



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 12:28 AM EST

PDB ID : 1COM  
Title : THE MONOFUNCTIONAL CHORISMATE MUTASE FROM BACILLUS SUBTILIS: STRUCTURE DETERMINATION OF CHORISMATE MUTASE AND ITS COMPLEXES WITH A TRANSITION STATE ANALOG AND PREPHENATE, AND IMPLICATIONS ON THE MECHANISM OF ENZY-MATIC REACTION  
Authors : Chook, Y.M.; Ke, H.; Lipscomb, W.N.  
Deposited on : unknown  
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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

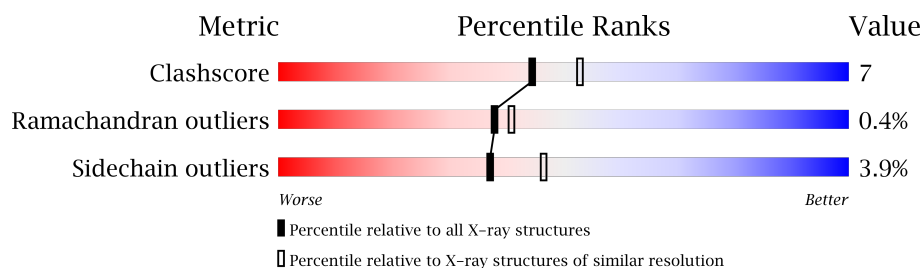
# 1 Overall quality at a glance

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))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (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 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	<div><div></div><div>66%20%••10%</div></div>
1	I	127	<div><div></div><div>68%20%•10%</div></div>
1	J	127	<div><div></div><div>72%16%•10%</div></div>
1	K	127	<div><div></div><div>65%23%•9%</div></div>
1	L	127	<div><div></div><div>65%23%•10%</div></div>

## 2 Entry composition

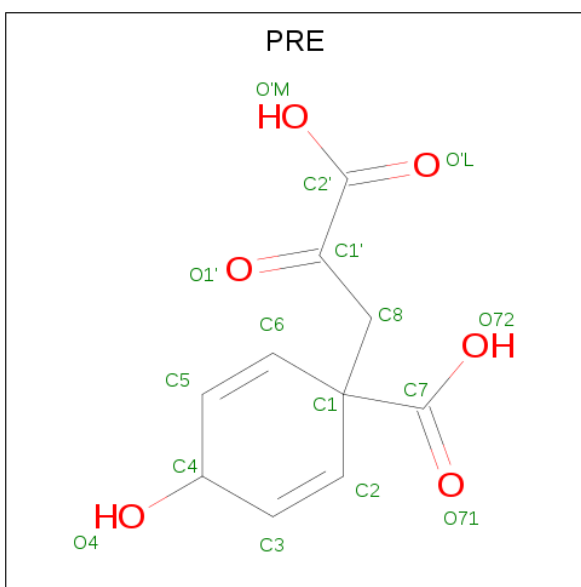
There are 3 unique types of molecules in this entry. The entry contains 15125 atoms, of which 3466 are hydrogens and 0 are deuteriums.

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	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	C	119	Total	C	H	N	O	S	0	0	0
			1156	594	211	164	179	8			
1	D	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	E	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	F	117	Total	C	H	N	O	S	0	0	0
			1139	585	208	162	176	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	116	Total	C	H	N	O	S	0	0	0
			1130	581	207	161	173	8			
1	L	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			

- Molecule 2 is PREPHENIC ACID (three-letter code: PRE) (formula: C<sub>10</sub>H<sub>10</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	10	1	6		
2	B	1	Total	C	H	O	0	0
			17	10	1	6		
2	C	1	Total	C	H	O	0	0
			17	10	1	6		
2	D	1	Total	C	H	O	0	0
			17	10	1	6		
2	E	1	Total	C	H	O	0	0
			17	10	1	6		
2	F	1	Total	C	H	O	0	0
			17	10	1	6		
2	G	1	Total	C	H	O	0	0
			17	10	1	6		
2	H	1	Total	C	H	O	0	0
			17	10	1	6		
2	K	1	Total	C	H	O	0	0
			17	10	1	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	36	Total	H	O	0	0
			108	72	36		
3	B	42	Total	H	O	0	0
			126	84	42		
3	C	44	Total	H	O	0	0
			132	88	44		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	37	Total	H	O	0	0
			111	74	37		
3	E	45	Total	H	O	0	0
			135	90	45		
3	F	57	Total	H	O	0	0
			171	114	57		
3	G	33	Total	H	O	0	0
			99	66	33		
3	H	16	Total	H	O	0	0
			48	32	16		
3	I	49	Total	H	O	0	0
			147	98	49		
3	J	36	Total	H	O	0	0
			108	72	36		
3	K	38	Total	H	O	0	0
			114	76	38		
3	L	70	Total	H	O	0	0
			210	140	70		

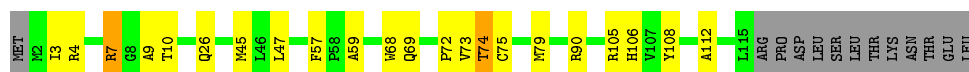
### 3 Residue-property plots

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.

