



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:59 AM UTC

PDB ID : 5TDX / pdb_00005tdx
Title : Resurrected Ancestral Hydroxynitrile Lyase from Flowering Plants
Authors : Jones, B.J.; Evans, R.; Wilmot, C.M.; Kazlauskas, R.J.
Deposited on : 2016-09-20
Resolution : 1.96 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

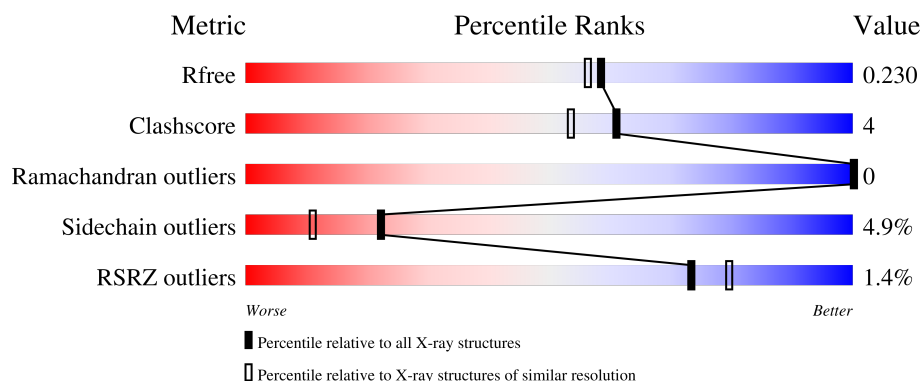
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	272	2% 75% 15% . . .
1	B	272	2% 73% 18% 5%
1	C	272	79% 17% . .
1	D	272	2% 74% 18% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8741 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 Ancestral Hydroxynitrile Lyase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	5	0
			2131	1373	341	408	9			
1	B	259	Total	C	N	O	S	0	4	0
			2112	1361	340	402	9			
1	C	265	Total	C	N	O	S	0	2	0
			2138	1380	342	407	9			
1	D	260	Total	C	N	O	S	0	5	0
			2132	1374	344	405	9			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

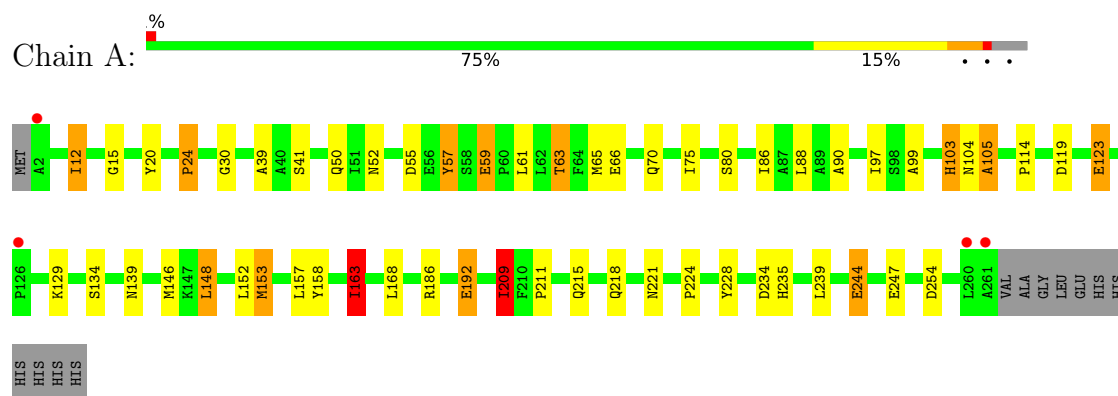
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	66	Total	O	0	0
			66	66		
3	C	54	Total	O	0	0
			54	54		
3	D	14	Total	O	0	0
			14	14		

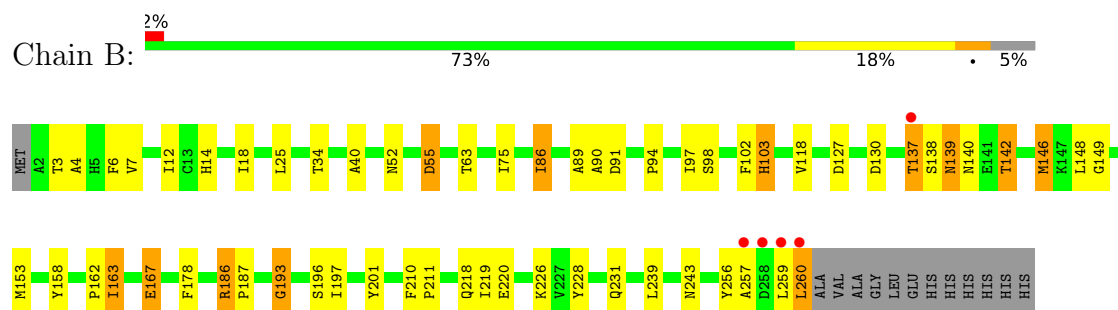
3 Residue-property plots [i](#)

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.

