



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:10 AM UTC

PDB ID : 6FPG / pdb_00006fpg
Title : Structure of the Ustilago maydis chorismate mutase 1 in complex with a Zea mays kiwellin
Authors : Altegoer, F.; Steinchen, W.; Bange, G.
Deposited on : 2018-02-09
Resolution : 1.80 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

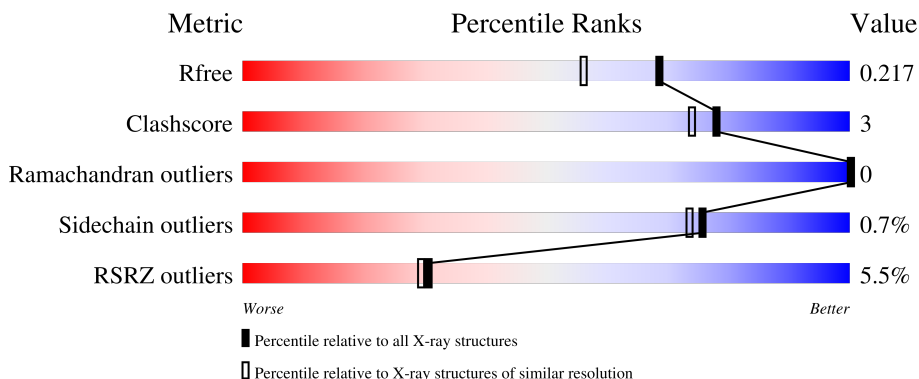
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	B	278	 6% 85% 9% • 5%
1	C	278	 4% 85% 9% 6%
1	F	278	 3% 88% 6% • •
1	G	278	 6% 87% 7% • 5%
2	D	175	 5% 82% • • 13%

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Mol	Chain	Length	Quality of chain
2	E	175	<p>9% 79% 10% 10%</p>
2	H	175	<p>5% 79% 8% 12%</p>
2	I	175	<p>6% 79% 9% 12%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	B	301	-	X	-	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14061 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
			Total	C	N	O	S			
1	C	262	2059	1298	365	393	3	0	0	0
1	B	264	2072	1306	368	395	3	0	0	0
1	F	266	2096	1321	372	400	3	0	1	0
1	G	265	2079	1310	369	397	3	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	MET	-	initiating methionine	UNP A0A0D1DWQ2
C	291	LEU	-	expression tag	UNP A0A0D1DWQ2
C	292	GLU	-	expression tag	UNP A0A0D1DWQ2
C	293	HIS	-	expression tag	UNP A0A0D1DWQ2
C	294	HIS	-	expression tag	UNP A0A0D1DWQ2
C	295	HIS	-	expression tag	UNP A0A0D1DWQ2
C	296	HIS	-	expression tag	UNP A0A0D1DWQ2
C	297	HIS	-	expression tag	UNP A0A0D1DWQ2
C	298	HIS	-	expression tag	UNP A0A0D1DWQ2
B	21	MET	-	initiating methionine	UNP A0A0D1DWQ2
B	291	LEU	-	expression tag	UNP A0A0D1DWQ2
B	292	GLU	-	expression tag	UNP A0A0D1DWQ2
B	293	HIS	-	expression tag	UNP A0A0D1DWQ2
B	294	HIS	-	expression tag	UNP A0A0D1DWQ2
B	295	HIS	-	expression tag	UNP A0A0D1DWQ2
B	296	HIS	-	expression tag	UNP A0A0D1DWQ2
B	297	HIS	-	expression tag	UNP A0A0D1DWQ2
B	298	HIS	-	expression tag	UNP A0A0D1DWQ2
F	21	MET	-	initiating methionine	UNP A0A0D1DWQ2
F	291	LEU	-	expression tag	UNP A0A0D1DWQ2
F	292	GLU	-	expression tag	UNP A0A0D1DWQ2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	293	HIS	-	expression tag	UNP A0A0D1DWQ2
F	294	HIS	-	expression tag	UNP A0A0D1DWQ2
F	295	HIS	-	expression tag	UNP A0A0D1DWQ2
F	296	HIS	-	expression tag	UNP A0A0D1DWQ2
F	297	HIS	-	expression tag	UNP A0A0D1DWQ2
F	298	HIS	-	expression tag	UNP A0A0D1DWQ2
G	21	MET	-	initiating methionine	UNP A0A0D1DWQ2
G	291	LEU	-	expression tag	UNP A0A0D1DWQ2
G	292	GLU	-	expression tag	UNP A0A0D1DWQ2
G	293	HIS	-	expression tag	UNP A0A0D1DWQ2
G	294	HIS	-	expression tag	UNP A0A0D1DWQ2
G	295	HIS	-	expression tag	UNP A0A0D1DWQ2
G	296	HIS	-	expression tag	UNP A0A0D1DWQ2
G	297	HIS	-	expression tag	UNP A0A0D1DWQ2
G	298	HIS	-	expression tag	UNP A0A0D1DWQ2

