



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:32 AM UTC

PDB ID : 6FPF / pdb_00006fpf
Title : Structure of the Ustilago maydis chorismate mutase 1
Authors : Altegoer, F.; Steinchen, W.; Bange, G.
Deposited on : 2018-02-09
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
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

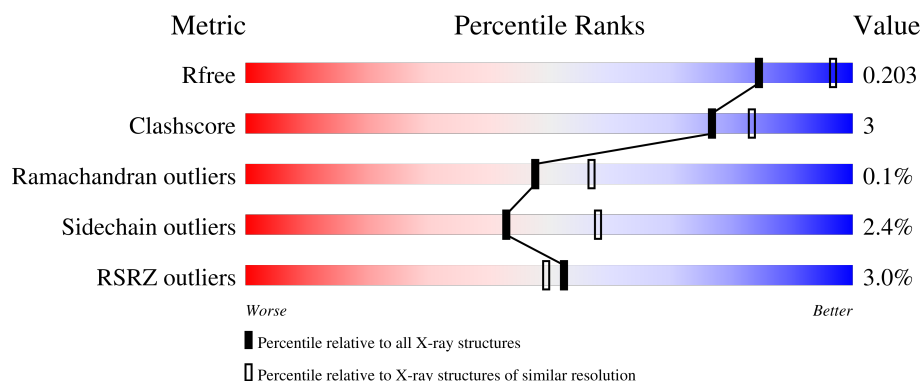
1 Overall quality at a glance

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))
R_{free}	180053	6164 (2.20-2.20)
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	278	2% 68% 23% • 8%
1	C	278	3% 76% 14% • 8%
1	D	278	2% 71% 19% • 8%
1	E	278	5% 69% 20% • • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8957 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 Chromosome 16, whole genome shotgun sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			2039	1285	363	388	3			
1	C	255	Total	C	N	O	S	0	2	0
			2022	1275	360	384	3			
1	D	257	Total	C	N	O	S	0	1	0
			2030	1280	361	386	3			
1	E	256	Total	C	N	O	S	0	2	0
			2030	1280	364	383	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	initiating methionine	UNP A0A0D1DWQ2
A	286	LEU	-	expression tag	UNP A0A0D1DWQ2
A	287	GLU	-	expression tag	UNP A0A0D1DWQ2
A	288	HIS	-	expression tag	UNP A0A0D1DWQ2
A	289	HIS	-	expression tag	UNP A0A0D1DWQ2
A	290	HIS	-	expression tag	UNP A0A0D1DWQ2
A	291	HIS	-	expression tag	UNP A0A0D1DWQ2
A	292	HIS	-	expression tag	UNP A0A0D1DWQ2
A	293	HIS	-	expression tag	UNP A0A0D1DWQ2
C	16	MET	-	initiating methionine	UNP A0A0D1DWQ2
C	286	LEU	-	expression tag	UNP A0A0D1DWQ2
C	287	GLU	-	expression tag	UNP A0A0D1DWQ2
C	288	HIS	-	expression tag	UNP A0A0D1DWQ2
C	289	HIS	-	expression tag	UNP A0A0D1DWQ2
C	290	HIS	-	expression tag	UNP A0A0D1DWQ2
C	291	HIS	-	expression tag	UNP A0A0D1DWQ2
C	292	HIS	-	expression tag	UNP A0A0D1DWQ2
C	293	HIS	-	expression tag	UNP A0A0D1DWQ2
D	16	MET	-	initiating methionine	UNP A0A0D1DWQ2
D	286	LEU	-	expression tag	UNP A0A0D1DWQ2
D	287	GLU	-	expression tag	UNP A0A0D1DWQ2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	288	HIS	-	expression tag	UNP A0A0D1DWQ2
D	289	HIS	-	expression tag	UNP A0A0D1DWQ2
D	290	HIS	-	expression tag	UNP A0A0D1DWQ2
D	291	HIS	-	expression tag	UNP A0A0D1DWQ2
D	292	HIS	-	expression tag	UNP A0A0D1DWQ2
D	293	HIS	-	expression tag	UNP A0A0D1DWQ2
E	16	MET	-	initiating methionine	UNP A0A0D1DWQ2
E	286	LEU	-	expression tag	UNP A0A0D1DWQ2
E	287	GLU	-	expression tag	UNP A0A0D1DWQ2
E	288	HIS	-	expression tag	UNP A0A0D1DWQ2
E	289	HIS	-	expression tag	UNP A0A0D1DWQ2
E	290	HIS	-	expression tag	UNP A0A0D1DWQ2
E	291	HIS	-	expression tag	UNP A0A0D1DWQ2
E	292	HIS	-	expression tag	UNP A0A0D1DWQ2
E	293	HIS	-	expression tag	UNP A0A0D1DWQ2