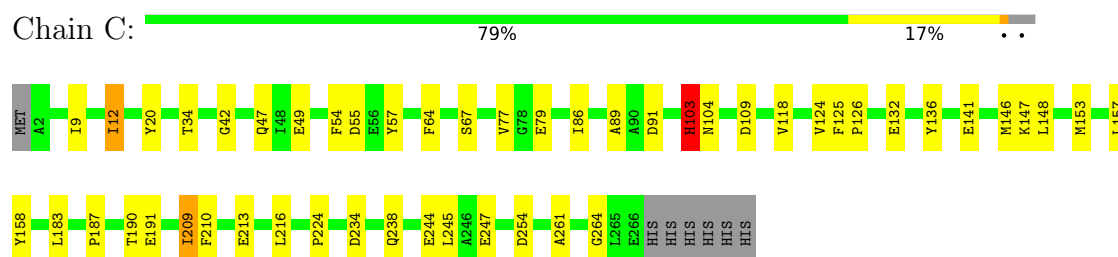
• Molecule 1: Ancestral Hydroxynitrile Lyase 1



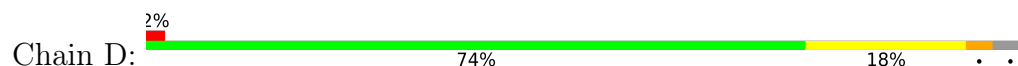
• Molecule 1: Ancestral Hydroxynitrile Lyase 1

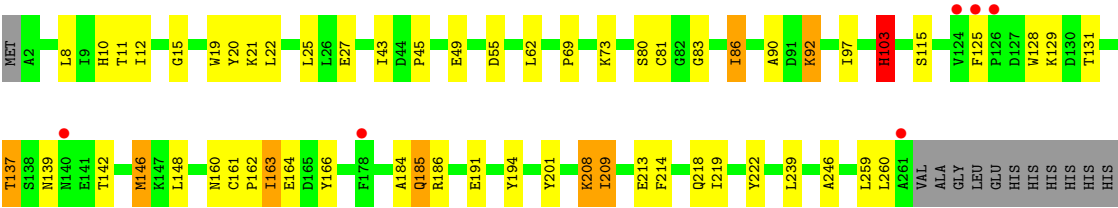


• Molecule 1: Ancestral Hydroxynitrile Lyase 1



• Molecule 1: Ancestral Hydroxynitrile Lyase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.27Å 108.27Å 201.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 1.96 29.32 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.32-1.96) 99.7 (29.32-1.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.177 , 0.227 0.186 , 0.230	Depositor DCC
R_{free} test set	4319 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8741	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: GOL

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	1.76	31/2188 (1.4%)	1.38	10/2969 (0.3%)
1	B	1.84	35/2172 (1.6%)	1.45	15/2947 (0.5%)
1	C	1.73	28/2195 (1.3%)	1.34	4/2980 (0.1%)
1	D	1.48	17/2192 (0.8%)	1.32	10/2974 (0.3%)
All	All	1.71	111/8747 (1.3%)	1.37	39/11870 (0.3%)

