



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:17 AM GMT

PDB ID : 2CHT
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 : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

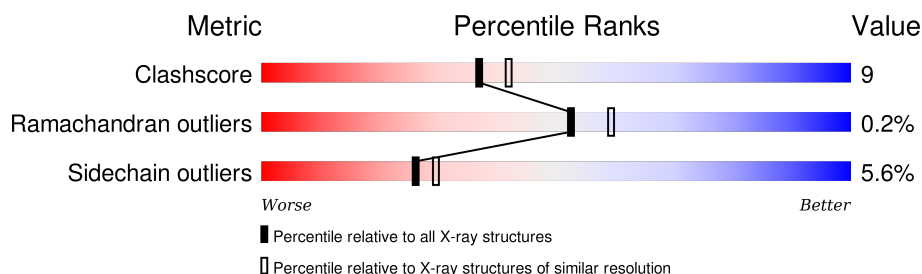
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 ≥ 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	 65%22%•9%
1	I	127	 61%26%••10%
1	J	127	 65%22%6%8%
1	K	127	 71%17%••8%
1	L	127	 56%30%•10%

2 Entry composition

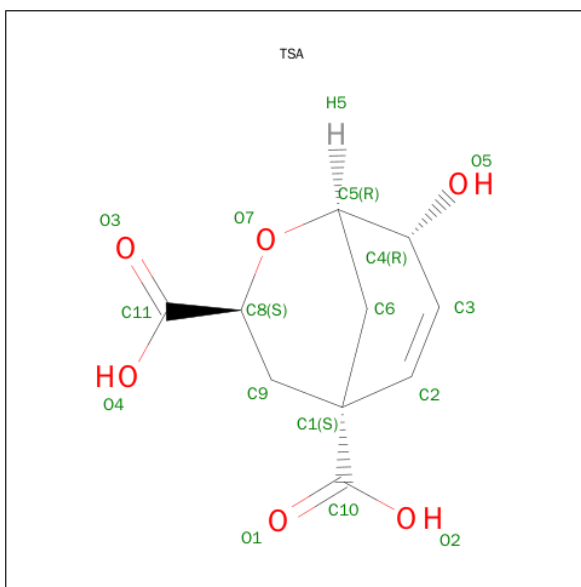
There are 3 unique types of molecules in this entry. The entry contains 15344 atoms, of which 3554 are hydrogens and 0 are deuteriums.

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	117	Total	C	H	N	O	S	0	0	0
			1139	585	208	162	176	8			
1	C	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	D	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	E	117	Total	C	H	N	O	S	0	0	0
			1139	585	208	162	176	8			
1	F	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	G	115	Total	C	H	N	O	S	0	0	0
			1123	576	207	160	172	8			
1	H	116	Total	C	H	N	O	S	0	0	0
			1130	581	207	161	173	8			
1	I	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	J	117	Total	C	H	N	O	S	0	0	0
			1139	585	208	162	176	8			
1	K	117	Total	C	H	N	O	S	0	0	0
			1139	585	208	162	176	8			
1	L	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			

- Molecule 2 is 8-HYDROXY-2-OXA-BICYCLO[3.3.1]NON-6-ENE-3,5-DICARBOXYLIC ACID (three-letter code: TSA) (formula: C₁₀H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	A	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	D	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	I	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	K	1	Total	C	H	O	0	0
			17	10	1	6		
2	L	1	Total	C	H	O	0	0
			17	10	1	6		
2	J	1	Total	C	H	O	0	0
			17	10	1	6		

- Molecule 3 is water.