Note EDS was not executed.

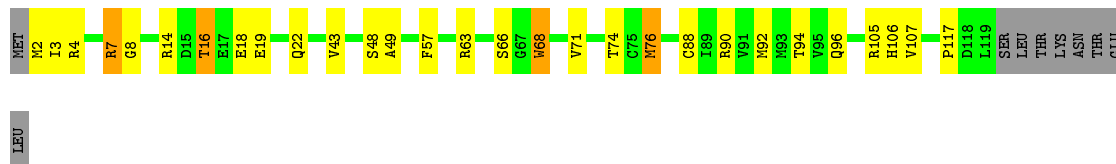
#### • Molecule 1: CHORISMATE MUTASE

Chain A: 



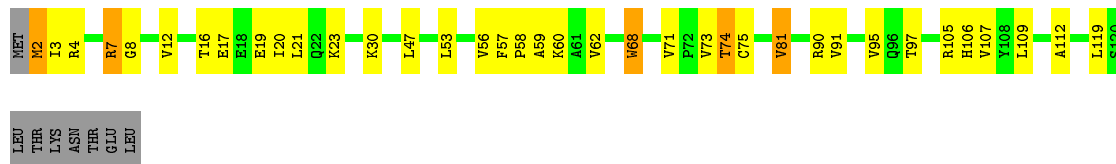
#### • Molecule 1: CHORISMATE MUTASE

Chain B: 



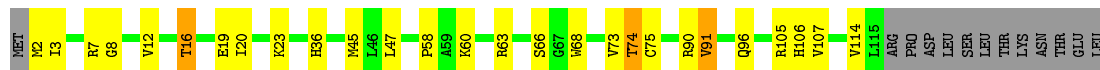
#### • Molecule 1: CHORISMATE MUTASE

Chain C: 



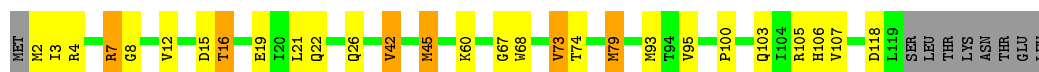
#### • Molecule 1: CHORISMATE MUTASE

Chain D: 

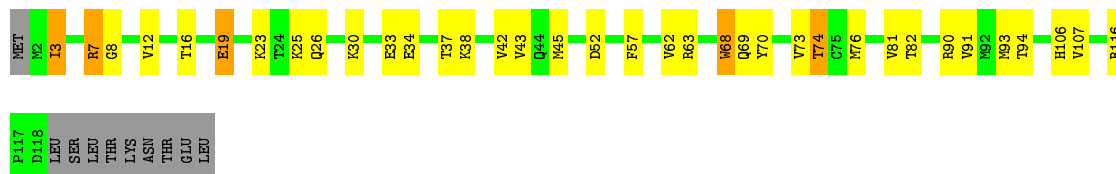


#### • Molecule 1: CHORISMATE MUTASE

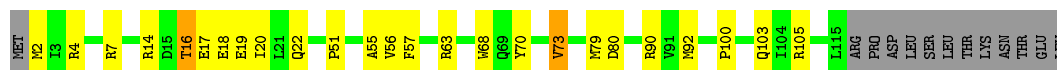
Chain E: 



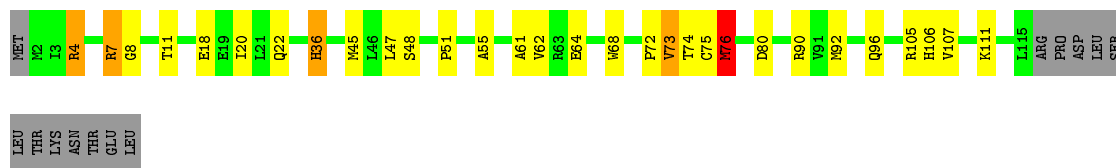
• Molecule 1: CHORISMATE MUTASE



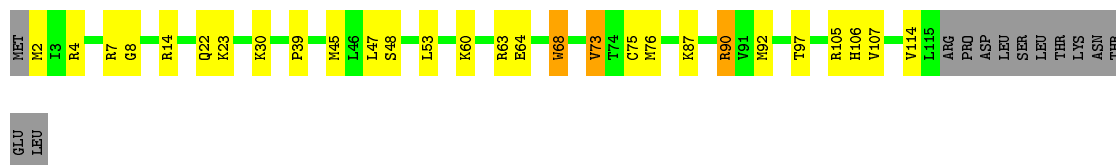
• Molecule 1: CHORISMATE MUTASE



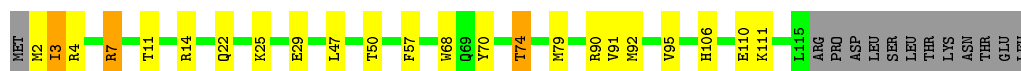
• Molecule 1: CHORISMATE MUTASE



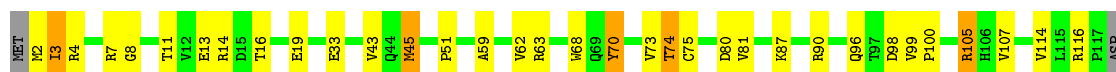
• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE