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0

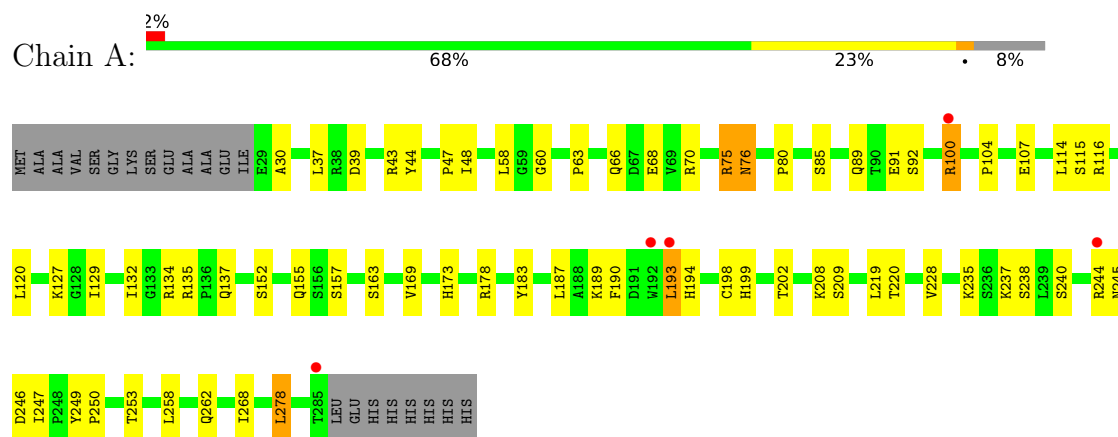
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	239	Total O 239 239	0	0
3	C	219	Total O 219 219	0	0
3	D	213	Total O 213 213	0	0
3	E	164	Total O 164 164	0	0

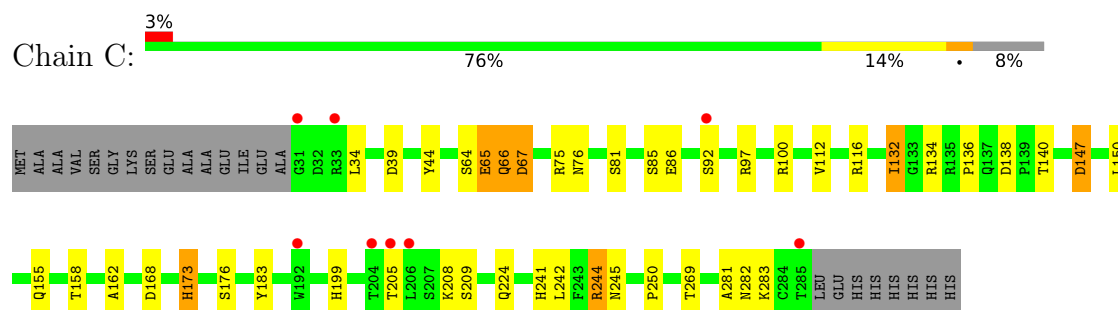
3 Residue-property plots [i](#)

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.

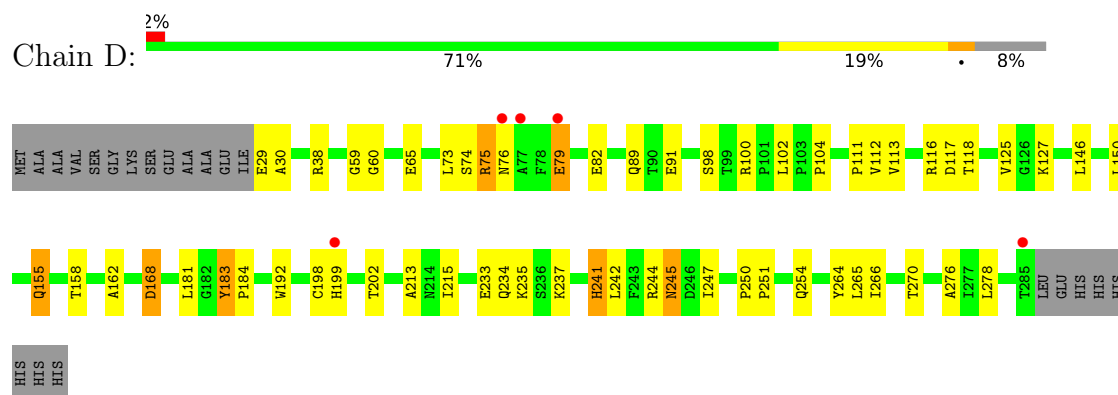
- Molecule 1: Chromosome 16, whole genome shotgun sequence