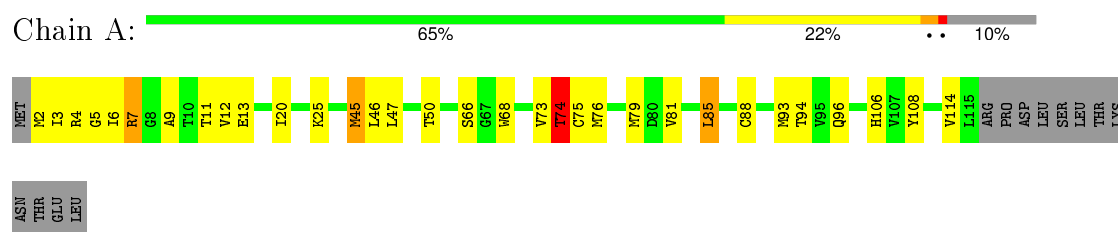
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	49	Total	H	O	0	0
			147	98	49		
3	B	37	Total	H	O	0	0
			111	74	37		
3	C	56	Total	H	O	0	0
			168	112	56		
3	D	53	Total	H	O	0	0
			159	106	53		
3	E	50	Total	H	O	0	0
			150	100	50		
3	F	48	Total	H	O	0	0
			144	96	48		
3	G	42	Total	H	O	0	0
			126	84	42		
3	H	36	Total	H	O	0	0
			108	72	36		
3	I	39	Total	H	O	0	0
			117	78	39		
3	J	37	Total	H	O	0	0
			111	74	37		
3	K	45	Total	H	O	0	0
			135	90	45		
3	L	45	Total	H	O	0	0
			135	90	45		

3 Residue-property plots [i](#)

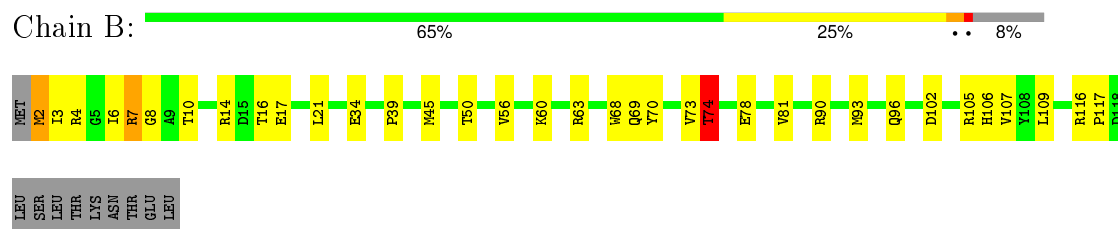
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

