



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:18 AM GMT

PDB ID : 2CHS  
Title : CRYSTAL STRUCTURES OF THE MONOFUNCTIONAL CHORISMATE  
MUTASE FROM BACILLUS SUBTILIS AND ITS COMPLEX WITH A  
TRANSITION STATE ANALOG  
Authors : Chook, Y.M.; Ke, H.; Lipscomb, W.N.  
Deposited on : 1994-04-08  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

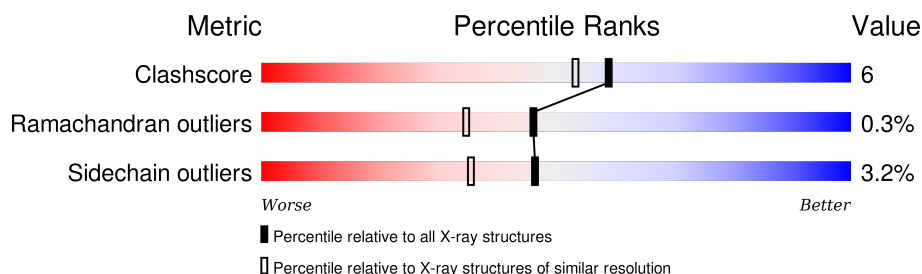
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)






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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	
1	C	127	
1	D	127	
1	E	127	
1	F	127	
1	G	127	

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Mol	Chain	Length	Quality of chain
1	H	127	 68%20%•10%
1	I	127	 76%13%•10%
1	J	127	 72%15%•10%
1	K	127	 70%18%•10%
1	L	127	 69%18%•10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14838 atoms, of which 3456 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 CHORISMATE MUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	B	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	C	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	D	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	E	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	F	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	G	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	H	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	I	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	J	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	K	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	L	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	49	Total	H	O	0	0
			147	98	49		
2	B	35	Total	H	O	0	0
			105	70	35		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	43	Total	H	O	0	0
			129	86	43		
2	D	56	Total	H	O	0	0
			168	112	56		
2	E	55	Total	H	O	0	0
			165	110	55		
2	F	32	Total	H	O	0	0
			96	64	32		
2	G	32	Total	H	O	0	0
			96	64	32		
2	H	10	Total	H	O	0	0
			30	20	10		
2	I	67	Total	H	O	0	0
			201	134	67		
2	J	35	Total	H	O	0	0
			105	70	35		
2	K	43	Total	H	O	0	0
			129	86	43		
2	L	65	Total	H	O	0	0
			195	130	65		

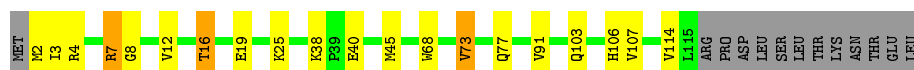
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

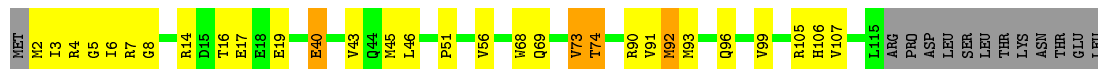
#### • Molecule 1: CHORISMATE MUTASE

Chain A: 



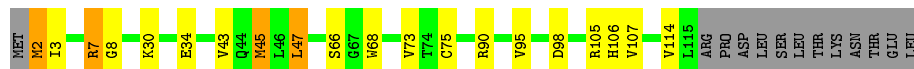
#### • Molecule 1: CHORISMATE MUTASE

Chain B: 




#### • Molecule 1: CHORISMATE MUTASE

Chain C: 



#### • Molecule 1: CHORISMATE MUTASE

Chain D: 



#### • Molecule 1: CHORISMATE MUTASE

Chain E: 