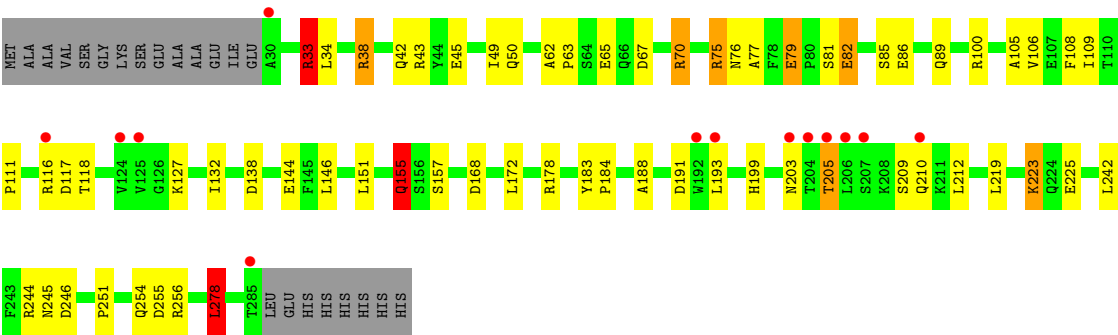
- Molecule 1: Chromosome 16, whole genome shotgun sequence



- Molecule 1: Chromosome 16, whole genome shotgun sequence



- Molecule 1: Chromosome 16, whole genome shotgun sequence



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.77Å 83.48Å 186.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.20 49.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.74-2.20) 99.9 (49.74-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.155 , 0.203 0.165 , 0.203	Depositor DCC
R_{free} test set	5251 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8957	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4049e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MN

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	2.03	60/2078 (2.9%)	1.52	22/2829 (0.8%)
1	C	1.89	32/2061 (1.6%)	1.47	16/2806 (0.6%)
1	D	2.02	46/2069 (2.2%)	1.50	14/2817 (0.5%)
1	E	1.87	32/2069 (1.5%)	1.47	16/2816 (0.6%)
All	All	1.95	170/8277 (2.1%)	1.49	68/11268 (0.6%)

