



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2019 – 02:30 PM EST

PDB ID : 6FPG  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

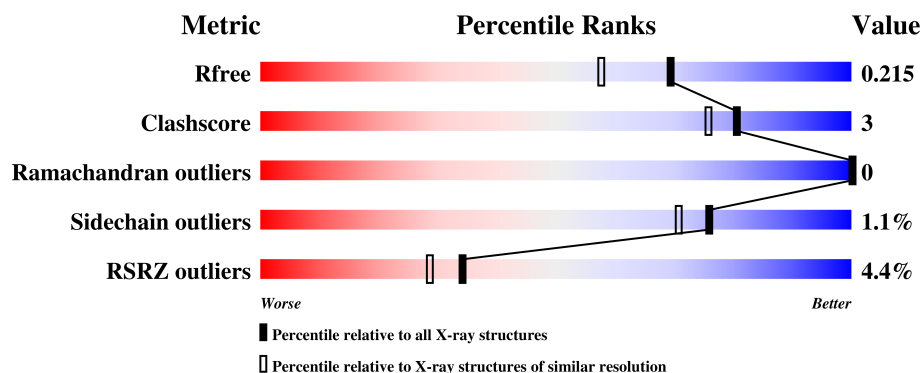
# 1 Overall quality at a glance

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))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>86% 8% • 5%</div> </div>
1	C	278	<div> <div>%</div> <div>87% 6% 6%</div> </div>
1	F	278	<div> <div>3%</div> <div>90% 6% •</div> </div>
1	G	278	<div> <div>3%</div> <div>89% 6% • 5%</div> </div>
2	D	175	<div> <div>6%</div> <div>83% • • 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	175	<div><div></div><div>11%</div><div>84%</div><div>5%</div><div>10%</div></div>
2	H	175	<div><div></div><div>5%</div><div>82%</div><div>5%</div><div>12%</div></div>
2	I	175	<div><div></div><div>5%</div><div>82%</div><div>6%</div><div>12%</div></div>

## 2 Entry composition

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
1	C	262	Total	C	N	O	S	0	0	0
			2059	1298	365	393	3			
1	B	264	Total	C	N	O	S	0	0	0
			2072	1306	368	395	3			
1	F	266	Total	C	N	O	S	0	1	0
			2096	1321	372	400	3			
1	G	265	Total	C	N	O	S	0	0	0
			2079	1310	369	397	3			

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

There are 36 discrepancies between the modelled and reference sequences:

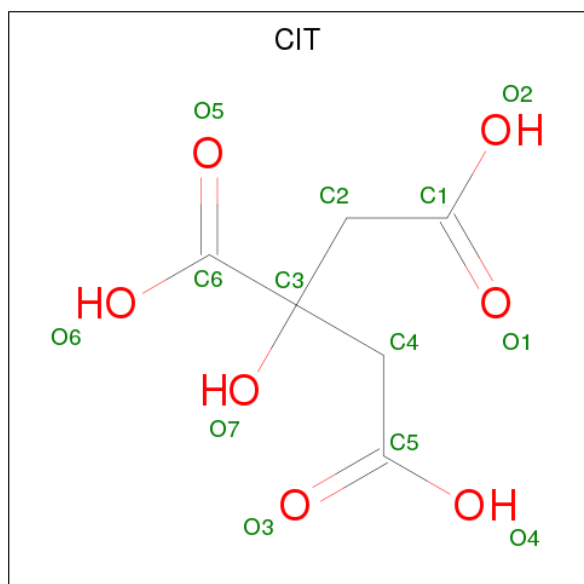
Chain	Residue	Modelled	Actual	Comment	Reference
D	32	MET	-	initiating methionine	UNP A0A1D6GNR3
D	199	LEU	-	expression tag	UNP A0A1D6GNR3
D	200	GLU	-	expression tag	UNP A0A1D6GNR3
D	201	HIS	-	expression tag	UNP A0A1D6GNR3
D	202	HIS	-	expression tag	UNP A0A1D6GNR3
D	203	HIS	-	expression tag	UNP A0A1D6GNR3
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 (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



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

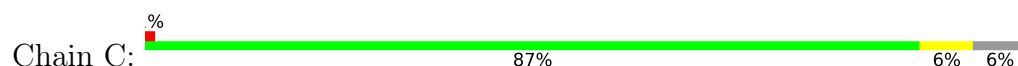
- Molecule 4 is water.