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	ASP	C-O	8.82	1.30	1.24
1	A	57	TYR	CA-C	8.20	1.63	1.52
1	A	239	LEU	CA-C	-7.80	1.44	1.52
1	B	3	THR	C-O	-7.40	1.14	1.23
1	B	153	MET	SD-CE	-7.33	1.61	1.79
1	B	4	ALA	N-CA	-7.11	1.37	1.45
1	B	103	HIS	CA-CB	7.01	1.62	1.53
1	A	218	GLN	N-CA	6.82	1.54	1.46
1	D	49	GLU	C-O	-6.77	1.15	1.24
1	C	20	TYR	N-CA	-6.76	1.37	1.46
1	C	216	LEU	C-O	-6.74	1.16	1.24
1	C	42	GLY	C-O	-6.73	1.14	1.24
1	B	210	PHE	N-CA	6.65	1.55	1.46
1	C	261	ALA	C-O	-6.62	1.16	1.24
1	B	102	PHE	C-O	-6.57	1.16	1.24
1	A	228	TYR	C-O	6.51	1.31	1.24
1	D	103	HIS	CA-C	6.50	1.61	1.53
1	A	50	GLN	C-O	-6.47	1.15	1.23
1	A	105	ALA	CA-C	-6.45	1.44	1.52
1	A	129	LYS	C-O	-6.44	1.15	1.24
1	C	54	PHE	N-CA	-6.36	1.38	1.46
1	D	129	LYS	C-O	-6.34	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	247	GLU	N-CA	-6.29	1.38	1.46
1	C	264	GLY	C-O	-6.27	1.15	1.23
1	C	34	THR	N-CA	-6.22	1.38	1.46
1	B	158	TYR	CA-CB	6.21	1.61	1.53
1	A	41	SER	CA-C	6.20	1.60	1.52
1	C	261	ALA	N-CA	6.20	1.53	1.46
1	D	166	TYR	N-CA	-6.19	1.38	1.46
1	A	244	GLU	CA-C	-6.18	1.44	1.52
1	A	148	LEU	CA-C	-6.17	1.45	1.52
1	A	12	ILE	C-O	6.10	1.31	1.24
1	A	75	ILE	CA-C	-6.08	1.45	1.52
1	B	91	ASP	N-CA	-5.99	1.38	1.46
1	A	41	SER	C-O	5.99	1.31	1.23
1	C	187	PRO	CA-C	5.96	1.60	1.52
1	D	239	LEU	N-CA	-5.95	1.38	1.46
1	B	219	ILE	C-O	-5.94	1.17	1.24
1	B	7	VAL	N-CA	-5.92	1.38	1.46
1	C	183	LEU	C-O	-5.91	1.17	1.24
1	D	43	ILE	C-O	-5.90	1.15	1.24
1	C	190	THR	C-O	5.90	1.30	1.23
1	C	153	MET	SD-CE	-5.89	1.64	1.79
1	D	194	TYR	CA-C	5.83	1.60	1.52
1	B	12	ILE	C-O	-5.75	1.17	1.24
1	A	221	ASN	C-O	-5.73	1.17	1.24
1	B	6	PHE	N-CA	-5.73	1.38	1.46
1	B	40	ALA	N-CA	-5.67	1.38	1.46
1	C	89	ALA	CA-C	-5.65	1.45	1.52
1	B	162	PRO	CA-C	5.61	1.59	1.52
1	B	139	ASN	CA-C	5.60	1.58	1.52
1	B	187	PRO	CA-C	5.59	1.59	1.52
1	B	231	GLN	C-O	-5.57	1.17	1.23
1	B	196	SER	C-O	-5.56	1.16	1.24
1	B	86	ILE	CB-CG1	-5.55	1.42	1.53
1	B	162	PRO	C-O	5.54	1.30	1.23
1	C	158	TYR	C-O	-5.54	1.16	1.24
1	A	66	GLU	CA-CB	5.53	1.61	1.53
1	A	134	SER	C-O	5.53	1.31	1.24
1	D	22	LEU	CA-C	5.52	1.59	1.52
1	B	193	GLY	C-O	5.50	1.31	1.23
1	D	246	ALA	CA-C	5.48	1.60	1.52
1	B	34	THR	N-CA	-5.47	1.39	1.46
1	A	119	ASP	N-CA	5.46	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	160	ASN	N-CA	5.45	1.53	1.46
1	A	55	ASP	C-O	-5.42	1.17	1.24
1	B	210	PHE	CA-C	-5.42	1.46	1.52
1	C	224	PRO	N-CA	-5.41	1.41	1.47
1	A	168	LEU	CA-CB	-5.39	1.44	1.53
1	A	15	GLY	N-CA	-5.39	1.39	1.45
1	B	127	ASP	N-CA	5.37	1.53	1.46
1	B	211	PRO	N-CA	-5.36	1.36	1.46
1	B	75	ILE	CA-CB	-5.36	1.47	1.54
1	C	67	SER	CA-C	5.35	1.60	1.52
1	D	260	LEU	CA-C	5.34	1.61	1.53
1	D	81	CYS	N-CA	5.33	1.53	1.46
1	C	57	TYR	N-CA	5.33	1.52	1.46
1	D	259	LEU	CA-C	5.31	1.59	1.52
1	C	245	LEU	C-O	-5.30	1.18	1.24