- Molecule 2 is a protein called Ripening-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	153	1124	678	205	230	11	0	0	0
2	E	157	1149	691	209	238	11	0	0	0
2	H	154	1131	682	206	232	11	0	0	0
2	I	154	1128	680	206	231	11	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

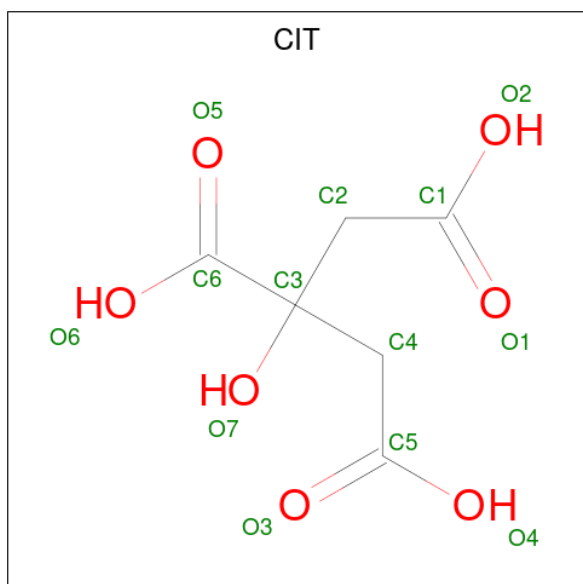
Chain	Residue	Modelled	Actual	Comment	Reference
D	32	MET	-	initiating methionine	UNP A0A1D6GNR3
D	199	LEU	-	expression tag	UNP A0A1D6GNR3
D	200	GLU	-	expression tag	UNP A0A1D6GNR3
D	201	HIS	-	expression tag	UNP A0A1D6GNR3
D	202	HIS	-	expression tag	UNP A0A1D6GNR3
D	203	HIS	-	expression tag	UNP A0A1D6GNR3
D	204	HIS	-	expression tag	UNP A0A1D6GNR3
D	205	HIS	-	expression tag	UNP A0A1D6GNR3
D	206	HIS	-	expression tag	UNP A0A1D6GNR3
E	32	MET	-	initiating methionine	UNP A0A1D6GNR3
E	199	LEU	-	expression tag	UNP A0A1D6GNR3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	200	GLU	-	expression tag	UNP A0A1D6GNR3
E	201	HIS	-	expression tag	UNP A0A1D6GNR3
E	202	HIS	-	expression tag	UNP A0A1D6GNR3
E	203	HIS	-	expression tag	UNP A0A1D6GNR3
E	204	HIS	-	expression tag	UNP A0A1D6GNR3
E	205	HIS	-	expression tag	UNP A0A1D6GNR3
E	206	HIS	-	expression tag	UNP A0A1D6GNR3
H	32	MET	-	initiating methionine	UNP A0A1D6GNR3
H	199	LEU	-	expression tag	UNP A0A1D6GNR3
H	200	GLU	-	expression tag	UNP A0A1D6GNR3
H	201	HIS	-	expression tag	UNP A0A1D6GNR3
H	202	HIS	-	expression tag	UNP A0A1D6GNR3
H	203	HIS	-	expression tag	UNP A0A1D6GNR3
H	204	HIS	-	expression tag	UNP A0A1D6GNR3
H	205	HIS	-	expression tag	UNP A0A1D6GNR3
H	206	HIS	-	expression tag	UNP A0A1D6GNR3
I	32	MET	-	initiating methionine	UNP A0A1D6GNR3
I	199	LEU	-	expression tag	UNP A0A1D6GNR3
I	200	GLU	-	expression tag	UNP A0A1D6GNR3
I	201	HIS	-	expression tag	UNP A0A1D6GNR3
I	202	HIS	-	expression tag	UNP A0A1D6GNR3
I	203	HIS	-	expression tag	UNP A0A1D6GNR3
I	204	HIS	-	expression tag	UNP A0A1D6GNR3
I	205	HIS	-	expression tag	UNP A0A1D6GNR3
I	206	HIS	-	expression tag	UNP A0A1D6GNR3

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).