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

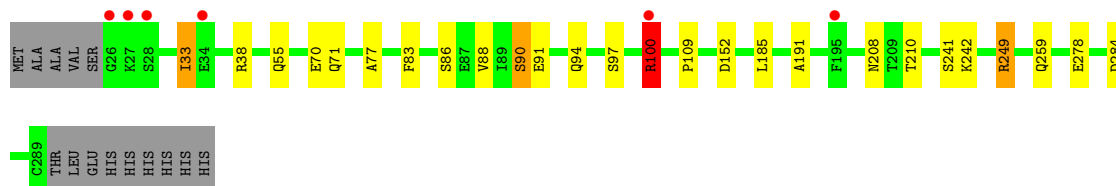
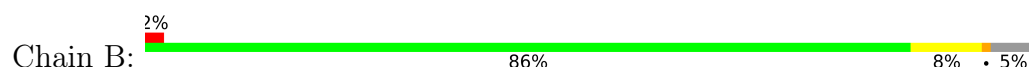
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

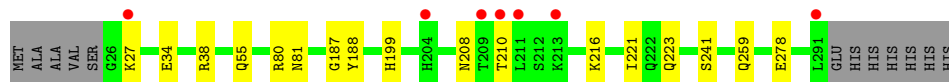
- Molecule 1: Chromosome 16, whole genome shotgun sequence



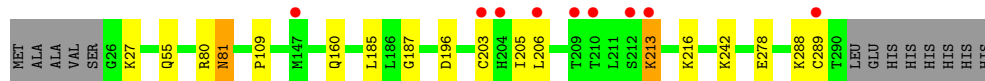
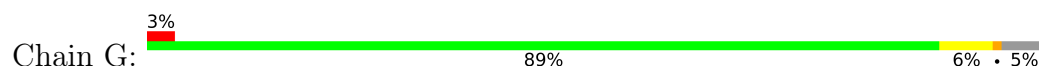
- Molecule 1: Chromosome 16, whole genome shotgun sequence



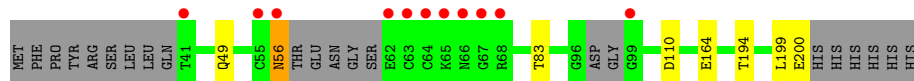
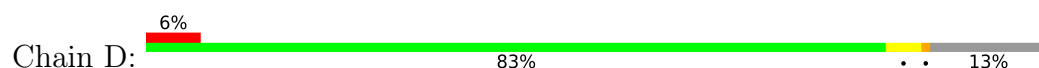
- Molecule 1: Chromosome 16, whole genome shotgun sequence