LEU  
SER  
LEU  
THR  
LYS  
ASN  
THR  
GLU  
LEU

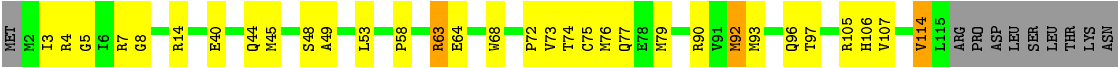
● Molecule 1: CHORISMATE MUTASE

Chain L: 

65%

23%

• 10%



THR  
GLU  
LEU

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PRE

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	0.80	0/917	1.46	12/1240 (1.0%)
1	B	0.79	0/952	1.46	14/1288 (1.1%)
1	C	0.76	0/958	1.47	13/1296 (1.0%)
1	D	0.82	0/917	1.47	7/1240 (0.6%)
1	E	0.81	0/952	1.53	14/1288 (1.1%)
1	F	0.79	0/944	1.44	16/1277 (1.3%)
1	G	0.79	0/917	1.47	16/1240 (1.3%)
1	H	0.76	0/917	1.43	12/1240 (1.0%)
1	I	0.81	0/917	1.48	12/1240 (1.0%)
1	J	0.80	0/917	1.51	13/1240 (1.0%)
1	K	0.78	0/936	1.47	17/1266 (1.3%)
1	L	0.82	0/917	1.54	19/1240 (1.5%)
All	All	0.79	0/11161	1.48	165/15095 (1.1%)

There are no bond length outliers.