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	245	ASN	N-CA	11.98	1.60	1.46
1	A	268	ILE	CA-CB	-9.49	1.42	1.54
1	A	92	SER	CA-C	9.44	1.64	1.52
1	C	112	VAL	C-O	-9.01	1.15	1.24
1	A	237	LYS	C-O	-8.88	1.13	1.23
1	D	116	ARG	NE-CZ	-8.86	1.23	1.33
1	E	109	ILE	C-O	-8.80	1.14	1.24
1	D	168	ASP	C-O	-8.47	1.14	1.24
1	D	112	VAL	C-O	-8.24	1.15	1.24
1	A	235	LYS	CA-C	-8.12	1.42	1.52
1	D	251	PRO	CA-C	8.05	1.63	1.52
1	D	76	ASN	CA-C	-7.96	1.43	1.53
1	A	66	GLN	CA-C	7.95	1.63	1.52
1	C	64	SER	CA-C	7.70	1.63	1.53
1	A	219	LEU	C-O	-7.57	1.14	1.24
1	C	199	HIS	CA-C	-7.57	1.42	1.52
1	A	155	GLN	N-CA	-7.56	1.36	1.46
1	A	91	GLU	C-O	-7.55	1.15	1.24
1	E	77	ALA	N-CA	-7.33	1.37	1.46
1	A	43	ARG	CD-NE	-7.18	1.36	1.46
1	D	82	GLU	C-O	-7.18	1.15	1.24
1	C	242	LEU	N-CA	-7.13	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	132	ILE	CB-CG1	-7.09	1.39	1.53
1	C	176	SER	CA-C	6.94	1.61	1.52
1	A	228	VAL	C-O	-6.82	1.16	1.24
1	C	116	ARG	CD-NE	-6.77	1.36	1.46
1	C	116	ARG	CZ-NH2	-6.77	1.24	1.33
1	E	76	ASN	CA-C	-6.71	1.43	1.53
1	D	155	GLN	N-CA	-6.68	1.37	1.46
1	A	76	ASN	CB-CG	-6.65	1.35	1.52
1	D	73	LEU	CA-C	6.65	1.61	1.52
1	E	67	ASP	C-O	-6.63	1.16	1.24
1	E	255	ASP	C-O	-6.63	1.16	1.24
1	D	276	ALA	N-CA	-6.62	1.38	1.46
1	D	74	SER	C-O	-6.61	1.16	1.24
1	E	251	PRO	CA-CB	6.58	1.62	1.53
1	A	137	GLN	C-O	-6.57	1.15	1.24
1	E	172	LEU	C-O	6.56	1.31	1.24
1	A	47	PRO	CA-CB	-6.54	1.44	1.53
1	C	100	ARG	CA-C	6.53	1.59	1.53
1	D	75	ARG	CD-NE	-6.51	1.37	1.46
1	D	241	HIS	CB-CG	-6.48	1.41	1.50
1	A	183	TYR	CA-C	6.47	1.59	1.52
1	C	76	ASN	C-O	6.42	1.30	1.23
1	D	113	VAL	C-O	-6.42	1.16	1.24
1	D	111	PRO	N-CA	6.41	1.54	1.46
1	C	81	SER	N-CA	6.38	1.54	1.45
1	E	242	LEU	N-CA	-6.38	1.38	1.46
1	D	89	GLN	C-O	-6.36	1.15	1.24
1	D	116	ARG	CD-NE	-6.33	1.37	1.46
1	D	91	GLU	N-CA	-6.32	1.38	1.46
1	D	125	VAL	C-O	-6.32	1.17	1.24
1	A	278	LEU	C-O	-6.31	1.16	1.24
1	D	198	CYS	C-O	-6.31	1.16	1.24
1	E	116	ARG	CD-NE	-6.29	1.37	1.46
1	E	245	ASN	CA-CB	-6.25	1.45	1.53
1	C	147	ASP	CA-C	6.23	1.60	1.52
1	E	138	ASP	CA-C	-6.22	1.46	1.53
1	D	250	PRO	CA-CB	6.22	1.59	1.53
1	C	44	TYR	C-O	6.20	1.32	1.24
1	E	75	ARG	CD-NE	-6.15	1.37	1.46
1	A	135	ARG	N-CA	6.14	1.53	1.46
1	A	116	ARG	CZ-NH2	-6.14	1.25	1.33
1	D	158	THR	N-CA	-6.11	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	LEU	C-O	-6.08	1.16	1.24
1	A	220	THR	C-O	-6.07	1.16	1.24
1	E	49	ILE	CA-C	-6.07	1.45	1.52
1	A	114	LEU	N-CA	-6.04	1.38	1.45
1	C	67	ASP	CA-C	6.02	1.60	1.52
1	D	98	SER	C-O	-5.93	1.16	1.23
1	D	183	TYR	C-O	-5.93	1.19	1.24
1	A	63	PRO	N-CA	5.89	1.54	1.47
1	D	127	LYS	N-CA	5.88	1.53	1.45
1	A	262	GLN	N-CA	5.88	1.53	1.46
1	E	50	GLN	N-CA	-5.85	1.39	1.46
1	E	138	ASP	N-CA	5.85	1.54	1.45
1	C	66	GLN	CD-OE1	5.84	1.34	1.23
1	D	146	LEU	N-CA	5.83	1.53	1.46
1	D	235	LYS	CA-C	-5.82	1.45	1.52
1	D	60	GLY	C-O	5.82	1.29	1.23
1	A	240	SER	CA-C	-5.81	1.45	1.52
1	E	246	ASP	C-O	-5.79	1.16	1.23
1	D	213	ALA	C-O	5.79	1.30	1.24
1	A	100	ARG	CD-NE	-5.74	1.38	1.46