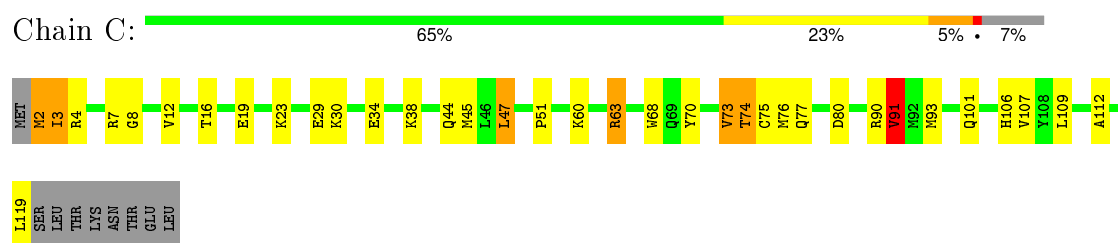
• Molecule 1: CHORISMATE MUTASE



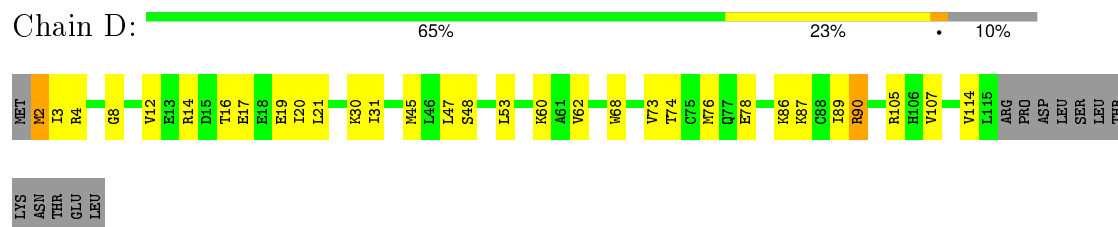
• Molecule 1: CHORISMATE MUTASE



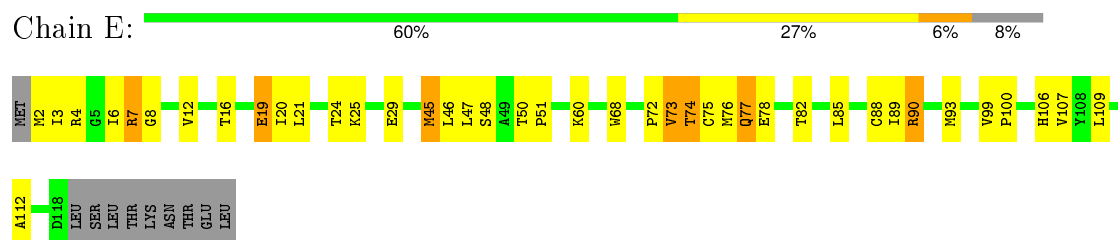
• Molecule 1: CHORISMATE MUTASE



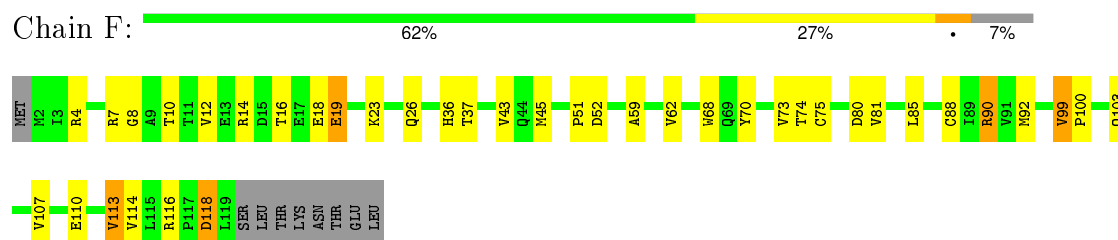
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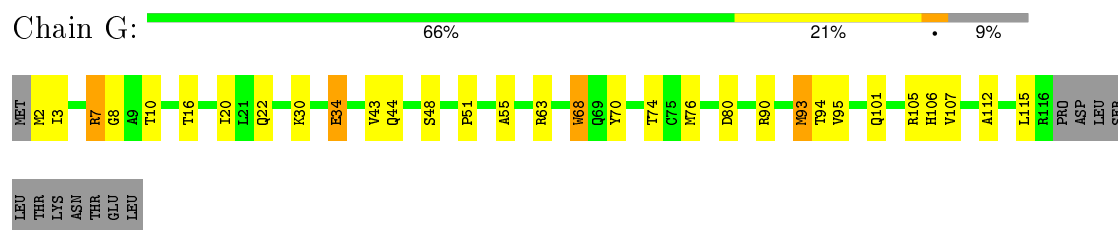
- Molecule 1: CHORISMATE MUTASE



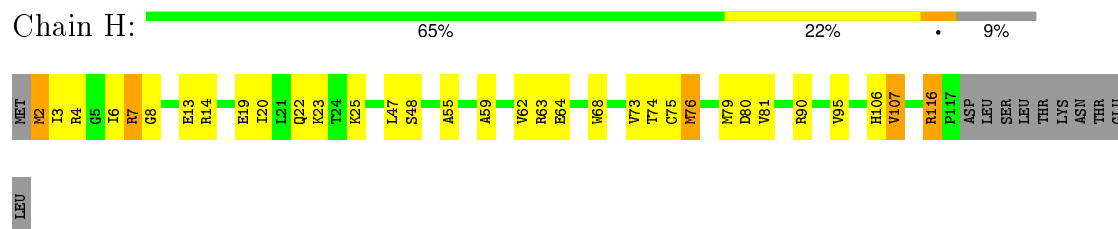
- Molecule 1: CHORISMATE MUTASE



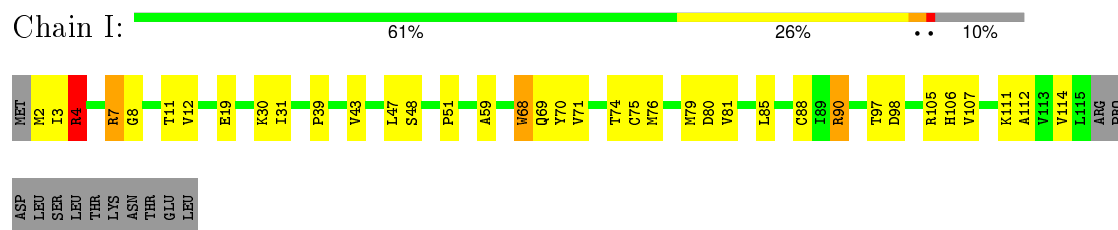
- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE

