1
1	A	153	LEU	3.1
1	A	144	ILE	3.1
1	B	207	GLN	3.1
1	B	258	ALA	3.1
1	B	28	ARG	3.1
1	B	138	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	ARG	3.1
1	B	19	TRP	3.0
1	A	91	ASP	3.0
1	B	182	ASN	3.0
1	A	187	ARG	3.0
1	B	155	ARG	3.0
1	B	184	LEU	3.0
1	B	12	ILE	3.0
1	B	131	THR	3.0
1	A	115	SER	3.0
1	B	53	SER	3.0
1	A	170	ALA	3.0
1	A	68	LEU	3.0
1	A	12	ILE	3.0
1	A	195	TYR	3.0
1	B	195	TYR	3.0
1	A	131	THR	3.0
1	A	64	PHE	3.0
1	B	126	PRO	3.0
1	A	51	ILE	3.0
1	A	155	ARG	3.0
1	A	157	ASN	3.0
1	B	180	PHE	2.9
1	B	68	LEU	2.9
1	B	70	GLN	2.9
1	A	89	ALA	2.9
1	B	33	VAL	2.9
1	B	210	ILE	2.9
1	B	133	TYR	2.9
1	B	67	LYS	2.9
1	B	244	GLU	2.9
1	A	15	GLY	2.9
1	B	77	VAL	2.9
1	A	202	TYR	2.8
1	B	112	HIS	2.8
1	A	102	PHE	2.8
1	A	185	ALA	2.8
1	A	94	VAL	2.8
1	A	17	TRP	2.8
1	A	108	PRO	2.8
1	A	257	TYR	2.8
1	B	107	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	180	PHE	2.8
1	B	17	TRP	2.8
1	A	88	ILE	2.8
1	B	76	ILE	2.8
1	A	255	ASP	2.8
1	A	30	GLY	2.8
1	A	132	GLU	2.8
1	B	21	LYS	2.8
1	B	176	LYS	2.8
1	A	118	VAL	2.8
1	B	110	THR	2.8
1	B	146	THR	2.8
1	A	119	GLU	2.8
1	B	192	GLU	2.8
1	A	158	LEU	2.8
1	B	238	LEU	2.8
1	A	242	LYS	2.8
1	A	240	LEU	2.7
1	B	47	GLN	2.7
1	B	104	ASN	2.7
1	B	135	THR	2.7
1	A	142	GLU	2.7
1	A	120	LYS	2.7
1	B	38	MET	2.7
1	A	212	LEU	2.7
1	B	250	LEU	2.7
1	A	6	PHE	2.7
1	A	181	GLN	2.7
1	A	251	GLN	2.7
1	B	246	VAL	2.7
1	A	140	THR	2.7
1	A	244	GLU	2.7
1	B	215	PHE	2.7
1	A	171	LYS	2.7
1	A	243	THR	2.7
1	A	60	PRO	2.7
1	B	84	LEU	2.7
1	B	120	LYS	2.6
1	B	159	PHE	2.6
1	B	228	VAL	2.6
1	B	13	CYS	2.6
1	B	216	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	227	LYS	2.6
1	A	164	ASP	2.6
1	B	92	ARG	2.6
1	B	229	TYR	2.6
1	B	34	THR	2.6
1	B	188	PRO	2.6
1	B	20	HIS	2.6
1	B	35	ALA	2.6
1	B	222	ASN	2.6
1	B	71	GLY	2.6
1	B	243	THR	2.6
1	B	65	LEU	2.6
1	A	137	THR	2.6
1	A	191	THR	2.6
1	B	152	VAL	2.6
1	A	21	LYS	2.6
1	A	50	GLN	2.5
1	A	245	GLU	2.5
1	B	169	LEU	2.5
1	A	222	ASN	2.5
1	B	164	ASP	2.5
1	B	201	VAL	2.5
1	A	52	ASN	2.5
1	A	198	ILE	2.5
1	B	122	LEU	2.5
1	A	172	MET	2.5
1	B	143	THR	2.5
1	A	203	ILE	2.5
1	B	158	LEU	2.5
1	B	127	ASP	2.5
1	B	40	ALA	2.5
1	A	246	VAL	2.4
1	B	154	LEU	2.4
1	A	174	MET	2.4
1	B	148	LYS	2.4
1	B	224	LYS	2.4
1	A	248	HIS	2.4
1	A	97	ILE	2.4
1	B	231	VAL	2.4
1	B	22	LEU	2.4
1	B	236	HIS	2.4
1	B	100	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	80	SER	2.4
1	A	48	ILE	2.4
1	B	118	VAL	2.4
1	B	144	ILE	2.4
1	B	5	HIS	2.4
1	A	23	LYS	2.4
1	B	145	THR	2.4
1	B	136	PHE	2.4
1	A	47	GLN	2.4
1	B	86	ILE	2.3
1	B	101	VAL	2.3
1	A	26	LEU	2.3
1	B	123	GLU	2.3
1	A	33	VAL	2.3
1	B	190	PHE	2.3
1	A	65	LEU	2.3
1	A	37	ASP	2.3
1	B	85	ASN	2.3
1	B	194	GLY	2.3
1	B	137	THR	2.3
1	B	179	LEU	2.3
1	A	5	HIS	2.3
1	B	58	SER	2.3
1	A	59	GLU	2.3
1	A	9	ILE	2.3
1	B	73	LYS	2.3
1	B	220	ILE	2.3
1	B	242	LYS	2.3
1	A	122	LEU	2.2
1	A	16	ALA	2.2
1	A	209	LYS	2.2
1	B	227	LYS	2.2
1	B	173	VAL	2.2
1	B	109	ASP	2.2
1	A	1	MET	2.2
1	A	168	GLU	2.2
1	A	236	HIS	2.2
1	A	8	LEU	2.2
1	B	59	GLU	2.2
1	B	189	LYS	2.2
1	A	216	GLN	2.2
1	A	57	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	ALA	2.1
1	B	124	SER	2.1
1	A	86	ILE	2.1
1	B	61	LEU	2.1
1	B	56	GLU	2.1
1	A	129	ARG	2.1
1	A	53	SER	2.1
1	B	99	ALA	2.1
1	B	37	ASP	2.1
1	B	211	PHE	2.1
1	B	113	SER	2.1
1	A	87	ALA	2.1
1	A	75	ILE	2.1
1	B	187	ARG	2.1
1	A	161	LYS	2.0
1	A	11	THR	2.0
1	A	58	SER	2.0
1	B	239	GLN	2.0
1	B	111	VAL	2.0
1	A	96	LYS	2.0
1	B	140	THR	2.0
1	B	156	GLU	2.0
1	B	89	ALA	2.0
1	B	212	LEU	2.0
1	B	129	ARG	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. 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($\text{\AA}^2$)	Q<0.9
1	CSA	A	81	10/11	0.65	0.20	23,26,35,35	0
1	CSA	B	81	10/11	0.83	0.14	23,25,36,38	0

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($\text{\AA}^2$)	Q<0.9
2	ATO	A	1259	5/5	0.79	0.19	39,39,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.