1	A	43	ARG	CZ-NH2	-5.72	1.26	1.33
1	E	151	LEU	C-O	-5.72	1.16	1.24
1	E	106	VAL	N-CA	-5.72	1.40	1.46
1	C	134	ARG	CA-C	5.69	1.60	1.52
1	A	30	ALA	CA-C	5.69	1.60	1.52
1	D	118	THR	N-CA	5.69	1.53	1.46
1	A	178	ARG	CZ-NH1	-5.67	1.24	1.32
1	A	80	PRO	CA-C	5.66	1.59	1.52
1	D	270	THR	N-CA	-5.64	1.39	1.46
1	D	116	ARG	CZ-NH2	-5.64	1.26	1.33
1	D	38	ARG	C-O	5.64	1.30	1.24
1	A	202	THR	N-CA	5.63	1.53	1.46
1	E	219	LEU	C-O	-5.63	1.16	1.24
1	E	157	SER	C-O	-5.62	1.16	1.24
1	D	215	ILE	CA-C	5.60	1.59	1.52
1	E	38	ARG	CA-C	-5.60	1.45	1.52
1	A	104	PRO	C-O	5.58	1.30	1.23
1	A	58	LEU	C-O	-5.57	1.17	1.24
1	C	162	ALA	C-O	-5.57	1.17	1.24
1	A	48	ILE	CA-CB	-5.56	1.47	1.54
1	D	264	TYR	CA-C	5.54	1.57	1.52
1	A	253	THR	CA-C	5.54	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	ARG	CA-C	-5.53	1.47	1.53
1	A	68	GLU	CA-C	-5.49	1.45	1.52
1	D	162	ALA	N-CA	5.47	1.53	1.46
1	A	253	THR	N-CA	-5.47	1.39	1.46
1	D	254	GLN	CG-CD	5.45	1.65	1.52
1	E	33	ARG	CA-C	5.44	1.60	1.52
1	A	173	HIS	CA-C	-5.42	1.45	1.52
1	A	187	LEU	C-O	-5.41	1.17	1.24
1	C	92	SER	CA-C	5.41	1.59	1.52
1	D	158	THR	CA-C	5.41	1.59	1.52
1	A	44	TYR	C-O	-5.41	1.17	1.24
1	A	134	ARG	C-O	5.41	1.30	1.23
1	D	266	ILE	C-O	-5.41	1.17	1.24
1	A	116	ARG	CD-NE	-5.40	1.38	1.46
1	C	224	GLN	CA-C	5.39	1.60	1.52
1	A	169	VAL	C-O	5.39	1.30	1.24
1	D	234	GLN	C-O	5.38	1.30	1.24
1	C	250	PRO	N-CA	-5.38	1.39	1.46
1	A	246	ASP	C-O	-5.38	1.17	1.23
1	D	265	LEU	C-O	5.36	1.30	1.24
1	A	249	TYR	C-O	-5.35	1.17	1.23
1	A	39	ASP	CB-CG	5.34	1.65	1.52
1	E	254	GLN	N-CA	5.34	1.52	1.46
1	C	158	THR	CA-C	5.33	1.59	1.52
1	C	241	HIS	CB-CG	-5.31	1.42	1.50
1	E	111	PRO	CA-CB	5.29	1.60	1.53
1	A	107	GLU	CA-C	-5.29	1.45	1.52
1	C	97	ARG	C-O	-5.28	1.17	1.24
1	C	183	TYR	CA-C	5.27	1.58	1.52
1	D	202	THR	N-CA	5.26	1.52	1.46
1	A	152	SER	CA-C	5.26	1.60	1.52
1	C	281	ALA	N-CA	5.26	1.53	1.46
1	D	244	ARG	N-CA	-5.25	1.39	1.46
1	C	75	ARG	CZ-NH1	5.24	1.40	1.32
1	A	43	ARG	CZ-NH1	-5.24	1.25	1.32
1	A	190	PHE	C-O	-5.24	1.18	1.24
1	C	150	LEU	CA-CB	-5.23	1.45	1.53
1	C	250	PRO	CA-C	5.22	1.54	1.51
1	C	140	THR	CB-CG2	5.20	1.69	1.52
1	A	89	GLN	N-CA	5.20	1.52	1.46
1	E	178	ARG	CA-C	5.20	1.59	1.52
1	A	76	ASN	C-N	-5.19	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	SER	CA-C	-5.18	1.46	1.52
1	A	238	SER	C-O	-5.18	1.18	1.24
1	E	256	ARG	C-O	-5.18	1.17	1.24
1	A	60	GLY	C-O	5.16	1.28	1.23
1	E	225	GLU	CA-C	5.16	1.59	1.52
1	A	37	LEU	N-CA	5.12	1.52	1.46
1	A	258	LEU	C-O	5.12	1.29	1.24
1	C	136	PRO	CA-CB	5.10	1.61	1.53
1	A	76	ASN	CA-CB	-5.09	1.45	1.53
1	D	181	LEU	N-CA	-5.08	1.39	1.46
1	E	105	ALA	N-CA	-5.08	1.39	1.46
1	C	269	THR	CA-C	5.08	1.59	1.52
1	E	146	LEU	N-CA	5.06	1.52	1.46
1	E	118	THR	C-O	5.06	1.29	1.23
1	D	150	LEU	C-O	-5.04	1.18	1.24
1	C	173	HIS	CA-CB	5.02	1.61	1.53
1	E	278	LEU	CA-C	-5.02	1.46	1.52
1	A	157	SER	C-O	-5.02	1.17	1.24
1	A	127	LYS	N-CA	5.02	1.52	1.45
1	A	194	HIS	C-O	5.02	1.29	1.24
1	A	129	ILE	C-O	5.00	1.29	1.23
1	E	155	GLN	C-O	5.00	1.29	1.23