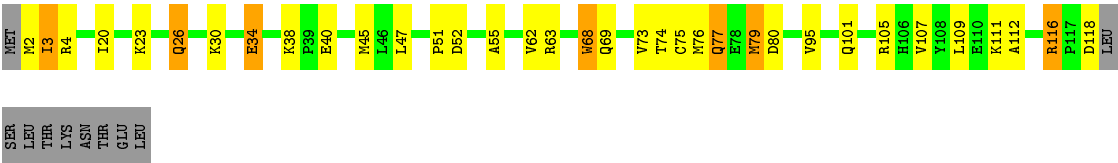


- Molecule 1: CHORISMATE MUTASE

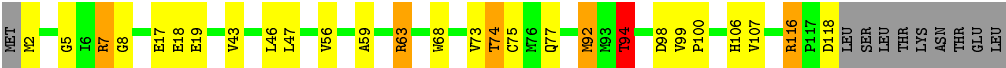


- Molecule 1: CHORISMATE MUTASE

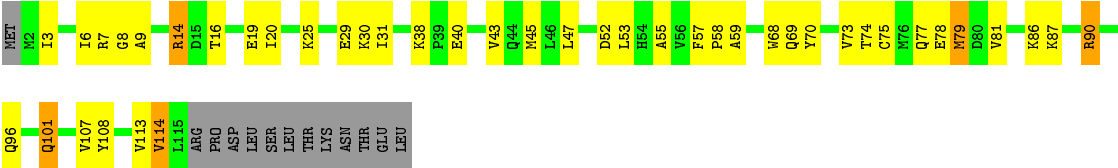




• Molecule 1: CHORISMATE MUTASE



• 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, α , β , γ	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}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15344	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: TSA