- Molecule 1: Chromosome 16, whole genome shotgun sequence

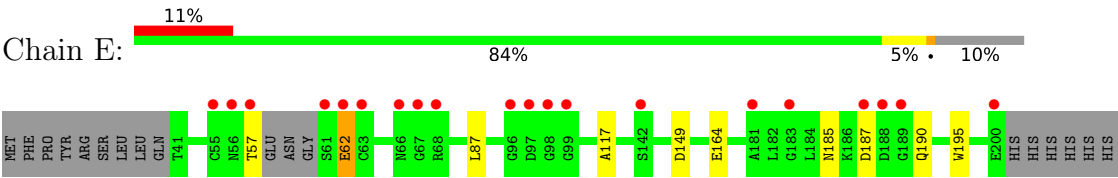


- Molecule 2: Ripening-related protein 3

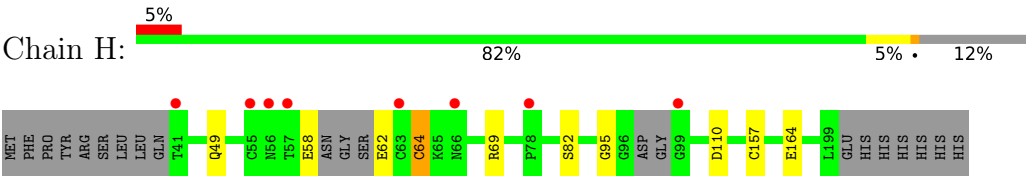




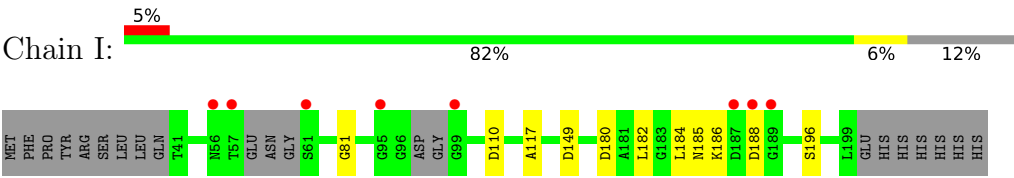
● Molecule 2: Ripening-related protein 3



● Molecule 2: Ripening-related protein 3



● Molecule 2: Ripening-related protein 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.186 , 0.216 0.187 , 0.215	Depositor DCC
$R_{free}$ test set	8386 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14061	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.71	2/2111 (0.1%)	0.75	5/2872 (0.2%)
1	C	0.61	0/2098	0.71	5/2856 (0.2%)
1	F	0.67	2/2135 (0.1%)	0.62	0/2905
1	G	0.63	1/2118 (0.0%)	0.72	6/2882 (0.2%)
2	D	0.79	2/1143 (0.2%)	0.70	0/1545
2	E	0.81	2/1169 (0.2%)	0.76	0/1582
2	H	0.78	2/1150 (0.2%)	0.75	2/1555 (0.1%)
2	I	0.62	0/1147	0.70	3/1551 (0.2%)
All	All	0.69	11/13071 (0.1%)	0.71	21/17748 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	164	GLU	CD-OE1	-8.01	1.16	1.25
1	B	241	SER	CB-OG	-6.73	1.33	1.42
2	H	164	GLU	CD-OE1	-6.53	1.18	1.25
2	D	164	GLU	CD-OE2	-5.98	1.19	1.25
2	E	164	GLU	CD-OE1	-5.83	1.19	1.25
1	B	70	GLU	C-O	-5.53	1.12	1.23
1	F	216	LYS	CD-CE	5.40	1.64	1.51
2	E	195	TRP	CE3-CZ3	-5.26	1.29	1.38
2	H	164	GLU	CD-OE2	-5.25	1.19	1.25
1	G	81	ASN	CA-C	-5.19	1.39	1.52
1	F	221	ILE	C-O	-5.02	1.13	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	ARG	NE-CZ-NH1	-12.58	114.01	120.30
2	H	64	CYS	CA-CB-SG	10.23	132.41	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	B	33	ILE	CA-CB-CG1	-6.99	97.72	111.00
1	C	121	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	38	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	C	29	GLU	CB-CA-C	-6.49	97.41	110.40
2	I	110	ASP	CB-CG-OD2	-6.49	112.45	118.30
1	C	72	ASP	CB-CG-OD1	6.41	124.07	118.30
1	G	213	LYS	CA-CB-CG	6.17	126.97	113.40
1	G	213	LYS	CG-CD-CE	5.96	129.77	111.90
1	B	83	PHE	C-N-CA	-5.93	106.87	121.70
1	G	213	LYS	C-N-CA	-5.78	107.25	121.70
2	H	95	GLY	N-CA-C	5.69	127.32	113.10
1	G	242	LYS	CB-CA-C	5.54	121.48	110.40
2	I	110	ASP	CB-CA-C	-5.33	99.73	110.40
1	G	242	LYS	CA-CB-CG	5.32	125.11	113.40
1	B	249	ARG	NE-CZ-NH1	-5.31	117.64	120.30
2	I	110	ASP	CB-CG-OD1	5.04	122.84	118.30
1	G	160	GLN	N-CA-CB	5.03	119.65	110.60
1	C	72	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	13	0
1	C	2059	0	2079	11	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	73	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 (73) 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
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:ND2	2:D:56:ASN:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:THR:O	2:E:57:THR:HG22	2.02	0.58
1:B:94:GLN:HA	1:B:94:GLN:NE2	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: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
1:G:203:CYS:HA	1:G:289:CYS:SG	2.54	0.48
2:I:180:ASP:OD1	2:I:186:LYS:NZ	2.38	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
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:D:56:ASN:C	2:D:56:ASN:ND2	2.72	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
1:B:71:GLN:CD	1:B:152:ASP:OD1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLU:HA	1:C:90:SER:HG	1.85	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:HG3	1:B:100:ARG:H	1.60	0.41
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.87	0.41
1:B:97:SER:HG	1:B:284:ASP:CG	2.24	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