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	ARG	CG-CD-NE	-8.55	93.18	112.00
1	A	70	ARG	NE-CZ-NH2	8.12	126.51	119.20
1	E	116	ARG	CG-CD-NE	-8.08	94.23	112.00
1	A	43	ARG	CG-CD-NE	-8.05	94.28	112.00
1	D	241	HIS	CB-CA-C	-7.63	100.17	111.77
1	D	199	HIS	N-CA-CB	-7.09	99.30	110.28
1	C	116	ARG	NE-CZ-NH1	7.04	128.54	121.50
1	E	33	ARG	CB-CA-C	7.02	124.16	110.67
1	A	75	ARG	CA-C-N	-6.98	110.59	122.67
1	A	75	ARG	C-N-CA	-6.98	110.59	122.67
1	A	70	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	C	100	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	D	247	ILE	N-CA-C	-6.78	102.31	108.95
1	C	245	ASN	N-CA-C	6.70	120.78	112.47
1	A	92	SER	N-CA-C	-6.56	103.75	111.03
1	A	115	SER	CB-CA-C	6.52	120.56	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	LEU	CD1-CG-CD2	-6.38	96.77	110.80
1	A	245	ASN	N-CA-C	6.31	120.77	113.38
1	E	45	GLU	CB-CA-C	-6.08	101.59	110.96
1	E	79	GLU	N-CA-CB	6.03	117.33	110.03
1	A	199	HIS	N-CA-CB	-6.02	101.03	110.06
1	C	132	ILE	CA-CB-CG2	6.00	120.70	110.50
1	C	65	GLU	N-CA-C	-5.97	104.77	111.28
1	D	30	ALA	CA-C-N	5.97	126.61	119.98
1	D	30	ALA	C-N-CA	5.97	126.61	119.98
1	C	39	ASP	CA-C-O	-5.96	114.23	120.55
1	E	70	ARG	NE-CZ-NH2	5.96	124.57	119.20
1	E	42	GLN	N-CA-C	5.95	118.55	111.71
1	E	117	ASP	CB-CA-C	-5.82	99.53	110.01
1	C	199	HIS	CB-CA-C	-5.80	100.82	110.68
1	A	100	ARG	CA-CB-CG	-5.77	102.56	114.10
1	A	100	ARG	CB-CG-CD	-5.76	98.04	111.30
1	E	116	ARG	CB-CA-C	-5.72	99.03	110.42
1	C	75	ARG	CD-NE-CZ	-5.68	116.45	124.40
1	E	45	GLU	N-CA-C	5.58	117.06	110.97
1	E	210	GLN	CB-CG-CD	-5.58	103.12	112.60
1	C	92	SER	CA-C-N	5.57	127.10	120.14
1	C	92	SER	C-N-CA	5.57	127.10	120.14
1	D	244	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	D	79	GLU	N-CA-C	-5.55	102.66	110.31
1	A	85	SER	N-CA-CB	-5.54	101.98	110.01
1	A	193	LEU	N-CA-C	-5.53	103.80	110.88
1	D	74	SER	CB-CA-C	-5.49	101.68	110.79
1	C	138	ASP	CA-C-O	5.43	124.59	119.76
1	C	100	ARG	CG-CD-NE	-5.41	100.09	112.00
1	A	247	ILE	N-CA-C	5.31	113.20	108.63
1	E	199	HIS	N-CA-C	5.30	118.54	111.75
1	A	120	LEU	N-CA-C	5.30	119.82	112.45
1	A	237	LYS	CB-CA-C	-5.26	100.93	110.56
1	A	189	LYS	N-CA-CB	5.26	117.85	110.12
1	D	104	PRO	N-CA-C	5.21	119.27	111.14
1	A	43	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	D	74	SER	CA-CB-OG	-5.20	100.70	111.10
1	A	198	CYS	CA-C-O	5.20	126.06	120.55
1	D	250	PRO	O-C-N	5.19	123.70	121.31
1	A	157	SER	N-CA-C	-5.19	106.97	113.72
1	D	192	TRP	CA-CB-CG	5.16	123.41	113.60
1	A	75	ARG	N-CA-C	-5.15	106.78	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ASP	CB-CA-C	-5.14	101.50	110.09
1	C	85	SER	CB-CA-C	-5.11	102.86	110.88
1	C	34	LEU	N-CA-C	5.11	116.66	111.14
1	E	33	ARG	CA-CB-CG	5.09	124.27	114.10
1	E	199	HIS	CB-CA-C	-5.07	100.63	110.46
1	E	108	PHE	N-CA-C	5.05	117.62	110.10
1	E	100	ARG	NH1-CZ-NH2	-5.05	112.74	119.30
1	C	86	GLU	N-CA-C	-5.03	105.69	111.07
1	E	116	ARG	N-CA-C	5.01	121.48	110.80
1	A	250	PRO	CB-CA-C	-5.00	106.69	111.39