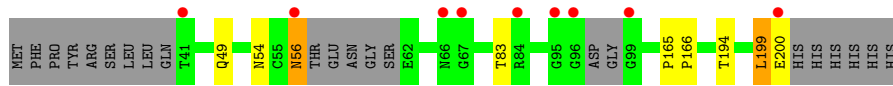
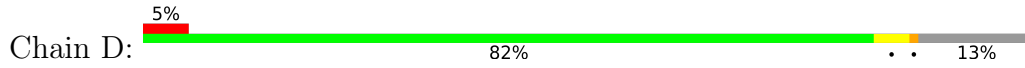


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		

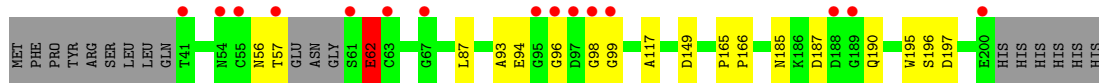
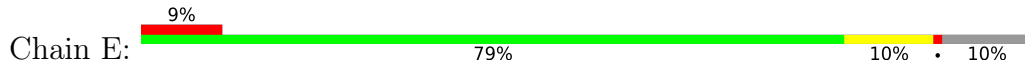
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	186	Total	O	0	0
			186	186		
4	B	167	Total	O	0	0
			167	167		
4	D	75	Total	O	0	0
			75	75		
4	E	87	Total	O	0	0
			87	87		
4	F	255	Total	O	0	0
			255	255		
4	G	220	Total	O	0	0
			220	220		
4	H	81	Total	O	0	0
			81	81		
4	I	100	Total	O	0	0
			100	100		

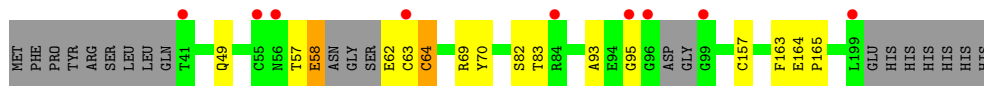
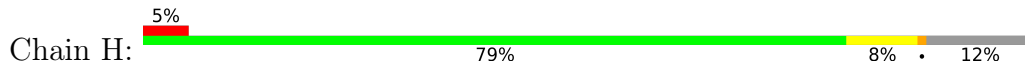
• Molecule 2: Ripening-related protein 3



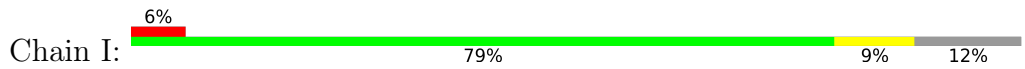
• Molecule 2: Ripening-related protein 3



• Molecule 2: Ripening-related protein 3



• Molecule 2: Ripening-related protein 3



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.51Å 85.66Å 95.78Å 96.16° 92.39° 90.37°	Depositor
Resolution (Å)	48.50 – 1.80 48.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.50-1.80) 96.6 (48.50-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.79Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.186 , 0.216 0.190 , 0.217	Depositor DCC
R_{free} test set	8389 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14061	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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: CIT

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	B	0.88	11/2111 (0.5%)	0.77	1/2872 (0.0%)
1	C	0.78	13/2098 (0.6%)	0.66	3/2856 (0.1%)
1	F	0.84	12/2135 (0.6%)	0.63	1/2905 (0.0%)
1	G	0.81	12/2118 (0.6%)	0.79	7/2882 (0.2%)
2	D	0.83	3/1143 (0.3%)	0.79	3/1545 (0.2%)
2	E	0.94	8/1169 (0.7%)	0.85	6/1582 (0.4%)
2	H	0.89	7/1150 (0.6%)	0.82	6/1555 (0.4%)
2	I	0.77	5/1147 (0.4%)	0.67	0/1551
All	All	0.84	71/13071 (0.5%)	0.74	27/17748 (0.2%)