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	0.77	0/917	1.49	8/1240 (0.6%)
1	B	0.81	0/944	1.51	13/1277 (1.0%)
1	C	0.78	0/952	1.47	12/1288 (0.9%)
1	D	0.77	0/917	1.47	8/1240 (0.6%)
1	E	0.79	0/944	1.45	9/1277 (0.7%)
1	F	0.78	0/952	1.49	14/1288 (1.1%)
1	G	0.76	0/928	1.48	12/1254 (1.0%)
1	H	0.75	0/936	1.39	10/1266 (0.8%)
1	I	0.76	0/917	1.44	10/1240 (0.8%)
1	J	0.80	0/944	1.41	9/1277 (0.7%)
1	K	0.77	0/944	1.47	10/1277 (0.8%)
1	L	0.80	0/917	1.52	11/1240 (0.9%)
All	All	0.78	0/11212	1.47	126/15164 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	THR	CA-CB-CG2	10.42	126.98	112.40
1	L	7	ARG	NE-CZ-NH2	-9.62	115.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	90	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	C	68	TRP	CD1-CG-CD2	8.94	113.45	106.30
1	G	7	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	74	THR	CA-CB-OG1	-8.86	90.39	109.00
1	D	4	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	4	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	J	68	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	L	7	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	K	7	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	I	4	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	F	68	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	C	68	TRP	CE2-CD2-CG	-8.23	100.71	107.30
1	J	68	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	L	68	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	F	68	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	I	79	MET	CA-CB-CG	7.89	126.72	113.30
1	L	79	MET	CA-CB-CG	7.84	126.63	113.30
1	L	68	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	I	68	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	K	63	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	E	90	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	E	68	TRP	CG-CD2-CE3	7.66	140.79	133.90
1	A	68	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	I	68	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	E	68	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	G	90	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	68	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	G	68	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	H	63	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	68	TRP	CE2-CD2-CG	-7.44	101.34	107.30
1	B	68	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	G	68	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	H	68	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	L	14	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	4	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	H	68	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	F	4	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	K	68	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	F	92	MET	CG-SD-CE	-7.23	88.64	100.20
1	D	68	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	H	4	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	K	68	TRP	CD1-CG-CD2	7.11	111.99	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	K	94	THR	CA-CB-CG2	6.98	122.17	112.40
1	A	7	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	B	116	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	E	68	TRP	CD1-CG-CD2	6.77	111.72	106.30
1	G	70	TYR	CB-CG-CD2	-6.70	116.98	121.00
1	D	68	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	B	7	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	D	90	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	81	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	K	7	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	L	90	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	F	70	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	A	74	THR	CA-CB-CG2	6.45	121.43	112.40
1	I	68	TRP	CG-CD2-CE3	6.36	139.62	133.90
1	E	7	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	G	90	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	L	68	TRP	CG-CD2-CE3	6.30	139.57	133.90
1	E	4	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	L	114	VAL	N-CA-CB	-6.28	97.68	111.50
1	D	2	MET	CA-CB-CG	-6.27	102.64	113.30
1	F	81	VAL	CA-CB-CG2	-6.21	101.58	110.90
1	H	4	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	K	92	MET	CA-CB-CG	6.05	123.59	113.30
1	F	116	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	68	TRP	CB-CG-CD1	-5.99	119.21	127.00
1	G	63	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	4	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	H	7	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	K	94	THR	CA-CB-OG1	-5.92	96.56	109.00
1	C	2	MET	CA-CB-CG	-5.84	103.37	113.30
1	F	26	GLN	CA-CB-CG	-5.82	100.59	113.40
1	J	68	TRP	CG-CD2-CE3	5.82	139.13	133.90
1	C	91	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	H	116	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	I	7	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	68	TRP	CG-CD2-CE3	5.75	139.07	133.90
1	G	22	GLN	CA-CB-CG	5.73	126.01	113.40
1	L	101	GLN	CA-CB-CG	5.72	125.98	113.40
1	D	14	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	102	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	70	TYR	CB-CG-CD1	-5.64	117.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	68	TRP	CB-CG-CD1	-5.60	119.71	127.00
1	A	7	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	74	THR	CA-CB-CG2	5.55	120.18	112.40
1	G	68	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	F	90	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	J	116	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	G	63	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	68	TRP	CG-CD2-CE3	5.44	138.80	133.90
1	J	4	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	L	19	GLU	CA-CB-CG	-5.44	101.43	113.40
1	F	81	VAL	CA-CB-CG1	5.40	119.00	110.90
1	D	105	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	J	79	MET	CG-SD-CE	5.38	108.80	100.20
1	C	29	GLU	CA-CB-CG	-5.37	101.58	113.40
1	J	116	ARG	N-CA-C	-5.36	96.54	111.00
1	I	90	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	K	116	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	H	107	VAL	CG1-CB-CG2	-5.25	102.49	110.90
1	E	72	PRO	N-CA-CB	5.25	109.60	103.30
1	G	93	MET	CG-SD-CE	-5.25	91.80	100.20
1	C	68	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	C	73	VAL	CB-CA-C	-5.20	101.52	111.40
1	H	68	TRP	CG-CD2-CE3	5.18	138.56	133.90
1	H	80	ASP	CB-CG-OD1	5.17	122.96	118.30
1	F	118	ASP	CA-CB-CG	5.17	124.77	113.40
1	B	116	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	G	68	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	K	63	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	68	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	C	4	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	F	99	VAL	CG1-CB-CG2	-5.10	102.73	110.90
1	I	4	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	19	GLU	N-CA-CB	-5.10	101.42	110.60
1	J	3	ILE	N-CA-C	-5.10	97.23	111.00
1	B	14	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	119	LEU	CA-CB-CG	5.08	126.99	115.30
1	I	81	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	J	116	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	86	LYS	CA-CB-CG	5.00	124.41	113.40
1	F	68	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	116	ARG	Peptide
1	J	116	ARG	Peptide

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	18	0
1	B	931	208	960	14	0
1	C	939	209	971	20	0
1	D	905	201	936	17	0
1	E	931	208	960	23	0
1	F	939	209	971	19	0
1	G	916	207	949	19	0
1	H	923	207	956	19	0
1	I	905	201	936	24	0
1	J	931	208	960	24	0
1	K	931	208	960	14	0
1	L	905	201	936	25	2
2	A	16	1	10	0	0
2	B	16	1	10	1	0
2	C	16	1	10	2	0
2	D	16	1	10	1	0
2	E	16	1	10	1	0
2	F	16	1	10	1	0
2	G	16	1	10	1	0
2	H	16	1	10	1	0
2	I	16	1	10	1	0
2	J	16	1	10	1	0
2	K	16	1	10	1	0
2	L	16	1	10	1	0
3	A	49	98	0	0	0
3	B	37	74	0	0	0
3	C	56	112	0	0	0
3	D	53	106	0	0	1
3	E	50	100	0	0	0
3	F	48	96	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	42	84	0	0	0
3	H	36	72	0	0	0
3	I	39	78	0	0	0
3	J	37	74	0	0	0
3	K	45	90	0	0	0
3	L	45	90	0	0	0
All	All	11790	3554	11551	215	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 9.