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	2039	0	2059	10	1
1	C	2022	0	2045	10	0
1	D	2030	0	2052	14	0
1	E	2030	0	2053	22	1
2	A	1	0	0	0	0
3	A	239	0	0	3	1
3	C	219	0	0	4	0
3	D	213	0	0	2	1
3	E	164	0	0	4	0
All	All	8957	0	8209	48	2

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 3.

All (48) 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:155:GLN:OE1	3:D:301:HOH:O	1.91	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:NH2	3:A:401:HOH:O	2.12	0.81
1:A:76:ASN:C	1:A:76:ASN:OD1	2.19	0.80
1:C:244:ARG:HG3	1:C:244:ARG:NH1	1.97	0.76
1:C:244:ARG:HG3	1:C:244:ARG:HH11	1.53	0.72
1:E:155:GLN:NE2	3:E:302:HOH:O	2.23	0.71
1:A:100:ARG:HD3	1:D:237:LYS:HD3	1.72	0.71
1:C:244:ARG:HH11	1:C:244:ARG:CG	2.03	0.70
1:E:43[B]:ARG:NH1	3:E:303:HOH:O	2.28	0.66
1:A:100:ARG:HE	1:D:233:GLU:CD	2.04	0.65
1:E:144:GLU:OE1	3:E:301:HOH:O	2.14	0.63
1:E:203:ASN:ND2	1:E:205:THR:CG2	2.62	0.62
1:D:237:LYS:O	1:D:241:HIS:HD2	1.82	0.62
1:C:173:HIS:HE1	3:C:360:HOH:O	1.88	0.57
1:C:155:GLN:NE2	3:C:301:HOH:O	2.18	0.56
1:E:212:LEU:HD12	1:E:278:LEU:CD1	2.37	0.55
1:E:70:ARG:HH11	1:E:70:ARG:HG3	1.72	0.54
1:C:67:ASP:OD2	3:C:302:HOH:O	2.18	0.54
1:E:203:ASN:ND2	1:E:205:THR:HG21	2.22	0.53
1:E:65:GLU:OE2	1:E:168:ASP:OD2	2.29	0.50
1:E:82:GLU:O	1:E:86:GLU:HG3	2.12	0.49
1:E:70:ARG:HH11	1:E:70:ARG:CG	2.27	0.48
1:D:59:GLY:HA2	1:E:43[B]:ARG:HH21	1.79	0.47
1:E:62:ALA:HB1	1:E:63:PRO:HD2	1.96	0.47
1:C:66:GLN:HG2	1:C:147:ASP:OD1	2.15	0.47
1:E:81:SER:O	1:E:85:SER:HB2	2.14	0.47
1:C:282:ASN:OD1	1:C:283:LYS:N	2.48	0.46
1:E:223:LYS:HB3	1:E:223:LYS:HE3	1.61	0.46
1:A:75:ARG:HG2	1:D:241:HIS:HB3	1.98	0.46
1:A:100:ARG:NH1	3:A:408:HOH:O	2.47	0.45
1:A:132:ILE:HD12	1:A:132:ILE:HG23	1.74	0.45
1:E:33:ARG:HD2	1:E:188:ALA:HB2	2.00	0.44
1:A:100:ARG:NE	1:D:233:GLU:HG2	2.32	0.44
1:D:245:ASN:ND2	3:D:302:HOH:O	2.13	0.43
3:A:431:HOH:O	1:E:244:ARG:HD3	2.19	0.43
1:E:43[B]:ARG:HH11	1:E:43[B]:ARG:HG3	1.83	0.43
1:C:65:GLU:OE2	1:C:168:ASP:OD2	2.36	0.43
1:E:132:ILE:HG21	1:E:132:ILE:HD13	1.72	0.43
1:E:183:TYR:HB3	1:E:184:PRO:CD	2.49	0.43
1:A:100:ARG:HE	1:D:233:GLU:CG	2.31	0.42
1:A:100:ARG:HE	1:D:233:GLU:HG2	1.84	0.42
1:D:65:GLU:OE2	1:D:168:ASP:OD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:TYR:HB3	1:D:184:PRO:CD	2.49	0.42
1:D:75:ARG:HD3	1:E:75:ARG:O	2.20	0.42
1:E:34:LEU:HD21	1:E:38:ARG:HH21	1.85	0.42
1:D:100:ARG:HH11	1:D:100:ARG:HG3	1.85	0.41
1:C:173:HIS:HD2	3:C:485:HOH:O	2.04	0.41
1:E:155:GLN:CD	3:E:302:HOH:O	2.61	0.40