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	81	ASN	CA-C	-11.31	1.39	1.53
2	I	165	PRO	C-O	-9.74	1.13	1.24
1	B	70	GLU	C-O	-9.64	1.12	1.24
1	F	221	ILE	C-O	-8.86	1.13	1.24
1	C	37	ASP	C-O	-8.54	1.14	1.24
2	H	63	CYS	C-O	-8.50	1.13	1.23
2	I	164	GLU	C-O	-7.77	1.15	1.23
1	F	34	GLU	C-O	-7.55	1.15	1.24
1	B	88	VAL	C-O	-7.51	1.15	1.24
1	F	33	ILE	C-O	-7.48	1.15	1.24
2	D	166	PRO	C-O	-7.29	1.15	1.23
1	F	80	ARG	C-O	-7.21	1.15	1.24
1	F	37	ASP	C-O	-7.14	1.15	1.24
1	G	208	ASN	C-O	-7.08	1.15	1.24
1	C	161	SER	C-O	-7.07	1.15	1.23
1	G	222	GLN	C-O	-7.05	1.15	1.24
2	D	165	PRO	C-O	-7.02	1.16	1.24
1	G	205	ILE	C-O	-7.00	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	242	LYS	C-O	-6.92	1.16	1.24
1	C	39	LEU	C-O	-6.72	1.16	1.24
1	B	71	GLN	C-O	-6.71	1.16	1.24
1	F	222	GLN	C-O	-6.71	1.16	1.24
1	G	82	ALA	N-CA	-6.66	1.38	1.46
1	C	121	ARG	C-O	-6.54	1.16	1.24
1	F	83	PHE	C-O	-6.48	1.16	1.24
1	F	38	ARG	C-O	-6.43	1.16	1.24
1	F	82	ALA	C-O	-6.28	1.16	1.24
2	H	83	THR	C-O	-6.24	1.16	1.24
1	C	122	ASP	C-O	-6.19	1.15	1.24
2	H	70	TYR	C-O	-6.16	1.16	1.24
2	E	93	ALA	C-O	-6.15	1.16	1.23
2	H	163	PHE	C-O	-6.11	1.15	1.23
1	C	34	GLU	C-O	-6.10	1.17	1.24
1	C	70	GLU	C-O	-6.09	1.17	1.24
1	C	33	ILE	C-O	-5.96	1.17	1.24
1	G	82	ALA	CA-C	-5.95	1.45	1.52
2	H	93	ALA	C-O	-5.89	1.16	1.23
2	E	196	SER	C-O	-5.87	1.16	1.23
1	C	71	GLN	C-O	-5.82	1.17	1.24
1	G	29	GLU	C-O	-5.80	1.17	1.24
1	G	29	GLU	N-CA	-5.80	1.39	1.46
1	B	243	SER	C-O	-5.79	1.17	1.24
2	E	165	PRO	C-O	-5.76	1.18	1.24
1	F	35	ALA	C-O	-5.76	1.17	1.24
1	F	84	GLU	C-O	-5.73	1.16	1.23
1	B	241	SER	C-O	-5.71	1.17	1.24
1	B	275	THR	C-O	-5.68	1.17	1.24
2	E	166	PRO	C-O	-5.64	1.17	1.23
1	G	251	ASP	C-O	-5.62	1.16	1.23
2	E	195	TRP	C-O	-5.61	1.16	1.23
1	B	282	ILE	C-O	-5.59	1.17	1.24
1	B	283	LEU	C-O	-5.58	1.17	1.24
2	E	62	GLU	C-O	-5.45	1.17	1.23
2	I	55	CYS	C-O	-5.37	1.17	1.23
1	F	223	GLN	C-O	-5.35	1.17	1.24
2	H	164	GLU	C-O	-5.29	1.18	1.23
1	G	82	ALA	C-O	-5.25	1.17	1.24
2	H	165	PRO	C-O	-5.25	1.18	1.24
1	C	38	ARG	C-O	-5.20	1.18	1.24
2	I	183	GLY	C-O	-5.20	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	ASP	C-O	-5.16	1.18	1.24
1	C	40	ASP	C-O	-5.13	1.18	1.24
1	B	97	SER	C-O	-5.13	1.18	1.24
2	I	166	PRO	C-O	-5.08	1.18	1.23
1	B	281	ALA	C-O	-5.08	1.18	1.24
1	C	121	ARG	CA-C	-5.05	1.46	1.52
2	E	197	ASP	C-O	-5.04	1.17	1.23
1	G	249	ARG	CA-C	-5.04	1.45	1.52
2	E	197	ASP	N-CA	-5.01	1.40	1.46
1	G	80	ARG	C-O	-5.01	1.18	1.24
2	D	54	ASN	C-O	-5.00	1.17	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	199	LEU	N-CA-C	9.82	121.75	111.14
2	H	95	GLY	N-CA-C	8.78	127.32	111.34
1	C	29	GLU	CB-CA-C	-8.58	97.41	110.88
1	G	213	LYS	CA-C-N	-8.19	107.25	121.66
1	G	213	LYS	C-N-CA	-8.19	107.25	121.66
1	G	213	LYS	CG-CD-CE	8.03	129.77	111.30
2	H	64	CYS	CA-CB-SG	7.83	132.41	114.40
1	C	80	ARG	NE-CZ-NH1	-7.49	114.01	121.50
1	B	33	ILE	CA-CB-CG1	-7.46	97.72	110.40
2	E	99	GLY	N-CA-C	6.89	123.83	110.73
1	G	160	GLN	N-CA-CB	6.50	119.65	109.83
1	G	213	LYS	CA-CB-CG	6.44	126.97	114.10
2	H	63	CYS	CB-CA-C	6.36	120.24	109.50
1	G	242	LYS	CB-CA-C	5.89	121.48	110.70
1	F	80	ARG	N-CA-C	5.86	117.75	111.36
2	H	57	THR	CA-C-N	5.83	132.19	121.70
2	H	57	THR	C-N-CA	5.83	132.19	121.70
2	E	98	GLY	N-CA-C	-5.72	105.44	112.77
2	E	96	GLY	N-CA-C	5.63	120.76	113.27
1	C	29	GLU	N-CA-CB	5.52	118.01	110.01
1	G	242	LYS	CA-CB-CG	5.50	125.11	114.10
2	E	56	ASN	CA-C-N	5.38	131.39	121.70
2	E	56	ASN	C-N-CA	5.38	131.39	121.70
2	D	165	PRO	CA-C-N	5.34	125.26	119.76
2	D	165	PRO	C-N-CA	5.34	125.26	119.76
2	H	57	THR	N-CA-C	5.24	117.27	109.25
2	E	94	GLU	N-CA-C	5.22	116.66	111.07