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	D	105	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	H	4	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	B	4	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	E	4	ARG	NE-CZ-NH1	10.19	125.40	120.30
1	I	105	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	J	68	TRP	CD1-CG-CD2	9.49	113.89	106.30
1	G	7	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	E	7	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	L	63	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	L	68	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	L	4	ARG	NE-CZ-NH2	-8.51	116.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	14	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	E	68	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	C	68	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	I	2	MET	CG-SD-CE	-8.32	86.89	100.20
1	E	68	TRP	CE2-CD2-CG	-8.32	100.65	107.30
1	F	68	TRP	CD1-CG-CD2	8.28	112.93	106.30
1	B	68	TRP	CE2-CD2-CG	-8.24	100.70	107.30
1	J	68	TRP	CE2-CD2-CG	-8.23	100.72	107.30
1	J	7	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	I	68	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	G	68	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	4	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	K	7	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	E	45	MET	CG-SD-CE	-7.94	87.50	100.20
1	K	7	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	L	68	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	J	79	MET	CA-CB-CG	7.71	126.40	113.30
1	J	90	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	G	68	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	F	68	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	C	68	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	D	68	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	I	68	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	D	68	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	B	68	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	68	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	K	68	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	G	90	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	H	68	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	B	74	THR	CA-CB-CG2	7.39	122.75	112.40
1	H	7	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	E	7	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	G	14	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	L	4	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	I	90	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	L	90	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	I	105	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	H	68	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	A	26	GLN	CA-CB-CG	6.98	128.75	113.40
1	A	68	TRP	CD1-CG-CD2	6.95	111.86	106.30
1	L	14	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	G	22	GLN	CA-CB-CG	6.90	128.58	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	G	4	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	K	68	TRP	CD1-CG-CD2	6.68	111.65	106.30
1	H	36	HIS	CA-CB-CG	6.67	124.93	113.60
1	L	97	THR	CA-C-N	-6.59	102.70	117.20
1	F	116	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	F	63	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	L	77	GLN	CA-CB-CG	-6.51	99.07	113.40
1	I	4	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	14	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	K	74	THR	CA-CB-CG2	6.43	121.40	112.40
1	J	4	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	68	TRP	CG-CD2-CE3	6.32	139.59	133.90
1	L	114	VAL	N-CA-CB	-6.32	97.61	111.50
1	G	90	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	K	81	VAL	CA-CB-CG2	-6.29	101.47	110.90
1	E	79	MET	CA-CB-CG	6.28	123.98	113.30
1	B	74	THR	CA-CB-OG1	-6.24	95.89	109.00
1	E	68	TRP	CG-CD2-CE3	6.19	139.47	133.90
1	A	4	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	F	33	GLU	CA-CB-CG	6.14	126.91	113.40
1	F	90	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	7	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	K	68	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	I	4	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	G	92	MET	CG-SD-CE	-6.09	90.46	100.20
1	L	14	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	H	92	MET	CG-SD-CE	-6.07	90.48	100.20
1	F	63	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	K	70	TYR	CB-CG-CD1	-6.06	117.36	121.00
1	F	7	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	105	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	7	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	105	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	H	76	MET	CA-CB-CG	5.96	123.43	113.30
1	C	91	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	I	14	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	H	90	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	7	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	F	68	TRP	CG-CD2-CE3	5.85	139.17	133.90
1	H	7	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	J	14	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	68	TRP	CG-CD2-CE3	5.83	139.15	133.90
1	A	68	TRP	CG-CD2-CE3	5.82	139.14	133.90
1	J	4	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	F	91	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	D	90	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	L	105	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	105	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	F	3	ILE	CG1-CB-CG2	-5.78	98.67	111.40
1	J	68	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	F	116	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	G	7	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	7	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	K	90	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	7	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	G	68	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	B	4	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	L	92	MET	CG-SD-CE	-5.64	91.17	100.20
1	A	90	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	H	105	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	63	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	68	TRP	CG-CD2-CE3	5.62	138.95	133.90
1	K	45	MET	CA-CB-CG	5.61	122.84	113.30
1	J	70	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	B	105	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	K	63	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	F	52	ASP	CB-CG-OD1	5.55	123.29	118.30
1	K	4	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	4	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	4	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	E	105	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	E	15	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	F	7	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	E	42	VAL	CG1-CB-CG2	-5.45	102.17	110.90
1	L	68	TRP	CG-CD2-CE3	5.45	138.80	133.90
1	F	70	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	C	68	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	E	15	ASP	CB-CG-OD1	5.41	123.16	118.30
1	B	68	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	F	68	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	H	73	VAL	CG1-CB-CG2	-5.33	102.36	110.90
1	C	68	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	C	119	LEU	N-CA-C	-5.32	96.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	105	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	E	73	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	K	68	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	E	45	MET	CA-CB-CG	5.23	122.19	113.30
1	K	4	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	79	MET	CA-CB-CG	5.22	122.17	113.30
1	I	97	THR	CA-C-N	-5.22	105.73	117.20
1	G	73	VAL	CB-CA-C	-5.19	101.54	111.40
1	C	81	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	I	68	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	J	110	GLU	CA-C-N	5.17	128.57	117.20
1	L	74	THR	CA-CB-CG2	5.16	119.62	112.40
1	G	4	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	L	68	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	J	68	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	G	105	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	91	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	H	74	THR	CA-CB-CG2	5.11	119.55	112.40
1	L	79	MET	CA-CB-CG	5.10	121.97	113.30
1	G	79	MET	CA-CB-CG	5.10	121.97	113.30
1	B	90	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	K	74	THR	CA-CB-OG1	-5.08	98.33	109.00
1	L	93	MET	CG-SD-CE	-5.07	92.08	100.20
1	G	70	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	K	3	ILE	N-CA-C	-5.07	97.32	111.00
1	A	90	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	L	105	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	A	905	201	936	13	0
1	B	939	209	971	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	945	211	976	27	0
1	D	905	201	936	18	2
1	E	939	209	971	19	1
1	F	931	208	960	19	1
1	G	905	201	936	6	0
1	H	905	201	936	15	1
1	I	905	201	936	12	0
1	J	905	201	936	9	0
1	K	923	207	956	15	1
1	L	905	201	936	12	1
2	A	16	1	8	4	0
2	B	16	1	8	2	0
2	C	16	1	8	1	0
2	D	16	1	8	3	0
2	E	16	1	8	1	0
2	F	16	1	8	1	0
2	G	16	1	8	0	0
2	H	16	1	8	1	0
2	K	16	1	8	2	0
3	A	36	72	0	0	0
3	B	42	84	0	0	0
3	C	44	88	0	0	0
3	D	37	74	0	0	1
3	E	45	90	0	0	1
3	F	57	114	0	0	0
3	G	33	66	0	0	0
3	H	16	32	0	0	0
3	I	49	98	0	0	0
3	J	36	72	0	0	0
3	K	38	76	0	1	0
3	L	70	140	0	0	3
All	All	11659	3466	11458	169	6

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 7.