1	D	162	PRO	C-O	5.27	1.29	1.23
1	B	201	TYR	CA-C	5.25	1.58	1.52
1	D	27	GLU	C-O	-5.25	1.17	1.24
1	B	167	GLU	CD-OE2	5.22	1.35	1.25
1	A	247	GLU	CA-C	5.22	1.59	1.52
1	C	244	GLU	CA-C	5.22	1.59	1.52
1	C	132	GLU	C-O	-5.21	1.17	1.24
1	A	153	MET	SD-CE	-5.20	1.66	1.79
1	B	89	ALA	C-O	5.19	1.30	1.24
1	C	234	ASP	CA-C	5.19	1.59	1.52
1	A	24	PRO	N-CA	-5.18	1.40	1.47
1	A	88	LEU	N-CA	-5.16	1.40	1.46
1	A	30	GLY	N-CA	5.15	1.52	1.45
1	A	254	ASP	C-O	-5.15	1.17	1.24
1	B	142	THR	CA-C	-5.14	1.46	1.52
1	A	99	ALA	C-O	5.11	1.29	1.23
1	C	224	PRO	C-O	-5.11	1.17	1.23
1	C	77	VAL	CA-CB	-5.11	1.47	1.54
1	C	12	ILE	CA-CB	-5.10	1.49	1.54
1	D	222	TYR	C-O	5.09	1.30	1.23
1	B	137	THR	C-O	5.09	1.30	1.24
1	B	220	GLU	CA-C	5.08	1.59	1.52
1	B	14	HIS	CA-CB	-5.08	1.46	1.53
1	C	109	ASP	C-O	5.08	1.30	1.24
1	D	208	LYS	C-O	-5.06	1.17	1.24
1	B	14	HIS	C-N	-5.05	1.27	1.33
1	B	243	ASN	CA-C	5.05	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ASN	CA-C	5.04	1.59	1.52
1	A	224	PRO	C-O	5.03	1.29	1.23
1	A	152	LEU	N-CA	5.03	1.52	1.46
1	C	254	ASP	C-O	-5.02	1.18	1.24
1	C	147	LYS	N-CA	5.02	1.52	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ILE	N-CA-CB	8.69	125.51	110.65
1	B	86	ILE	CB-CA-C	-8.57	100.57	112.14
1	B	257	ALA	N-CA-C	-8.53	95.34	109.24
1	B	163	ILE	CB-CA-C	-8.00	99.77	112.16
1	D	86	ILE	CB-CA-C	-7.81	101.88	111.88
1	D	161	CYS	CA-C-N	-7.56	112.54	120.03
1	D	161	CYS	C-N-CA	-7.56	112.54	120.03
1	A	209	ILE	CB-CA-C	7.40	118.47	111.44
1	B	118	VAL	N-CA-C	-7.24	103.41	110.72
1	D	218	GLN	CA-C-N	7.07	129.54	120.70
1	D	218	GLN	C-N-CA	7.07	129.54	120.70
1	D	214	PHE	N-CA-C	6.43	118.37	111.36
1	A	20	TYR	N-CA-C	6.32	118.38	111.50
1	A	163	ILE	N-CA-CB	6.27	120.39	110.54
1	B	63	THR	N-CA-C	6.25	118.61	111.11
1	D	218	GLN	O-C-N	6.15	128.63	122.12
1	D	137	THR	N-CA-C	6.14	119.56	109.85
1	B	211	PRO	N-CA-C	6.07	118.11	110.70
1	A	59	GLU	CA-C-N	-5.96	112.73	119.28
1	A	59	GLU	C-N-CA	-5.96	112.73	119.28
1	D	20	TYR	N-CA-C	5.93	118.53	111.71
1	C	103	HIS	N-CA-CB	-5.60	101.17	110.47
1	B	186	ARG	CB-CA-C	-5.56	99.38	109.45
1	A	158	TYR	CA-C-N	5.40	127.83	120.54
1	A	158	TYR	C-N-CA	5.40	127.83	120.54
1	A	123	GLU	N-CA-C	5.35	118.03	111.82
1	B	259	LEU	N-CA-C	5.29	118.03	110.68
1	C	64	PHE	N-CA-C	-5.27	105.61	111.36
1	C	191	GLU	N-CA-C	5.27	117.03	111.28
1	B	137	THR	CA-C-N	-5.23	113.37	122.37
1	B	137	THR	C-N-CA	-5.23	113.37	122.37
1	B	256	TYR	CA-C-N	-5.22	115.52	122.72
1	B	256	TYR	C-N-CA	-5.22	115.52	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASN	N-CA-C	5.20	119.67	113.23
1	D	21	LYS	CG-CD-CE	5.18	123.22	111.30
1	C	118	VAL	N-CA-C	-5.18	105.66	110.53
1	A	235	HIS	N-CA-C	5.17	117.66	111.71
1	B	218	GLN	N-CA-CB	5.17	117.72	110.12
1	B	197	ILE	CB-CA-C	-5.05	104.52	111.49