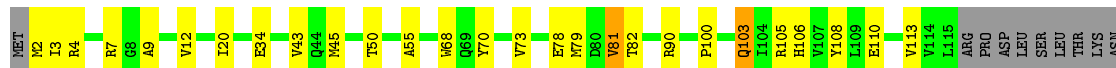


#### • Molecule 1: CHORISMATE MUTASE

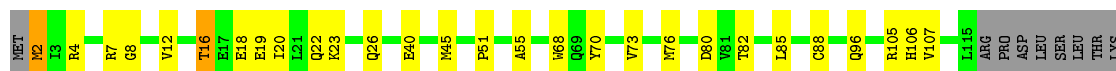
Chain F: 



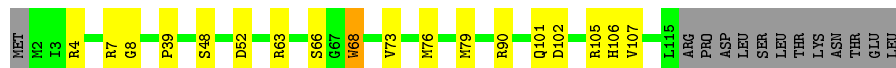
• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE



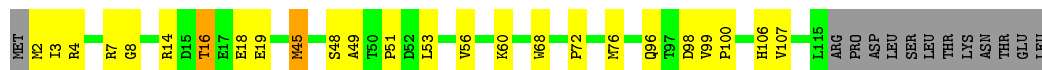
• Molecule 1: CHORISMATE MUTASE



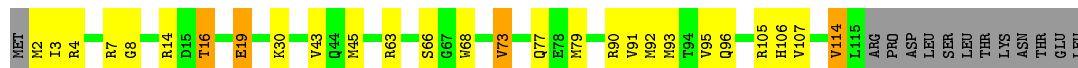
• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.40 Å 68.30 Å 102.80 Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.81	0/917	1.46	10/1240 (0.8%)
1	B	0.81	0/917	1.42	11/1240 (0.9%)
1	C	0.76	0/917	1.42	9/1240 (0.7%)
1	D	0.79	0/917	1.49	12/1240 (1.0%)
1	E	0.77	0/917	1.37	5/1240 (0.4%)
1	F	0.73	0/917	1.39	10/1240 (0.8%)
1	G	0.78	0/917	1.46	8/1240 (0.6%)
1	H	0.76	0/917	1.33	5/1240 (0.4%)
1	I	0.76	0/917	1.48	15/1240 (1.2%)
1	J	0.78	0/917	1.43	14/1240 (1.1%)
1	K	0.78	0/917	1.33	4/1240 (0.3%)
1	L	0.78	0/917	1.49	19/1240 (1.5%)
All	All	0.78	0/11004	1.42	122/14880 (0.8%)