All (169) 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:H:45:MET:HB3	1:H:73:VAL:HG12	1.58	0.84
1:G:100:PRO:HG2	1:G:103:GLN:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ARG:H	1:B:106:HIS:HD2	1.34	0.76
1:F:7:ARG:H	1:F:106:HIS:HD2	1.31	0.74
1:D:7:ARG:H	1:D:106:HIS:HD2	1.33	0.74
1:D:3:ILE:HD13	1:E:3:ILE:HD11	1.70	0.74
1:C:7:ARG:H	1:C:106:HIS:HD2	1.36	0.73
1:E:74:THR:HA	2:F:225:PRE:H5	1.71	0.70
2:A:223:PRE:H5	1:C:74:THR:HA	1.72	0.70
1:H:7:ARG:H	1:H:106:HIS:HD2	1.37	0.70
1:E:7:ARG:H	1:E:106:HIS:HD2	1.39	0.69
1:F:62:VAL:HG21	1:F:73:VAL:HG11	1.75	0.68
1:D:45:MET:HB3	1:D:73:VAL:HG12	1.75	0.68
1:H:11:THR:HG21	1:H:111:LYS:HB2	1.75	0.68
1:L:7:ARG:H	1:L:106:HIS:HD2	1.42	0.68
1:D:60:LYS:HA	1:D:63:ARG:NH1	2.09	0.67
1:I:7:ARG:H	1:I:106:HIS:HD2	1.44	0.66
1:H:62:VAL:HG21	1:H:73:VAL:HG11	1.78	0.66
1:D:74:THR:HA	2:E:224:PRE:H5	1.78	0.65
1:J:11:THR:HG21	1:J:111:LYS:HB2	1.77	0.65
1:E:45:MET:HE3	1:E:93:MET:HG3	1.77	0.65
1:J:92:MET:HE1	1:L:72:PRO:HB2	1.77	0.65
1:K:14:ARG:HH21	1:K:16:THR:HG21	1.63	0.64
1:G:20:ILE:HD12	1:G:55:ALA:HB3	1.79	0.64
1:B:16:THR:HG23	1:B:19:GLU:HB2	1.81	0.63
1:D:16:THR:HG23	1:D:19:GLU:HB3	1.81	0.62
1:J:2:MET:HG2	1:J:3:ILE:H	1.66	0.61
1:K:3:ILE:HD13	1:K:96:GLN:HA	1.82	0.61
1:C:20:ILE:HD11	1:C:53:LEU:HD22	1.84	0.60
1:G:16:THR:HG23	1:G:19:GLU:HB2	1.83	0.60
1:A:3:ILE:HD11	1:C:3:ILE:HG21	1.82	0.59
1:A:45:MET:HB3	1:A:73:VAL:HG12	1.84	0.59
1:L:8:GLY:HA2	1:L:107:VAL:O	2.03	0.59
1:A:7:ARG:H	1:A:106:HIS:HD2	1.48	0.59
1:C:12:VAL:HG12	1:C:23:LYS:HG3	1.85	0.58
1:K:51:PRO:HG3	1:K:80:ASP:HB2	1.84	0.58
1:C:62:VAL:HG21	1:C:73:VAL:HG11	1.83	0.58
1:H:8:GLY:HA2	1:H:107:VAL:O	2.04	0.58
1:K:59:ALA:HB2	1:K:75:CYS:SG	2.43	0.58
1:E:45:MET:HB3	1:E:73:VAL:HG12	1.85	0.58
2:D:226:PRE:H5	1:F:74:THR:HA	1.85	0.58
2:D:226:PRE:H3	1:F:57:PHE:CD1	2.39	0.57
1:L:45:MET:HB3	1:L:73:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:GLY:HA2	1:I:107:VAL:O	2.04	0.57
1:L:49:ALA:HB1	1:L:53:LEU:HD12	1.86	0.57
1:G:51:PRO:HG3	1:G:80:ASP:HB2	1.87	0.56
1:E:16:THR:HG22	1:E:19:GLU:CB	2.36	0.55
1:F:8:GLY:HA2	1:F:107:VAL:O	2.07	0.55
1:A:7:ARG:H	1:A:106:HIS:CD2	2.24	0.55
1:D:60:LYS:HA	1:D:63:ARG:HH11	1.71	0.55
1:E:12:VAL:HB	1:E:19:GLU:HG3	1.89	0.55
1:H:7:ARG:H	1:H:106:HIS:CD2	2.22	0.55
1:I:60:LYS:HA	1:I:63:ARG:HD3	1.89	0.54
2:D:226:PRE:H3	1:F:57:PHE:CG	2.43	0.54
1:G:57:PHE:CG	2:H:227:PRE:H3	2.43	0.54
1:F:12:VAL:HG12	1:F:23:LYS:HG3	1.90	0.54
1:C:16:THR:HG23	1:C:19:GLU:H	1.72	0.54
1:D:3:ILE:HD11	1:F:3:ILE:HG21	1.89	0.54
1:J:74:THR:HA	2:K:230:PRE:H5	1.91	0.53
1:L:3:ILE:HD13	1:L:96:GLN:HA	1.91	0.53
1:K:62:VAL:HG21	1:K:73:VAL:HG11	1.91	0.52
1:E:21:LEU:HD11	1:E:60:LYS:HD3	1.90	0.52
1:B:3:ILE:HD12	1:B:94:THR:CG2	2.39	0.52
2:A:223:PRE:H3	1:C:57:PHE:CE1	2.45	0.52
1:B:96:GLN:HB2	1:C:2:MET:SD	2.50	0.52
1:H:72:PRO:HB2	1:I:92:MET:HE1	1.91	0.52
1:D:47:LEU:O	1:D:75:CYS:HA	2.10	0.51
1:B:96:GLN:HB2	1:C:2:MET:CE	2.41	0.51
1:C:2:MET:N	1:C:97:THR:O	2.43	0.51
1:J:7:ARG:H	1:J:106:HIS:CD2	2.28	0.51
1:D:2:MET:HE2	1:D:3:ILE:O	2.10	0.51
1:D:7:ARG:H	1:D:106:HIS:CD2	2.21	0.51
1:A:72:PRO:HB2	1:B:92:MET:HE3	1.94	0.50
1:B:8:GLY:HA2	1:B:107:VAL:O	2.12	0.50
1:A:72:PRO:HB2	1:B:92:MET:CE	2.41	0.50
1:E:8:GLY:HA2	1:E:107:VAL:O	2.12	0.49
1:B:48:SER:HA	1:B:76:MET:O	2.12	0.49
1:H:4:ARG:HH11	1:H:4:ARG:HG2	1.77	0.49
1:K:16:THR:HG23	1:K:19:GLU:H	1.78	0.49
1:A:57:PHE:CD1	2:B:221:PRE:H3	2.47	0.49
1:C:47:LEU:O	1:C:75:CYS:HA	2.12	0.49
1:D:2:MET:HG2	1:D:3:ILE:H	1.78	0.49
1:H:20:ILE:HD12	1:H:55:ALA:HB3	1.94	0.49