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	2131	0	2078	18	0
1	B	2112	0	2066	11	1
1	C	2138	0	2094	17	0
1	D	2132	0	2088	27	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
2	C	12	0	16	0	0
2	D	6	0	8	0	0
3	A	58	0	0	2	0
3	B	66	0	0	0	0
3	C	54	0	0	0	0
3	D	14	0	0	0	0
All	All	8741	0	8374	71	1

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 4.

All (71) 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:D:185:GLN:C	1:D:185:GLN:HE21	1.88	0.80
1:D:186[B]:ARG:HB2	1:D:186[B]:ARG:NH1	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:O	1:A:63[A]:THR:HG23	1.93	0.68
1:C:12:ILE:HD11	1:C:146:MET:HE2	1.74	0.67
1:D:213[A]:GLU:OE2	1:D:213[A]:GLU:HA	1.94	0.67
1:D:186[B]:ARG:HB2	1:D:186[B]:ARG:HH11	1.59	0.67
1:A:12:ILE:HD11	1:A:146:MET:HE2	1.79	0.65
1:C:157:LEU:CD1	1:C:209:ILE:HD11	2.27	0.65
1:B:146:MET:HE1	1:B:178:PHE:CE2	2.33	0.63
1:D:163[A]:ILE:HD12	1:D:164:GLU:OE1	2.03	0.57
1:C:103:HIS:CD2	1:C:103:HIS:O	2.58	0.57
1:A:244:GLU:HG3	3:A:447:HOH:O	2.06	0.55
1:C:157:LEU:HD12	1:C:209:ILE:HD11	1.89	0.55
1:D:137:THR:HG22	1:D:142:THR:HG22	1.89	0.54
1:C:103:HIS:CD2	1:C:103:HIS:C	2.88	0.52
1:D:125:PHE:CZ	1:D:209:ILE:HD12	2.44	0.52
1:A:104:ASN:ND2	1:A:215:GLN:HE22	2.08	0.51
1:C:9:ILE:HD13	1:C:86[B]:ILE:CD1	2.41	0.51
1:B:18:ILE:CD1	1:B:239:LEU:HD11	2.41	0.50
1:D:12:ILE:HD11	1:D:146:MET:HE2	1.93	0.50
1:A:80:SER:HA	1:A:105:ALA:HA	1.93	0.50
1:C:103:HIS:O	1:C:103:HIS:HD2	1.92	0.49
1:B:52:ASN:ND2	1:B:138:SER:OG	2.44	0.49
1:D:185:GLN:O	1:D:185:GLN:NE2	2.34	0.49
1:C:49:GLU:HA	1:C:136:TYR:CE1	2.48	0.49
1:C:103:HIS:HE1	1:C:238:GLN:HB3	1.78	0.48
1:D:90:ALA:HA	1:D:97:ILE:HD12	1.94	0.48
1:A:163:ILE:HD11	3:A:455:HOH:O	2.12	0.48
1:D:10:HIS:CD2	1:D:15:GLY:HA2	2.48	0.47