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	90	ARG	NE-CZ-NH1	15.71	128.15	120.30
1	A	4	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	4	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	L	14	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	D	2	MET	CA-CB-CG	-10.34	95.71	113.30
1	I	105	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	E	90	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	I	4	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	G	90	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	I	90	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	B	68	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	J	90	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	F	7	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	I	68	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	68	TRP	CE2-CD2-CG	-8.31	100.65	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	68	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	D	105	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	G	68	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	I	68	TRP	CE2-CD2-CG	-8.08	100.84	107.30
1	B	68	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	L	14	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	L	68	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	I	73	VAL	CG1-CB-CG2	-7.84	98.36	110.90
1	B	4	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	68	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	C	68	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	D	77	GLN	CA-CB-CG	-7.70	96.47	113.40
1	H	68	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	F	73	VAL	CG1-CB-CG2	-7.62	98.71	110.90
1	F	68	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	J	68	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	G	4	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	K	68	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	D	68	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B	91	VAL	CG1-CB-CG2	-7.32	99.19	110.90
1	H	68	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	A	68	TRP	CG-CD2-CE3	7.19	140.37	133.90
1	C	68	TRP	CG-CD2-CE3	7.17	140.35	133.90
1	D	7	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	C	90	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	J	2	MET	CG-SD-CE	7.09	111.54	100.20
1	J	90	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	K	68	TRP	CD1-CG-CD2	7.07	111.95	106.30
1	J	2	MET	CA-CB-CG	-7.05	101.31	113.30
1	D	68	TRP	CD1-CG-CD2	7.04	111.94	106.30
1	A	77	GLN	CA-CB-CG	-6.98	98.05	113.40
1	B	4	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	F	7	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	C	2	MET	CG-SD-CE	6.90	111.24	100.20
1	E	68	TRP	CD1-CG-CD2	6.88	111.80	106.30
1	G	68	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	G	81	VAL	CG1-CB-CG2	-6.82	99.99	110.90
1	E	68	TRP	CE2-CD2-CG	-6.79	101.86	107.30
1	J	68	TRP	CG-CD2-CE3	6.77	139.99	133.90
1	D	2	MET	CG-SD-CE	6.71	110.94	100.20
1	A	68	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	F	68	TRP	CE2-CD2-CG	-6.66	101.97	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	68	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	F	90	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	D	73	VAL	CG1-CB-CG2	-6.59	100.36	110.90
1	J	22	GLN	CA-CB-CG	6.54	127.78	113.40
1	L	105	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	14	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	105	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	L	91	VAL	CG1-CB-CG2	-6.37	100.70	110.90
1	B	40	GLU	CA-CB-CG	6.37	127.42	113.40
1	I	68	TRP	CG-CD2-CE3	6.30	139.57	133.90
1	B	92	MET	CG-SD-CE	-6.25	90.19	100.20
1	J	7	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	F	79	MET	CA-CB-CG	6.20	123.84	113.30
1	L	4	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	E	63	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	I	105	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	7	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	J	68	TRP	CB-CG-CD1	-5.99	119.21	127.00
1	K	45	MET	CG-SD-CE	5.96	109.74	100.20
1	I	4	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	I	63	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	L	79	MET	CA-CB-CG	5.90	123.33	113.30
1	B	105	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	7	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	G	79	MET	CA-CB-CG	5.85	123.25	113.30
1	A	68	TRP	CB-CG-CD1	-5.85	119.40	127.00
1	H	68	TRP	CG-CD2-CE3	5.82	139.14	133.90
1	C	45	MET	CA-CB-CG	5.81	123.17	113.30
1	L	90	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	I	79	MET	CA-CB-CG	5.71	123.01	113.30
1	H	4	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	L	68	TRP	CG-CD2-CE3	5.69	139.02	133.90
1	L	114	VAL	N-CA-CB	-5.68	99.00	111.50
1	E	73	VAL	CG1-CB-CG2	-5.68	101.82	110.90
1	L	2	MET	CA-CB-CG	5.67	122.94	113.30
1	J	79	MET	CA-CB-CG	5.67	122.93	113.30
1	G	70	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	I	68	TRP	CB-CG-CD1	-5.58	119.75	127.00
1	D	2	MET	CB-CG-SD	5.58	129.13	112.40
1	B	99	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	A	73	VAL	CG1-CB-CG2	-5.51	102.09	110.90
1	I	68	TRP	CG-CD1-NE1	-5.35	104.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	105	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	45	MET	CA-CB-CG	5.30	122.31	113.30
1	L	77	GLN	CA-CB-CG	-5.30	101.74	113.40
1	J	73	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	L	63	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	L	68	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	K	4	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	L	114	VAL	CA-CB-CG2	-5.20	103.11	110.90
1	L	68	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	D	19	GLU	CA-CB-CG	5.16	124.75	113.40
1	F	2	MET	CA-CB-CG	5.15	122.06	113.30
1	D	68	TRP	CG-CD2-CE3	5.15	138.54	133.90
1	F	68	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	C	68	TRP	CB-CG-CD1	-5.10	120.37	127.00
1	I	102	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	103	GLN	CA-CB-CG	5.09	124.60	113.40
1	L	73	VAL	CG1-CB-CG2	-5.07	102.78	110.90
1	J	69	GLN	CA-CB-CG	5.07	124.56	113.40
1	I	52	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	7	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	90	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	H	105	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	J	19	GLU	CA-CB-CG	-5.04	102.32	113.40