### 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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1646/1812 (91%)	1610 (98%)	36 (2%)	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	B	232/244 (95%)	227 (98%)	5 (2%)	55	42
1	C	231/244 (95%)	229 (99%)	2 (1%)	81	77
1	F	235/244 (96%)	234 (100%)	1 (0%)	92	91
1	G	233/244 (96%)	231 (99%)	2 (1%)	81	77
2	D	122/142 (86%)	120 (98%)	2 (2%)	65	57
2	E	125/142 (88%)	124 (99%)	1 (1%)	83	80
2	H	123/142 (87%)	121 (98%)	2 (2%)	65	57
2	I	123/142 (87%)	123 (100%)	0	100	100
All	All	1424/1544 (92%)	1409 (99%)	15 (1%)	76	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	34	GLU
1	C	160	GLN
1	B	88	VAL
1	B	90	SER
1	B	91	GLU
1	B	100	ARG
1	B	249	ARG
2	D	56	ASN
2	D	110	ASP
2	E	62	GLU
1	F	27	LYS
1	G	27	LYS

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Mol	Chain	Res	Type
1	G	213	LYS
2	H	62	GLU
2	H	110	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	B	94	GLN
1	B	246	HIS
2	D	56	ASN
2	E	43	GLN
2	E	66	ASN
2	E	185	ASN
1	G	81	ASN
1	G	267	GLN
2	H	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 carbohydrates 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	B	301	-	3,12,12	3.44	3 (100%)	3,17,17	2.67	3 (100%)
3	CIT	C	301	-	3,12,12	1.24	0	3,17,17	2.28	2 (66%)
3	CIT	F	301	-	3,12,12	1.10	0	3,17,17	1.57	1 (33%)
3	CIT	G	301	-	3,12,12	1.08	0	3,17,17	1.54	0