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	B	2072	0	2095	12	0
1	C	2059	0	2079	10	0
1	F	2096	0	2120	16	0
1	G	2079	0	2104	19	0
2	D	1124	0	1039	5	0
2	E	1149	0	1061	7	0
2	H	1131	0	1049	6	0
2	I	1128	0	1045	7	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	F	13	0	5	0	0
3	G	13	0	5	0	0
4	B	167	0	0	0	0
4	C	186	0	0	2	0
4	D	75	0	0	0	0
4	E	87	0	0	1	2
4	F	255	0	0	3	0
4	G	220	0	0	0	0
4	H	81	0	0	0	0
4	I	100	0	0	0	2
All	All	14061	0	12612	71	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 (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)
2:H:64:CYS:SG	2:H:157:CYS:SG	1.40	1.33
1:G:203:CYS:CB	1:G:289:CYS:SG	2.32	1.17
1:G:203:CYS:SG	1:G:289:CYS:SG	1.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:ASN:HD22	1:G:81:ASN:HD21	1.13	0.95
1:G:206:LEU:O	1:G:216:LYS:HE2	1.70	0.89
2:H:64:CYS:SG	2:H:157:CYS:CB	2.60	0.89
1:G:203:CYS:SG	1:G:289:CYS:CB	2.62	0.88
1:F:81:ASN:HD22	1:G:81:ASN:ND2	1.74	0.85
1:F:80:ARG:HE	1:G:81:ASN:HB3	1.49	0.78
2:D:56:ASN:O	2:D:56:ASN:ND2	2.19	0.75
1:F:34:GLU:OE1	4:F:401:HOH:O	2.05	0.74
1:B:86:SER:O	1:B:90:SER:OG	2.07	0.72
1:C:81:ASN:HD21	1:B:77:ALA:HA	1.58	0.67
1:F:81:ASN:ND2	1:G:81:ASN:ND2	2.42	0.66
1:G:206:LEU:O	1:G:216:LYS:CE	2.43	0.66
1:F:34:GLU:HG3	1:F:38:ARG:HH12	1.61	0.66
1:G:196:ASP:OD1	1:G:288:LYS:HE2	1.98	0.64
2:H:58:GLU:HG2	2:H:58:GLU:O	1.98	0.63
1:G:205:ILE:O	1:G:216:LYS:HE3	2.00	0.62
1:G:203:CYS:CA	1:G:289:CYS:SG	2.89	0.60
1:B:242:LYS:HG2	1:B:259:GLN:OE1	2.02	0.60
1:F:34:GLU:HG3	1:F:38:ARG:NH1	2.15	0.60
1:C:81:ASN:ND2	1:B:77:ALA:HA	2.17	0.58
2:E:57:THR:HG22	2:E:57:THR:O	2.02	0.58
1:B:94:GLN:NE2	1:B:94:GLN:HA	2.18	0.58
1:C:76:ALA:O	1:C:80:ARG:HG3	2.03	0.58
2:I:182:LEU:CB	2:I:184:LEU:HD12	2.35	0.57
1:F:80:ARG:HD2	1:G:80:ARG:O	2.05	0.56
1:F:55:GLN:OE1	1:G:55:GLN:OE1	2.25	0.55
1:F:241:SER:OG	1:F:259[A]:GLN:HG2	2.06	0.54
2:H:82:SER:O	2:H:82:SER:OG	2.25	0.53
1:B:208:ASN:OD1	1:B:210:THR:HB	2.09	0.53
1:F:81:ASN:ND2	1:G:81:ASN:HD21	1.94	0.53
1:C:28:SER:N	4:C:405:HOH:O	2.43	0.52
2:I:180:ASP:OD1	2:I:186:LYS:NZ	2.38	0.51
2:I:185:ASN:O	2:I:188:ASP:HB2	2.10	0.51
2:I:182:LEU:HB3	2:I:184:LEU:HD12	1.93	0.50
1:C:287:ASN:OD1	1:C:288:LYS:HG2	2.13	0.48
1:B:191:ALA:HB2	1:B:278:GLU:HA	1.96	0.48
2:D:56:ASN:ND2	2:D:56:ASN:C	2.72	0.48
1:G:203:CYS:HA	1:G:289:CYS:SG	2.54	0.48
1:B:71:GLN:CD	1:B:152:ASP:OD1	2.58	0.47
2:I:182:LEU:HB2	2:I:184:LEU:HD12	1.98	0.46
1:F:188:TYR:HE1	4:F:406:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:49:GLN:OE1	2:H:69:ARG:NH1	2.49	0.45
2:E:117:ALA:HB2	2:E:149:ASP:HB3	1.98	0.45
1:C:191:ALA:HB2	1:C:278:GLU:HA	1.98	0.45
1:B:109:PRO:HB2	1:B:185:LEU:HD11	1.99	0.44
2:D:199:LEU:HG	2:D:200:GLU:HG2	1.99	0.44
1:G:187:GLY:O	1:G:278:GLU:HG2	2.18	0.44
1:C:55:GLN:OE1	1:B:55:GLN:OE1	2.35	0.44
2:D:83:THR:O	2:D:194:THR:HA	2.18	0.43
1:F:208:ASN:OD1	1:F:210:THR:HB	2.18	0.43
1:F:223:GLN:O	1:F:223:GLN:HG3	2.18	0.43
1:G:109:PRO:HB2	1:G:185:LEU:HD11	2.01	0.43
2:E:62:GLU:O	2:E:62:GLU:HG2	2.19	0.43
2:E:87:LEU:O	2:E:190:GLN:HA	2.18	0.43
2:E:185:ASN:ND2	2:E:187:ASP:HB2	2.34	0.43
1:F:199:HIS:HE1	4:F:475:HOH:O	2.02	0.43
2:I:117:ALA:HB2	2:I:149:ASP:HB3	2.01	0.42
1:B:33:ILE:HD11	2:D:49:GLN:HG3	2.00	0.42
2:H:64:CYS:SG	2:H:157:CYS:CA	3.08	0.42
1:F:187:GLY:O	1:F:278:GLU:HG2	2.20	0.41
1:C:105:ARG:NH1	4:C:413:HOH:O	2.52	0.41
1:G:80:ARG:HH11	1:G:80:ARG:HD2	1.60	0.41
1:C:187:GLY:O	1:C:278:GLU:HG2	2.21	0.41
1:B:100:ARG:H	1:B:100:ARG:HG3	1.60	0.41
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.87	0.41
2:E:57:THR:HA	4:E:318:HOH:O	2.19	0.41
2:I:81:GLY:O	2:I:196:SER:HB3	2.22	0.40
2:E:185:ASN:HD21	2:E:187:ASP:HB2	1.86	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)
4:E:335:HOH:O	4:I:346:HOH:O[1_554]	1.77	0.43
4:E:353:HOH:O	4:I:302:HOH:O[1_554]	2.04	0.16