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	905	201	936	11	0
1	B	905	201	936	11	0
1	C	905	201	936	13	0
1	D	905	201	936	13	0
1	E	905	201	936	12	0
1	F	905	201	936	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	905	201	936	12	1
1	H	905	201	936	16	1
1	I	905	201	936	7	0
1	J	905	201	936	12	0
1	K	905	201	936	11	0
1	L	905	201	936	11	0
2	A	49	98	0	0	0
2	B	35	70	0	0	0
2	C	43	86	0	0	0
2	D	56	112	0	0	0
2	E	55	110	0	0	0
2	F	32	64	0	0	0
2	G	32	64	0	0	0
2	H	10	20	0	0	0
2	I	67	134	0	0	1
2	J	35	70	0	0	0
2	K	43	86	0	0	1
2	L	65	130	0	0	0
All	All	11382	3456	11232	129	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 6.

All (129) 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:3:ILE:HD13	1:E:3:ILE:HD11	1.58	0.85
1:A:45:MET:HB3	1:A:73:VAL:HG12	1.61	0.82
1:G:45:MET:HB3	1:G:73:VAL:HG12	1.64	0.79
1:C:45:MET:HB3	1:C:73:VAL:HG12	1.63	0.79
1:G:7:ARG:H	1:G:106:HIS:HD2	1.31	0.78
1:F:7:ARG:H	1:F:106:HIS:HD2	1.33	0.77
1:K:7:ARG:H	1:K:106:HIS:HD2	1.31	0.77
1:C:2:MET:HG2	1:C:3:ILE:H	1.50	0.77
1:J:7:ARG:H	1:J:106:HIS:HD2	1.34	0.75
1:A:7:ARG:H	1:A:106:HIS:HD2	1.34	0.74
1:C:7:ARG:H	1:C:106:HIS:HD2	1.33	0.72
1:G:100:PRO:HG2	1:G:103:GLN:HG3	1.70	0.72
1:J:2:MET:HG2	1:J:3:ILE:H	1.52	0.71
1:L:7:ARG:H	1:L:106:HIS:HD2	1.38	0.71
1:H:12:VAL:HG12	1:H:23:LYS:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:16:THR:HG22	1:K:19:GLU:HB2	1.75	0.69
1:B:43:VAL:HG22	1:C:2:MET:HE3	1.79	0.65
1:D:7:ARG:H	1:D:106:HIS:HD2	1.46	0.63
1:G:20:ILE:HD12	1:G:55:ALA:HB3	1.81	0.62
1:B:7:ARG:H	1:B:106:HIS:HD2	1.47	0.61
1:D:2:MET:HG2	1:D:3:ILE:H	1.66	0.61
1:C:30:LYS:O	1:C:34:GLU:HG2	2.01	0.60
1:E:22:GLN:O	1:E:26:GLN:HG3	2.02	0.60
1:B:5:GLY:HA3	1:B:92:MET:HE1	1.83	0.59
1:B:96:GLN:HB2	1:C:2:MET:SD	2.43	0.59
1:B:8:GLY:HA2	1:B:107:VAL:O	2.03	0.58
1:G:3:ILE:HD11	1:H:2:MET:HE1	1.86	0.58
1:F:11:THR:HG21	1:F:111:LYS:HB2	1.85	0.58
1:D:16:THR:HG22	1:D:19:GLU:HB3	1.86	0.57
1:L:16:THR:HG22	1:L:19:GLU:HB2	1.87	0.57
1:J:2:MET:HG2	1:J:3:ILE:N	2.17	0.56
1:L:45:MET:HB3	1:L:73:VAL:HG12	1.88	0.56
1:I:8:GLY:HA2	1:I:107:VAL:O	2.05	0.56