1:H:61:ALA:HA	1:H:64:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:16:THR:HG22	1:K:19:GLU:HB2	1.95	0.48
1:H:18:GLU:O	1:H:22:GLN:HB2	2.13	0.47
1:C:8:GLY:HA2	1:C:107:VAL:O	2.15	0.47
1:E:16:THR:HG22	1:E:19:GLU:HB3	1.96	0.47
1:L:45:MET:O	1:L:73:VAL:HA	2.14	0.47
1:G:17:GLU:HG3	1:G:56:VAL:HB	1.95	0.47
1:A:74:THR:HA	2:B:221:PRE:H5	1.96	0.47
1:D:12:VAL:HG11	1:D:20:ILE:HA	1.96	0.46
1:A:7:ARG:N	1:A:106:HIS:HD2	2.13	0.46
1:K:8:GLY:HA2	1:K:107:VAL:O	2.15	0.46
1:A:9:ALA:HB3	1:A:108:TYR:HD1	1.80	0.46
1:C:7:ARG:N	1:C:106:HIS:HD2	2.11	0.46
1:H:51:PRO:HG3	1:H:80:ASP:HB2	1.97	0.46
1:E:16:THR:HG22	1:E:19:GLU:HB2	1.98	0.46
1:E:42:VAL:HG22	1:E:95:VAL:HG12	1.98	0.46
1:K:45:MET:HB3	1:K:73:VAL:HG12	1.97	0.46
1:K:11:THR:HA	1:K:87:LYS:O	2.16	0.46
1:B:57:PHE:CG	2:C:222:PRE:H3	2.51	0.46
1:E:100:PRO:HG2	1:E:103:GLN:HB2	1.97	0.46
1:A:47:LEU:O	1:A:75:CYS:HA	2.16	0.46
1:J:3:ILE:HA	1:J:95:VAL:O	2.16	0.45
1:B:68:TRP:CE3	1:B:71:VAL:HG21	2.51	0.45
1:E:45:MET:O	1:E:73:VAL:HA	2.16	0.45
1:J:47:LEU:HD23	1:J:91:VAL:HB	1.99	0.45
1:K:105:ARG:HA	3:K:676:HOH:O	2.15	0.45
1:C:59:ALA:HB2	1:C:75:CYS:SG	2.57	0.45
1:C:47:LEU:HD13	1:C:58:PRO:HB2	1.98	0.45
1:C:21:LEU:HD21	1:C:60:LYS:HB3	1.98	0.45
1:E:7:ARG:H	1:E:106:HIS:CD2	2.26	0.45
1:F:42:VAL:HG21	1:F:68:TRP:CH2	2.52	0.45
1:F:42:VAL:HG21	1:F:68:TRP:CZ3	2.52	0.45
1:F:23:LYS:HA	1:F:26:GLN:HE21	1.81	0.44
1:L:58:PRO:HD2	1:L:75:CYS:SG	2.56	0.44
1:E:21:LEU:HD21	1:E:60:LYS:HB3	2.00	0.44
1:D:12:VAL:HB	1:D:19:GLU:HG3	1.99	0.44
1:F:30:LYS:O	1:F:34:GLU:HG2	2.18	0.44
1:E:16:THR:HG22	1:E:19:GLU:H	1.83	0.44
1:L:48:SER:HA	1:L:76:MET:O	2.18	0.44
1:F:45:MET:HG3	1:F:93:MET:HG3	2.00	0.43
1:F:12:VAL:HB	1:F:19:GLU:HG2	1.99	0.43
1:D:58:PRO:HD2	1:E:79:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:TRP:CE3	1:C:71:VAL:HG21	2.54	0.43
1:I:30:LYS:HB3	1:I:107:VAL:HG11	1.99	0.43
1:K:99:VAL:HA	1:K:100:PRO:HD3	1.89	0.43
2:A:223:PRE:H3	1:C:57:PHE:CD1	2.53	0.43
1:B:16:THR:CG2	1:B:19:GLU:HB2	2.46	0.43
1:C:7:ARG:H	1:C:106:HIS:CD2	2.25	0.43
1:B:43:VAL:HG11	1:C:3:ILE:HG22	2.00	0.43
1:K:43:VAL:HG22	1:L:3:ILE:O	2.18	0.43
1:B:3:ILE:HD12	1:B:94:THR:HG22	2.01	0.43
1:H:4:ARG:HG2	1:H:4:ARG:NH1	2.34	0.42
1:D:3:ILE:HG12	1:F:3:ILE:HG12	2.01	0.42
1:C:17:GLU:HG3	1:C:56:VAL:HB	2.01	0.42
1:B:7:ARG:HG2	1:B:92:MET:HE3	2.01	0.42
1:F:16:THR:HG23	1:F:19:GLU:HB3	2.01	0.42
1:I:48:SER:HA	1:I:76:MET:O	2.20	0.42
1:D:12:VAL:HG12	1:D:23:LYS:HG3	2.00	0.42
1:C:109:LEU:O	1:C:112:ALA:HB3	2.20	0.42
1:C:3:ILE:HA	1:C:95:VAL:O	2.20	0.42
1:E:22:GLN:O	1:E:26:GLN:HG3	2.20	0.42
1:K:16:THR:CG2	1:K:19:GLU:HB2	2.50	0.42
1:A:59:ALA:HB2	1:A:75:CYS:SG	2.60	0.41
1:H:47:LEU:O	1:H:75:CYS:HA	2.20	0.41
1:I:22:GLN:OE1	1:I:23:LYS:HE3	2.19	0.41
1:J:57:PHE:CG	2:K:230:PRE:H3	2.55	0.41
1:A:108:TYR:HB3	1:A:112:ALA:O	2.20	0.41
1:B:16:THR:HG23	1:B:19:GLU:CB	2.49	0.41
1:L:7:ARG:N	1:L:106:HIS:HD2	2.15	0.41
1:K:14:ARG:NH2	1:K:16:THR:HG21	2.31	0.41
2:A:223:PRE:H2	1:C:57:PHE:CD2	2.55	0.41
1:I:53:LEU:HD21	1:I:87:LYS:HG2	2.01	0.41
1:B:49:ALA:HA	1:B:88:CYS:O	2.21	0.41
1:C:30:LYS:HA	1:C:30:LYS:HD2	1.89	0.41
1:D:8:GLY:HA2	1:D:107:VAL:O	2.21	0.41
1:F:23:LYS:HA	1:F:23:LYS:HD3	1.89	0.41
1:F:25:LYS:HB3	1:F:25:LYS:HE2	1.82	0.41
1:B:96:GLN:HB2	1:C:2:MET:HE1	2.02	0.41
1:F:43:VAL:HB	1:F:94:THR:HB	2.03	0.41
1:I:47:LEU:O	1:I:75:CYS:HA	2.21	0.40
1:I:48:SER:OG	1:I:90:ARG:HB2	2.20	0.40
1:J:25:LYS:O	1:J:29:GLU:HG3	2.21	0.40
1:L:5:GLY:HA3	1:L:92:MET:HE1	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:SER:HA	1:H:76:MET:O	2.21	0.40
1:I:45:MET:O	1:I:73:VAL:HA	2.20	0.40
1:I:39:PRO:HG3	1:I:68:TRP:NE1	2.36	0.40