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	B	301	-	-	0/6/16/16	0/0/0/0
3	CIT	C	301	-	-	0/6/16/16	0/0/0/0
3	CIT	F	301	-	-	0/6/16/16	0/0/0/0
3	CIT	G	301	-	-	0/6/16/16	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	CIT	C4-C3	-4.23	1.48	1.54
3	B	301	CIT	C2-C3	-3.04	1.50	1.54
3	B	301	CIT	O7-C3	-2.91	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	CIT	C3-C2-C1	-3.12	110.26	114.95
3	F	301	CIT	C3-C4-C5	-2.57	111.10	114.95
3	C	301	CIT	C3-C4-C5	-2.39	111.36	114.95
3	B	301	CIT	C3-C4-C5	2.16	118.19	114.95
3	B	301	CIT	C4-C3-C2	2.23	115.22	109.70
3	B	301	CIT	C3-C2-C1	3.42	120.08	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	264/278 (94%)	-0.02	6 (2%) 60 56	21, 36, 64, 85	0
1	C	262/278 (94%)	0.04	4 (1%) 73 70	21, 36, 60, 92	0
1	F	266/278 (95%)	0.14	7 (2%) 56 51	19, 30, 61, 90	0
1	G	265/278 (95%)	0.13	9 (3%) 45 40	18, 33, 66, 87	0
2	D	153/175 (87%)	0.10	11 (7%) 15 12	27, 43, 71, 81	0
2	E	157/175 (89%)	0.53	20 (12%) 3 2	29, 48, 76, 118	0
2	H	154/175 (88%)	0.03	8 (5%) 27 22	26, 42, 70, 93	0
2	I	154/175 (88%)	0.06	8 (5%) 27 22	25, 41, 69, 88	0
All	All	1675/1812 (92%)	0.11	73 (4%) 34 29	18, 38, 67, 118	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	98	GLY	12.7
2	E	97	ASP	6.5
2	D	66	ASN	5.8
2	E	189	GLY	5.6
2	I	189	GLY	4.7
2	H	55	CYS	4.5
2	H	57	THR	4.4
2	H	56	ASN	4.4
1	G	213	LYS	4.2
1	F	291	LEU	4.2
1	G	289	CYS	4.1
2	D	55	CYS	4.0
2	D	56	ASN	3.9
2	E	188	ASP	3.8
2	E	56	ASN	3.7
2	E	96	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	61	SER	3.5
2	H	41	THR	3.5
1	F	27	LYS	3.5
2	H	66	ASN	3.3
1	B	28	SER	3.3
1	F	210	THR	3.3
1	F	213	LYS	3.2
2	E	57	THR	3.1
2	E	68	ARG	3.1
2	D	67	GLY	3.0
2	E	63	CYS	3.0
2	D	64	CYS	3.0
1	G	206	LEU	2.9
2	E	200	GLU	2.9
1	C	289	CYS	2.9
2	E	99	GLY	2.9
2	E	55	CYS	2.9
2	D	99	GLY	2.8
2	I	99	GLY	2.8
2	D	65	LYS	2.8
2	I	57	THR	2.8
1	F	204	HIS	2.8
2	D	68	ARG	2.8
2	E	187	ASP	2.6
2	E	67	GLY	2.6
2	I	187	ASP	2.6
2	E	62	GLU	2.6
2	I	56	ASN	2.6
2	H	99	GLY	2.6
2	D	62	GLU	2.6
1	C	30	ALA	2.5
1	F	211	LEU	2.5
2	D	41	THR	2.5
1	G	209	THR	2.5
2	H	78	PRO	2.4
1	B	26	GLY	2.4
1	G	210	THR	2.4
1	G	203	CYS	2.4
2	D	63	CYS	2.3
1	B	195	PHE	2.3
1	B	27	LYS	2.3
2	E	183	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	66	ASN	2.3
1	B	34	GLU	2.2
2	E	181	ALA	2.2
2	I	61	SER	2.2
1	C	29	GLU	2.2
1	G	147	MET	2.2
1	B	100	ARG	2.2
1	C	28	SER	2.2
2	I	95	GLY	2.2
1	F	209	THR	2.1
2	I	188	ASP	2.1
2	E	142	SER	2.1
1	G	204	HIS	2.1
1	G	212	SER	2.0
2	H	63	CYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CIT	B	301	13/13	0.87	0.17	44,57,73,73	0
3	CIT	F	301	13/13	0.89	0.15	39,45,54,54	0
3	CIT	G	301	13/13	0.90	0.15	38,47,52,52	0
3	CIT	C	301	13/13	0.92	0.11	31,35,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.