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	B	262/278 (94%)	258 (98%)	4 (2%)	0	100	100
1	C	260/278 (94%)	256 (98%)	4 (2%)	0	100	100
1	F	265/278 (95%)	261 (98%)	4 (2%)	0	100	100
1	G	263/278 (95%)	257 (98%)	6 (2%)	0	100	100
2	D	147/175 (84%)	143 (97%)	4 (3%)	0	100	100
2	E	153/175 (87%)	149 (97%)	4 (3%)	0	100	100
2	H	148/175 (85%)	143 (97%)	5 (3%)	0	100	100
2	I	148/175 (85%)	143 (97%)	5 (3%)	0	100	100
All	All	1646/1812 (91%)	1610 (98%)	36 (2%)	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	B	232/244 (95%)	227 (98%)	5 (2%)	45	34
1	C	231/244 (95%)	231 (100%)	0	100	100
1	F	235/244 (96%)	235 (100%)	0	100	100
1	G	233/244 (96%)	232 (100%)	1 (0%)	84	83
2	D	122/142 (86%)	121 (99%)	1 (1%)	73	70
2	E	125/142 (88%)	124 (99%)	1 (1%)	73	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	123/142 (87%)	121 (98%)	2 (2%)	55	47
2	I	123/142 (87%)	123 (100%)	0	100	100
All	All	1424/1544 (92%)	1414 (99%)	10 (1%)	76	73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88	VAL
1	B	90	SER
1	B	91	GLU
1	B	96	GLU
1	B	249	ARG
2	D	56	ASN
2	E	62	GLU
1	G	29	GLU
2	H	58	GLU
2	H	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	C	246	HIS
1	C	250	ASN
1	B	71	GLN
1	B	94	GLN
2	D	56	ASN
2	D	132	HIS
2	E	43	GLN
2	E	90	ASN
2	E	132	HIS
2	E	162	ASN
2	E	185	ASN
2	E	190	GLN
1	G	81	ASN
1	G	201	ASN
2	H	141	ASN
2	H	162	ASN
2	I	162	ASN