All (2) 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)
3:A:628:HOH:O	3:D:454:HOH:O[1_455]	2.16	0.04
1:A:244:ARG:NH2	1:E:79:GLU:OE2[1_455]	2.17	0.03

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	257/278 (92%)	253 (98%)	4 (2%)	0	100	100
1	C	255/278 (92%)	249 (98%)	6 (2%)	0	100	100
1	D	256/278 (92%)	249 (97%)	7 (3%)	0	100	100
1	E	256/278 (92%)	247 (96%)	8 (3%)	1 (0%)	30	34
All	All	1024/1112 (92%)	998 (98%)	25 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	191	ASP

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	230/244 (94%)	226 (98%)	4 (2%)	53	69
1	C	229/244 (94%)	224 (98%)	5 (2%)	45	61
1	D	229/244 (94%)	226 (99%)	3 (1%)	61	76
1	E	228/244 (93%)	218 (96%)	10 (4%)	25	34
All	All	916/976 (94%)	894 (98%)	22 (2%)	43	58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LEU
1	A	208	LYS
1	A	209	SER
1	A	278	LEU
1	C	132	ILE
1	C	205	THR
1	C	208	LYS
1	C	209	SER
1	C	244	ARG
1	D	29	GLU
1	D	79	GLU
1	D	278	LEU
1	E	33	ARG
1	E	82	GLU
1	E	89	GLN
1	E	127	LYS
1	E	155	GLN
1	E	193	LEU
1	E	205	THR
1	E	209	SER
1	E	223	LYS
1	E	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	155	GLN
1	C	173	HIS
1	C	194	HIS
1	C	252	HIS
1	C	254	GLN
1	D	196	ASN
1	D	241	HIS
1	E	155	GLN
1	E	194	HIS
1	E	203	ASN
1	E	210	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

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

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	257/278 (92%)	-0.34	5 (1%) 66 63	9, 27, 63, 91	2 (0%)
1	C	255/278 (91%)	-0.20	8 (3%) 51 48	12, 30, 78, 96	2 (0%)
1	D	257/278 (92%)	-0.34	5 (1%) 66 63	9, 28, 59, 86	1 (0%)
1	E	256/278 (92%)	-0.03	13 (5%) 33 30	12, 34, 87, 110	2 (0%)
All	All	1025/1112 (92%)	-0.23	31 (3%) 52 49	9, 30, 78, 110	7 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	203	ASN	4.5
1	E	204	THR	4.4
1	C	31	GLY	3.7
1	E	125	VAL	3.7
1	E	193	LEU	3.5
1	C	285	THR	3.4
1	D	285	THR	3.4
1	E	192	TRP	3.1
1	E	124	VAL	3.0
1	E	206	LEU	2.9
1	D	79	GLU	2.9
1	A	193	LEU	2.8
1	A	285	THR	2.8
1	E	210	GLN	2.7
1	C	192	TRP	2.7
1	C	206	LEU	2.7
1	E	285	THR	2.6
1	A	192	TRP	2.6
1	E	207	SER	2.5
1	A	244	ARG	2.4
1	C	33	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	30	ALA	2.4
1	D	199	HIS	2.3
1	E	116	ARG	2.3
1	C	204	THR	2.2
1	D	77	ALA	2.2
1	C	92	SER	2.1
1	A	100	ARG	2.1
1	D	76	ASN	2.1
1	C	205	THR	2.0
1	E	205	THR	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, 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	MN	A	301	1/1	0.98	0.10	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.