1:F:45:MET:HB3	1:F:73:VAL:HG12	1.87	0.56
1:J:85:LEU:HD21	1:J:112:ALA:HA	1.89	0.55
1:H:7:ARG:H	1:H:106:HIS:HD2	1.55	0.55
1:D:2:MET:HE3	1:F:43:VAL:HG22	1.90	0.54
1:J:45:MET:HB3	1:J:73:VAL:HG12	1.88	0.54
1:D:85:LEU:HD23	1:D:88:CYS:SG	2.47	0.54
1:K:72:PRO:HB2	1:L:92:MET:HE1	1.90	0.54
1:J:7:ARG:H	1:J:106:HIS:CD2	2.20	0.54
1:H:7:ARG:H	1:H:106:HIS:CD2	2.27	0.53
1:D:3:ILE:CD1	1:E:3:ILE:HD11	2.36	0.53
1:C:2:MET:HG2	1:C:3:ILE:N	2.19	0.53
1:H:20:ILE:HD12	1:H:55:ALA:HB3	1.90	0.52
1:C:8:GLY:HA2	1:C:107:VAL:O	2.10	0.52
1:D:2:MET:HG2	1:D:3:ILE:N	2.24	0.52
1:E:45:MET:HB3	1:E:73:VAL:HG12	1.91	0.52
1:J:2:MET:HE3	1:L:43:VAL:HG22	1.91	0.51
1:I:39:PRO:HG3	1:I:68:TRP:NE1	2.25	0.51
1:H:51:PRO:HG3	1:H:80:ASP:HB2	1.92	0.51
1:G:3:ILE:HD12	1:G:43:VAL:HG21	1.93	0.50
1:K:14:ARG:NH2	1:K:16:THR:HG21	2.26	0.50
1:K:49:ALA:HB1	1:K:53:LEU:HD12	1.94	0.50
1:H:16:THR:HG23	1:H:19:GLU:CB	2.42	0.50
1:E:16:THR:HG22	1:E:19:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:NZ	1:A:25:LYS:HB3	2.27	0.49
1:D:2:MET:SD	1:F:96:GLN:HB2	2.53	0.49
1:H:12:VAL:HB	1:H:19:GLU:HG3	1.94	0.49
1:G:34:GLU:HB3	1:G:105:ARG:HD3	1.94	0.48
1:H:8:GLY:HA2	1:H:107:VAL:O	2.13	0.48
1:E:7:ARG:H	1:E:106:HIS:HD2	1.61	0.48
1:J:2:MET:N	1:J:97:THR:O	2.46	0.48
1:I:7:ARG:H	1:I:106:HIS:HD2	1.60	0.47
1:B:46:LEU:HD23	1:B:74:THR:HG22	1.96	0.47
1:J:12:VAL:HG12	1:J:23:LYS:HG3	1.96	0.47
1:H:16:THR:HG23	1:H:19:GLU:HB2	1.97	0.47
1:F:47:LEU:O	1:F:75:CYS:HA	2.14	0.47
1:A:8:GLY:HA2	1:A:107:VAL:O	2.14	0.47
1:B:45:MET:HB3	1:B:73:VAL:HG12	1.97	0.46
1:F:7:ARG:H	1:F:106:HIS:CD2	2.23	0.46
1:J:3:ILE:HA	1:J:95:VAL:O	2.15	0.46
1:L:3:ILE:HD13	1:L:96:GLN:HA	1.97	0.46
1:J:9:ALA:HB3	1:J:108:TYR:HD1	1.81	0.46
1:F:62:VAL:HG21	1:F:73:VAL:HG11	1.98	0.46
1:D:12:VAL:HB	1:D:19:GLU:HG3	1.98	0.46
1:I:7:ARG:H	1:I:106:HIS:CD2	2.34	0.46
1:F:69:GLN:HE21	1:F:69:GLN:H	1.64	0.46
1:J:8:GLY:HA2	1:J:107:VAL:O	2.15	0.46
1:A:16:THR:HG23	1:A:19:GLU:CB	2.46	0.46
1:C:3:ILE:HA	1:C:95:VAL:O	2.16	0.46
1:G:3:ILE:HD11	1:H:2:MET:CE	2.46	0.46
1:F:8:GLY:HA2	1:F:107:VAL:O	2.15	0.45