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](#)

4 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
3	CIT	G	301	-	12,12,12	1.00	0	17,17,17	1.41	2 (11%)
3	CIT	C	301	-	12,12,12	0.96	0	17,17,17	1.63	3 (17%)
3	CIT	F	301	-	12,12,12	1.02	0	17,17,17	1.76	3 (17%)
3	CIT	B	301	-	12,12,12	2.44	7 (58%)	17,17,17	4.03	9 (52%)

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
3	CIT	G	301	-	-	2/16/16/16	-
3	CIT	C	301	-	-	7/16/16/16	-
3	CIT	F	301	-	-	5/16/16/16	-
3	CIT	B	301	-	-	10/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	CIT	C4-C3	-4.34	1.48	1.54
3	B	301	CIT	O2-C1	-3.90	1.17	1.30
3	B	301	CIT	O4-C5	-3.21	1.20	1.30
3	B	301	CIT	C2-C3	-2.94	1.50	1.54
3	B	301	CIT	C3-C6	2.49	1.56	1.53
3	B	301	CIT	O7-C3	-2.45	1.38	1.43
3	B	301	CIT	O6-C6	-2.12	1.22	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	CIT	C4-C3-C6	-8.34	91.59	110.03
3	B	301	CIT	O7-C3-C6	-7.57	98.21	108.96
3	B	301	CIT	O6-C6-C3	7.08	126.73	113.14
3	B	301	CIT	O7-C3-C4	6.08	123.24	109.38
3	C	301	CIT	O6-C6-C3	4.41	121.61	113.14
3	F	301	CIT	O6-C6-C3	4.32	121.42	113.14
3	B	301	CIT	C2-C3-C6	-4.05	101.08	110.03
3	B	301	CIT	O6-C6-O5	-3.90	111.37	123.86
3	G	301	CIT	O6-C6-C3	3.51	119.87	113.14
3	B	301	CIT	O7-C3-C2	3.45	117.25	109.38
3	F	301	CIT	O7-C3-C6	-3.40	104.14	108.96
3	B	301	CIT	C4-C3-C2	2.30	115.22	109.31
3	B	301	CIT	C3-C2-C1	2.25	120.08	113.92
3	C	301	CIT	O4-C5-C4	2.16	121.20	114.35
3	F	301	CIT	O2-C1-C2	2.15	121.16	114.35
3	C	301	CIT	O2-C1-C2	2.14	121.13	114.35
3	G	301	CIT	O2-C1-O1	-2.08	117.98	123.33

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	CIT	O7-C3-C6-O5
3	B	301	CIT	O7-C3-C6-O6
3	B	301	CIT	O7-C3-C4-C5
3	B	301	CIT	C2-C3-C6-O5
3	F	301	CIT	C4-C3-C6-O6
3	F	301	CIT	O7-C3-C6-O6
3	B	301	CIT	C2-C3-C6-O6
3	B	301	CIT	C4-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	301	CIT	C4-C3-C6-O5
3	F	301	CIT	C2-C3-C6-O6
3	B	301	CIT	C1-C2-C3-C4
3	C	301	CIT	C2-C3-C6-O5
3	C	301	CIT	C2-C3-C6-O6
3	C	301	CIT	C4-C3-C6-O5
3	C	301	CIT	C4-C3-C6-O6
3	F	301	CIT	C2-C3-C6-O5
3	B	301	CIT	O2-C1-C2-C3
3	C	301	CIT	C3-C4-C5-O4
3	C	301	CIT	C3-C4-C5-O3
3	B	301	CIT	O1-C1-C2-C3
3	F	301	CIT	O7-C3-C6-O5
3	C	301	CIT	O1-C1-C2-C3
3	G	301	CIT	O1-C1-C2-C3
3	G	301	CIT	O2-C1-C2-C3