All (6) 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:F:38:LYS:HZ2	1:H:36:HIS:HD1[2_656]	1.29	0.31
1:E:67:GLY:O	3:E:734:HOH:H2[2_756]	1.56	0.04
1:D:96:GLN:O	3:L:797:HOH:H2[2_756]	1.56	0.04
1:L:96:GLN:O	3:D:326:HOH:H1[2_746]	1.57	0.03
1:K:70:TYR:OH	3:L:501:HOH:H2[2_747]	1.60	0.00
1:D:36:HIS:O	3:L:495:HOH:H2[2_756]	1.60	0.00

## 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%)	110 (98%)	2 (2%)	0	100	100
1	B	116/127 (91%)	111 (96%)	4 (3%)	1 (1%)	20	18
1	C	117/127 (92%)	110 (94%)	7 (6%)	0	100	100
1	D	112/127 (88%)	105 (94%)	5 (4%)	2 (2%)	10	6
1	E	116/127 (91%)	112 (97%)	3 (3%)	1 (1%)	20	18
1	F	115/127 (91%)	111 (96%)	4 (4%)	0	100	100
1	G	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	H	112/127 (88%)	108 (96%)	4 (4%)	0	100	100
1	I	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	J	112/127 (88%)	110 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	114/127 (90%)	112 (98%)	2 (2%)	0	100	100
1	L	112/127 (88%)	108 (96%)	3 (3%)	1 (1%)	20	18
All	All	1362/1524 (89%)	1311 (96%)	46 (3%)	5 (0%)	38	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	118	ASP
1	L	44	GLN
1	B	117	PRO
1	D	66	SER
1	D	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%)	48	60
1	B	107/116 (92%)	101 (94%)	6 (6%)	25	29
1	C	108/116 (93%)	105 (97%)	3 (3%)	49	61
1	D	103/116 (89%)	100 (97%)	3 (3%)	48	60
1	E	107/116 (92%)	105 (98%)	2 (2%)	62	76
1	F	106/116 (91%)	99 (93%)	7 (7%)	19	21
1	G	103/116 (89%)	98 (95%)	5 (5%)	29	35
1	H	103/116 (89%)	101 (98%)	2 (2%)	62	76
1	I	103/116 (89%)	100 (97%)	3 (3%)	48	60
1	J	103/116 (89%)	99 (96%)	4 (4%)	37	46
1	K	105/116 (90%)	98 (93%)	7 (7%)	19	21
1	L	103/116 (89%)	99 (96%)	4 (4%)	37	46
All	All	1254/1392 (90%)	1205 (96%)	49 (4%)	37	46