1:L:7:ARG:H	1:L:106:HIS:CD2	2.28	0.45
1:G:81:VAL:HG12	1:G:82:THR:O	2.17	0.44
1:C:47:LEU:O	1:C:75:CYS:HA	2.16	0.44
1:F:23:LYS:HD3	1:F:23:LYS:HA	1.85	0.44
1:B:6:ILE:HD12	1:B:93:MET:HE3	1.98	0.44
1:K:8:GLY:HA2	1:K:107:VAL:O	2.18	0.44
1:K:7:ARG:H	1:K:106:HIS:CD2	2.22	0.44
1:K:3:ILE:HD13	1:K:96:GLN:HA	1.99	0.44
1:K:48:SER:HB3	1:K:76:MET:HG3	1.99	0.44
1:F:78:GLU:HG2	1:F:90:ARG:NH1	2.33	0.43
1:E:6:ILE:HD12	1:E:93:MET:CE	2.48	0.43
1:H:85:LEU:HD23	1:H:88:CYS:SG	2.58	0.43
1:D:72:PRO:HB2	1:E:92:MET:HE1	2.00	0.43
1:A:38:LYS:HB3	1:A:40:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:GLU:O	1:G:113:VAL:HG22	2.18	0.43
1:L:93:MET:HE3	1:L:95:VAL:HG11	2.00	0.43
1:H:22:GLN:O	1:H:26:GLN:HG3	2.19	0.43
1:E:7:ARG:HG2	1:E:92:MET:HE3	2.01	0.43
1:A:3:ILE:HG13	1:C:43:VAL:HG13	2.01	0.43
1:A:3:ILE:HG13	1:C:43:VAL:CG1	2.49	0.42
1:I:48:SER:HA	1:I:76:MET:O	2.19	0.42
1:E:42:VAL:HG22	1:E:95:VAL:HG12	2.01	0.42
1:K:56:VAL:CG2	1:K:60:LYS:HD2	2.50	0.42
1:L:8:GLY:HA2	1:L:107:VAL:O	2.19	0.42
1:A:7:ARG:N	1:A:106:HIS:HD2	2.10	0.42
1:H:70:TYR:HB3	1:I:101:GLN:HG2	2.02	0.41
1:K:99:VAL:HA	1:K:100:PRO:HD3	1.87	0.41
1:I:39:PRO:HG3	1:I:68:TRP:CD1	2.54	0.41
1:B:16:THR:HG22	1:B:19:GLU:HB2	2.02	0.41
1:D:7:ARG:H	1:D:106:HIS:CD2	2.32	0.41
1:F:110:GLU:O	1:F:113:VAL:HG22	2.20	0.41
1:D:7:ARG:HD3	1:F:74:THR:HB	2.03	0.41
1:L:7:ARG:N	1:L:106:HIS:HD2	2.12	0.41
1:E:6:ILE:HD12	1:E:93:MET:HE2	2.02	0.41
1:G:50:THR:HA	1:G:78:GLU:HB3	2.03	0.41
1:H:16:THR:HG23	1:H:19:GLU:HB3	2.03	0.40
1:F:99:VAL:HA	1:F:100:PRO:HD3	1.86	0.40
1:L:30:LYS:HA	1:L:30:LYS:HD2	1.87	0.40
1:G:9:ALA:HB3	1:G:108:TYR:HD1	1.87	0.40
1:C:7:ARG:H	1:C:106:HIS:CD2	2.24	0.40
1:F:12:VAL:HG12	1:F:23:LYS:HG3	2.03	0.40
1:A:3:ILE:HD13	1:B:3:ILE:HD11	2.02	0.40
1:A:12:VAL:HB	1:A:19:GLU:HG3	2.03	0.40
1:E:46:LEU:CD2	1:E:74:THR:HG22	2.51	0.40
1:H:45:MET:HB3	1:H:73:VAL:HG12	2.03	0.40
1:B:17:GLU:HG3	1:B:56:VAL:HB	2.03	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)
1:H:82:THR:OG1	2:K:153:HOH:H1[2_657]	1.55	0.05
1:G:12:VAL:O	2:I:183:HOH:H1[2_657]	1.57	0.03