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	B	264/278 (94%)	0.32	16 (6%) 27 25	21, 36, 64, 85	0
1	C	262/278 (94%)	0.29	10 (3%) 44 44	21, 36, 60, 92	0
1	F	266/278 (95%)	-0.00	7 (2%) 57 57	15, 30, 61, 90	1 (0%)
1	G	265/278 (95%)	0.22	16 (6%) 27 26	18, 33, 66, 87	0
2	D	153/175 (87%)	0.47	9 (5%) 28 27	27, 42, 71, 81	0
2	E	157/175 (89%)	0.84	15 (9%) 13 12	29, 48, 76, 118	0
2	H	154/175 (88%)	0.47	9 (5%) 29 27	26, 42, 70, 93	0
2	I	154/175 (88%)	0.47	10 (6%) 25 23	25, 41, 69, 88	0
All	All	1675/1812 (92%)	0.34	92 (5%) 30 29	15, 38, 67, 118	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	CYS	6.3
2	E	98	GLY	6.0
2	I	57	THR	4.8
1	C	203	CYS	4.6
2	H	99	GLY	4.4
1	F	291	LEU	4.3
2	E	189	GLY	4.1
2	E	96	GLY	4.0
1	G	289	CYS	3.9
2	D	66	ASN	3.9
2	D	96	GLY	3.8
2	H	96	GLY	3.8
2	I	99	GLY	3.7
1	G	290	THR	3.4
2	H	63	CYS	3.3
2	D	99	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	I	95	GLY	3.2
1	G	203	CYS	3.2
2	H	55	CYS	3.2
1	B	26	GLY	3.1
2	I	96	GLY	3.1
2	I	199	LEU	3.0
2	H	95	GLY	3.0
1	G	206	LEU	3.0
2	E	188	ASP	3.0
1	F	213	LYS	2.9
2	E	67	GLY	2.9
1	G	209	THR	2.9
2	D	84	ARG	2.9
1	G	147	MET	2.9
2	D	41	THR	2.8
2	I	189	GLY	2.8
2	E	57	THR	2.8
2	I	61	SER	2.8
1	G	286	ALA	2.8
1	B	100	ARG	2.7
1	C	31	ALA	2.6
1	C	30	ALA	2.6
2	E	97	ASP	2.6
1	C	29	GLU	2.6
2	D	67	GLY	2.6
1	B	38	ARG	2.6
1	G	207	THR	2.6
2	I	138	GLY	2.5
2	H	56	ASN	2.5
1	F	204	HIS	2.5
2	E	55	CYS	2.5
2	I	184	LEU	2.5
2	H	41	THR	2.5
1	C	122	ASP	2.5
2	E	63	CYS	2.4
2	E	41	THR	2.4
1	C	121	ARG	2.4
1	B	28	SER	2.4
1	G	214	SER	2.4
2	H	199	LEU	2.4
1	F	211	LEU	2.3
1	B	210	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	288	LYS	2.3
1	B	97	SER	2.3
1	F	210	THR	2.3
2	E	95	GLY	2.3
2	E	200	GLU	2.3
2	D	56	ASN	2.3
1	F	26	GLY	2.2
1	G	26	GLY	2.2
1	B	288	LYS	2.2
1	B	93	LEU	2.2
2	H	84	ARG	2.2
1	B	214	SER	2.1
1	B	27	LYS	2.1
1	C	97	SER	2.1
1	C	209	THR	2.1
1	C	68	PRO	2.1
1	G	211	LEU	2.1
1	G	219	ASN	2.1
1	B	252	ILE	2.1
1	G	242	LYS	2.1
2	D	95	GLY	2.1
2	I	56	ASN	2.1
1	B	289	CYS	2.1
1	B	96	GLU	2.0
1	G	213	LYS	2.0
2	D	200	GLU	2.0
1	G	285	HIS	2.0
1	B	88	VAL	2.0
1	B	30	ALA	2.0
2	E	61	SER	2.0
1	F	209	THR	2.0
1	B	287	ASN	2.0
2	E	54	ASN	2.0
2	E	99	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIT	B	301	13/13	0.90	0.12	44,57,73,73	0
3	CIT	G	301	13/13	0.90	0.10	38,47,52,52	0
3	CIT	F	301	13/13	0.91	0.09	39,45,54,54	0
3	CIT	C	301	13/13	0.94	0.07	31,35,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.