1:D:213[A]:GLU:OE2	1:D:213[A]:GLU:CA	2.62	0.47
1:D:8:LEU:HB3	1:D:19:TRP:CE2	2.50	0.47
1:A:103:HIS:C	1:A:103:HIS:CD2	2.92	0.47
1:A:104:ASN:HD22	1:A:215:GLN:HE22	1.62	0.47
1:B:226:LYS:HE3	1:B:228:TYR:CZ	2.49	0.47
1:D:103:HIS:C	1:D:103:HIS:HD1	2.23	0.47
1:D:185:GLN:C	1:D:185:GLN:NE2	2.66	0.47
1:D:201:TYR:CE2	1:D:219:ILE:HD11	2.49	0.47
1:D:103:HIS:C	1:D:103:HIS:ND1	2.73	0.47
1:C:47:GLN:OE1	1:D:45:PRO:HB3	2.15	0.46
1:C:9:ILE:HD13	1:C:86[B]:ILE:HD11	1.98	0.46
1:A:24:PRO:HD3	1:B:167:GLU:HG2	1.98	0.45
1:A:90:ALA:HA	1:A:97:ILE:HD12	1.98	0.45
1:D:11:THR:HB	1:D:80:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ILE:CD1	1:C:86[B]:ILE:HD11	2.47	0.45
1:B:18:ILE:HD11	1:B:239:LEU:HD11	1.98	0.45
1:C:209:ILE:HG22	1:C:210:PHE:CD1	2.52	0.44
1:C:103:HIS:O	1:C:104:ASN:C	2.61	0.44
1:D:11:THR:CB	1:D:80:SER:HB3	2.48	0.44
1:A:163:ILE:N	1:A:163:ILE:CD1	2.81	0.44
1:D:103:HIS:ND1	1:D:103:HIS:O	2.46	0.44
1:D:201:TYR:CD2	1:D:219:ILE:HD11	2.52	0.43
1:D:83:GLY:HA2	1:D:86:ILE:HD12	2.00	0.43
1:A:114:PRO:HG2	1:A:186:ARG:HG3	2.00	0.43
1:B:55:ASP:OD2	1:B:186:ARG:NH1	2.48	0.42
1:A:103:HIS:O	1:A:104:ASN:C	2.62	0.42
1:B:94:PRO:HG3	1:B:193:GLY:HA2	2.00	0.42
1:D:128:TRP:HB3	1:D:131:THR:HB	2.00	0.42
1:A:61:LEU:O	1:A:65:MET:HG2	2.19	0.42
1:C:157:LEU:HG	1:C:209:ILE:CD1	2.50	0.42
1:B:90:ALA:HA	1:B:97:ILE:HD12	2.01	0.42
1:D:90:ALA:HA	1:D:97:ILE:CD1	2.50	0.42
1:D:115:SER:OG	1:D:184:ALA:HA	2.20	0.41
1:D:92[B]:LYS:O	1:D:92[B]:LYS:HG3	2.21	0.41
1:A:153:MET:HG2	1:A:157:LEU:HD22	2.02	0.41
1:A:209:ILE:O	1:A:211:PRO:HD3	2.20	0.41
1:B:130:ASP:OD1	1:B:149:GLY:HA3	2.20	0.41
1:A:192:GLU:H	1:A:192:GLU:CD	2.29	0.41
1:C:125:PHE:CD1	1:C:126:PRO:HD2	2.55	0.41
1:B:260:LEU:HD23	1:B:260:LEU:N	2.36	0.40
1:A:39:ALA:HB3	1:A:57:TYR:HA	2.03	0.40