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

Mol	Chain	Res	Type
1	A	10	THR
1	A	69	GLN
1	A	74	THR
1	B	2	MET
1	B	16	THR
1	B	18	GLU
1	B	22	GLN
1	B	66	SER
1	B	76	MET
1	C	2	MET
1	C	74	THR
1	C	81	VAL
1	D	16	THR
1	D	74	THR
1	D	91	VAL
1	E	2	MET
1	E	16	THR
1	F	19	GLU
1	F	37	THR
1	F	69	GLN
1	F	74	THR
1	F	76	MET
1	F	81	VAL
1	F	82	THR
1	G	2	MET
1	G	16	THR
1	G	18	GLU
1	G	63	ARG
1	G	73	VAL
1	H	76	MET
1	H	96	GLN
1	I	64	GLU
1	I	73	VAL
1	I	114	VAL
1	J	3	ILE
1	J	22	GLN
1	J	50	THR
1	J	74	THR
1	K	2	MET
1	K	13	GLU
1	K	33	GLU
1	K	74	THR

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Mol	Chain	Res	Type
1	K	98	ASP
1	K	114	VAL
1	K	116	ARG
1	L	40	GLU
1	L	63	ARG
1	L	64	GLU
1	L	114	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	77	GLN
1	A	101	GLN
1	A	106	HIS
1	B	26	GLN
1	B	44	GLN
1	B	69	GLN
1	B	106	HIS
1	C	44	GLN
1	C	103	GLN
1	C	106	HIS
1	D	106	HIS
1	E	44	GLN
1	E	101	GLN
1	E	106	HIS
1	F	26	GLN
1	F	44	GLN
1	F	106	HIS
1	G	44	GLN
1	G	106	HIS
1	H	44	GLN
1	H	106	HIS
1	I	44	GLN
1	I	101	GLN
1	I	106	HIS
1	J	26	GLN
1	J	44	GLN
1	J	106	HIS
1	K	44	GLN
1	K	101	GLN
1	L	26	GLN

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Mol	Chain	Res	Type
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](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PRE	A	223	-	10,16,16	1.57	2 (20%)	6,23,23	1.17	0
2	PRE	B	221	-	10,16,16	1.32	0	6,23,23	1.11	0
2	PRE	C	222	-	10,16,16	1.50	1 (10%)	6,23,23	1.28	1 (16%)
2	PRE	D	226	-	10,16,16	1.56	2 (20%)	6,23,23	0.98	0
2	PRE	E	224	-	10,16,16	1.46	1 (10%)	6,23,23	1.17	0
2	PRE	F	225	-	10,16,16	1.41	0	6,23,23	1.06	0
2	PRE	G	229	-	10,16,16	1.41	1 (10%)	6,23,23	1.33	0
2	PRE	H	227	-	10,16,16	1.51	2 (20%)	6,23,23	1.78	2 (33%)
2	PRE	K	230	-	10,16,16	1.45	1 (10%)	6,23,23	1.34	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
2	PRE	A	223	-	-	0/5/27/27	0/1/1/1
2	PRE	B	221	-	-	0/5/27/27	0/1/1/1
2	PRE	C	222	-	-	0/5/27/27	0/1/1/1
2	PRE	D	226	-	-	0/5/27/27	0/1/1/1
2	PRE	E	224	-	-	0/5/27/27	0/1/1/1
2	PRE	F	225	-	-	0/5/27/27	0/1/1/1
2	PRE	G	229	-	-	0/5/27/27	0/1/1/1
2	PRE	H	227	-	-	0/5/27/27	0/1/1/1
2	PRE	K	230	-	-	0/5/27/27	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	230	PRE	C5-C6	2.15	1.36	1.32
2	H	227	PRE	C5-C6	2.15	1.36	1.32
2	H	227	PRE	C3-C2	2.28	1.36	1.32
2	E	224	PRE	C5-C6	2.36	1.36	1.32
2	D	226	PRE	C8-C1'	2.49	1.54	1.51
2	A	223	PRE	C5-C6	2.49	1.36	1.32
2	A	223	PRE	C8-C1'	2.52	1.54	1.51
2	D	226	PRE	C5-C6	2.59	1.36	1.32
2	C	222	PRE	C8-C1'	2.59	1.54	1.51
2	G	229	PRE	C8-C1'	2.82	1.54	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	227	PRE	O1'-C1'-C8	-3.29	116.26	120.58
2	H	227	PRE	O4-C4-C5	-2.08	105.90	117.56
2	C	222	PRE	O4-C4-C5	-2.06	106.02	117.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	223	PRE	4	0
2	B	221	PRE	2	0
2	C	222	PRE	1	0
2	D	226	PRE	3	0
2	E	224	PRE	1	0
2	F	225	PRE	1	0
2	H	227	PRE	1	0
2	K	230	PRE	2	0

## 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.