## 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	112/127 (88%)	108 (96%)	3 (3%)	1 (1%)	21	9
1	B	112/127 (88%)	108 (96%)	3 (3%)	1 (1%)	21	9
1	C	112/127 (88%)	103 (92%)	8 (7%)	1 (1%)	21	9
1	D	112/127 (88%)	106 (95%)	6 (5%)	0	100	100
1	E	112/127 (88%)	111 (99%)	1 (1%)	0	100	100
1	F	112/127 (88%)	106 (95%)	6 (5%)	0	100	100
1	G	112/127 (88%)	108 (96%)	4 (4%)	0	100	100
1	H	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	I	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
1	J	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
1	K	112/127 (88%)	107 (96%)	4 (4%)	1 (1%)	21	9
1	L	112/127 (88%)	109 (97%)	3 (3%)	0	100	100
All	All	1344/1524 (88%)	1293 (96%)	47 (4%)	4 (0%)	46	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	B	51	PRO
1	K	51	PRO
1	C	114	VAL

### 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	103/116 (89%)	100 (97%)	3 (3%)	50	40
1	B	103/116 (89%)	98 (95%)	5 (5%)	31	18
1	C	103/116 (89%)	100 (97%)	3 (3%)	50	40
1	D	103/116 (89%)	101 (98%)	2 (2%)	65	59
1	E	103/116 (89%)	99 (96%)	4 (4%)	39	27
1	F	103/116 (89%)	101 (98%)	2 (2%)	65	59
1	G	103/116 (89%)	101 (98%)	2 (2%)	65	59
1	H	103/116 (89%)	97 (94%)	6 (6%)	25	13
1	I	103/116 (89%)	102 (99%)	1 (1%)	82	81
1	J	103/116 (89%)	101 (98%)	2 (2%)	65	59
1	K	103/116 (89%)	98 (95%)	5 (5%)	31	18
1	L	103/116 (89%)	99 (96%)	4 (4%)	39	27
All	All	1236/1392 (89%)	1197 (97%)	39 (3%)	46	35

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	16	THR
1	A	91	VAL
1	B	2	MET
1	B	40	GLU
1	B	69	GLN
1	B	73	VAL
1	B	74	THR
1	C	47	LEU
1	C	66	SER
1	C	98	ASP
1	D	36	HIS
1	D	74	THR
1	E	2	MET
1	E	16	THR
1	E	22	GLN
1	E	74	THR
1	F	16	THR
1	F	69	GLN
1	G	2	MET

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Mol	Chain	Res	Type
1	G	103	GLN
1	H	2	MET
1	H	16	THR
1	H	18	GLU
1	H	40	GLU
1	H	76	MET
1	H	96	GLN
1	I	66	SER
1	J	3	ILE
1	J	66	SER
1	K	2	MET
1	K	16	THR
1	K	18	GLU
1	K	45	MET
1	K	98	ASP
1	L	16	THR
1	L	19	GLU
1	L	66	SER
1	L	114	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	44	GLN
1	A	106	HIS
1	B	26	GLN
1	B	44	GLN
1	B	106	HIS
1	C	44	GLN
1	C	106	HIS
1	D	26	GLN
1	D	103	GLN
1	D	106	HIS
1	E	44	GLN
1	E	106	HIS
1	F	69	GLN
1	F	106	HIS
1	G	26	GLN
1	G	44	GLN
1	G	77	GLN
1	G	106	HIS

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Mol	Chain	Res	Type
1	H	44	GLN
1	H	77	GLN
1	H	106	HIS
1	I	26	GLN
1	I	44	GLN
1	I	106	HIS
1	J	44	GLN
1	J	101	GLN
1	J	106	HIS
1	K	44	GLN
1	K	101	GLN
1	K	106	HIS
1	L	26	GLN
1	L	101	GLN
1	L	106	HIS

### 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](#)

There are no ligands in this entry.

### 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.