All (1) 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:B:137:THR:OG1	1:B:139:ASN:O[7_555]	2.19	0.01

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	263/272 (97%)	253 (96%)	10 (4%)	0	100	100
1	B	261/272 (96%)	247 (95%)	14 (5%)	0	100	100
1	C	265/272 (97%)	254 (96%)	11 (4%)	0	100	100
1	D	263/272 (97%)	252 (96%)	11 (4%)	0	100	100
All	All	1052/1088 (97%)	1006 (96%)	46 (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	231/236 (98%)	220 (95%)	11 (5%)	23	12
1	B	230/236 (98%)	218 (95%)	12 (5%)	21	9
1	C	231/236 (98%)	222 (96%)	9 (4%)	28	18
1	D	231/236 (98%)	214 (93%)	17 (7%)	13	4
All	All	923/944 (98%)	874 (95%)	49 (5%)	22	9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63[A]	THR
1	A	63[B]	THR
1	A	70	GLN
1	A	86[A]	ILE
1	A	86[B]	ILE
1	A	103	HIS
1	A	123	GLU
1	A	148	LEU

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Mol	Chain	Res	Type
1	A	163	ILE
1	A	192	GLU
1	A	209	ILE
1	B	25	LEU
1	B	55	ASP
1	B	86	ILE
1	B	98[A]	SER
1	B	98[B]	SER
1	B	103	HIS
1	B	140	ASN
1	B	142	THR
1	B	146	MET
1	B	148	LEU
1	B	163	ILE
1	B	260	LEU
1	C	55	ASP
1	C	79	GLU
1	C	91	ASP
1	C	103	HIS
1	C	124	VAL
1	C	141	GLU
1	C	148	LEU
1	C	209	ILE
1	C	213	GLU
1	D	25	LEU
1	D	55	ASP
1	D	62	LEU
1	D	69	PRO
1	D	73	LYS
1	D	92[A]	LYS
1	D	92[B]	LYS
1	D	103	HIS
1	D	139	ASN
1	D	146	MET
1	D	148	LEU
1	D	163[A]	ILE
1	D	163[B]	ILE
1	D	185	GLN
1	D	191	GLU
1	D	208	LYS
1	D	209	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	B	50	GLN
1	B	52	ASN
1	B	215	GLN
1	B	243	ASN
1	C	52	ASN
1	C	103	HIS
1	C	104	ASN
1	C	180	GLN
1	D	139	ASN
1	D	185	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](#)

6 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	GOL	B	300	-	5,5,5	0.73	0	5,5,5	1.24	1 (20%)
2	GOL	A	300	-	5,5,5	0.91	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	301	-	5,5,5	0.98	0	5,5,5	1.03	0
2	GOL	D	300	-	5,5,5	0.59	0	5,5,5	1.26	1 (20%)
2	GOL	C	301	-	5,5,5	0.88	0	5,5,5	1.12	0
2	GOL	C	300	-	5,5,5	1.47	1 (20%)	5,5,5	1.54	1 (20%)

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	GOL	B	300	-	-	3/4/4/4	-
2	GOL	A	300	-	-	2/4/4/4	-
2	GOL	B	301	-	-	4/4/4/4	-
2	GOL	D	300	-	-	2/4/4/4	-
2	GOL	C	301	-	-	3/4/4/4	-
2	GOL	C	300	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	GOL	C3-C2	2.01	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	GOL	O1-C1-C2	3.20	124.77	110.38
2	B	300	GOL	O3-C3-C2	2.63	122.21	110.38
2	D	300	GOL	O1-C1-C2	2.33	120.85	110.38

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	GOL	C1-C2-C3-O3
2	B	300	GOL	O1-C1-C2-C3
2	D	300	GOL	O1-C1-C2-C3
2	B	301	GOL	C1-C2-C3-O3
2	C	301	GOL	C1-C2-C3-O3
2	B	300	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	300	GOL	O1-C1-C2-O2
2	C	301	GOL	O2-C2-C3-O3
2	A	300	GOL	O2-C2-C3-O3
2	B	301	GOL	O2-C2-C3-O3
2	B	301	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-O2
2	B	300	GOL	O2-C2-C3-O3

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 [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	260/272 (95%)	-0.19	4 (1%) 72 78	12, 33, 51, 70	5 (1%)
1	B	259/272 (95%)	-0.26	5 (1%) 66 74	12, 29, 49, 86	4 (1%)
1	C	265/272 (97%)	-0.22	0 100 100	13, 33, 56, 69	2 (0%)
1	D	260/272 (95%)	0.21	6 (2%) 61 68	17, 47, 80, 108	5 (1%)
All	All	1044/1088 (95%)	-0.11	15 (1%) 73 79	12, 33, 65, 108	16 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	LEU	5.6
1	D	261	ALA	4.9
1	A	260	LEU	4.6
1	B	259	LEU	4.2
1	A	2	ALA	4.1
1	A	261	ALA	3.8
1	B	258	ASP	2.9
1	D	126	PRO	2.8
1	B	257	ALA	2.7
1	D	125	PHE	2.7
1	D	124	VAL	2.7
1	B	137	THR	2.6
1	D	178	PHE	2.5
1	A	126	PRO	2.4
1	D	140	ASN	2.1

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($\text{\AA}^2$)	Q<0.9
2	GOL	C	301	6/6	0.75	0.13	39,44,46,59	0
2	GOL	B	301	6/6	0.76	0.13	51,57,60,63	0
2	GOL	C	300	6/6	0.83	0.15	43,48,53,54	0
2	GOL	D	300	6/6	0.84	0.15	52,55,56,56	0
2	GOL	A	300	6/6	0.86	0.16	51,57,60,63	0
2	GOL	B	300	6/6	0.88	0.15	36,58,65,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.