All (215) 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:74:THR:HA	2:E:204:TSA:H3	1.52	0.89
1:J:45:MET:HB3	1:J:73:VAL:HG12	1.59	0.84
1:G:74:THR:HA	2:H:207:TSA:H3	1.60	0.84
1:J:74:THR:HA	2:K:210:TSA:H3	1.61	0.83
1:K:74:THR:HA	2:L:211:TSA:H3	1.61	0.81
2:G:209:TSA:H3	1:I:74:THR:HA	1.65	0.77
1:I:7:ARG:H	1:I:106:HIS:HD2	1.31	0.77
1:K:7:ARG:H	1:K:106:HIS:HD2	1.30	0.77
1:I:12:VAL:HB	1:I:19:GLU:HG3	1.68	0.76
1:K:43:VAL:HB	1:K:94:THR:HG22	1.65	0.76
1:E:7:ARG:H	1:E:106:HIS:HD2	1.34	0.74
1:D:3:ILE:HD13	1:E:3:ILE:HD11	1.68	0.73
1:D:2:MET:HG2	1:D:3:ILE:H	1.53	0.73
1:B:74:THR:HA	2:C:202:TSA:H3	1.72	0.72
1:D:12:VAL:HB	1:D:19:GLU:HG3	1.73	0.70
1:F:62:VAL:HG21	1:F:73:VAL:HG11	1.73	0.69
1:L:45:MET:HB3	1:L:73:VAL:HG12	1.73	0.69
1:G:3:ILE:HG21	1:H:3:ILE:HD11	1.77	0.67
1:E:74:THR:HA	2:F:205:TSA:H3	1.74	0.67
1:L:53:LEU:HD21	1:L:87:LYS:HG2	1.76	0.67
1:B:96:GLN:HB2	1:C:2:MET:SD	2.35	0.67
1:D:53:LEU:HD21	1:D:87:LYS:HG2	1.78	0.66
1:A:74:THR:HA	2:B:201:TSA:H3	1.79	0.65
2:J:212:TSA:H3	1:L:74:THR:HA	1.79	0.65
1:D:62:VAL:HG21	1:D:73:VAL:HG11	1.76	0.65
1:I:2:MET:HG2	1:I:3:ILE:H	1.60	0.64
1:I:51:PRO:HG3	1:I:80:ASP:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:HG11	1:E:20:ILE:HA	1.80	0.63
1:B:7:ARG:H	1:B:106:HIS:HD2	1.44	0.63
1:F:12:VAL:HG12	1:F:23:LYS:HG3	1.81	0.63
1:D:2:MET:HE3	1:F:43:VAL:HG22	1.81	0.63
1:I:4:ARG:HG3	1:I:97:THR:HG23	1.82	0.62
1:D:45:MET:HB3	1:D:73:VAL:HG12	1.80	0.62
1:F:45:MET:HB3	1:F:73:VAL:HG12	1.82	0.62
1:E:6:ILE:HD12	1:E:93:MET:HE2	1.83	0.61
1:H:7:ARG:H	1:H:106:HIS:HD2	1.50	0.60
1:E:7:ARG:H	1:E:106:HIS:CD2	2.17	0.60
1:F:16:THR:HG23	1:F:19:GLU:H	1.67	0.59
1:A:45:MET:HE3	1:A:73:VAL:HG12	1.84	0.59
1:I:30:LYS:HB3	1:I:107:VAL:HG11	1.83	0.59
1:A:12:VAL:HG11	1:A:20:ILE:HA	1.84	0.59
1:C:45:MET:HE2	1:C:93:MET:HG3	1.84	0.59
1:E:85:LEU:HD23	1:E:88:CYS:SG	2.44	0.58
1:D:2:MET:HG2	1:D:3:ILE:N	2.19	0.58
1:F:100:PRO:HD2	1:F:103:GLN:HG3	1.85	0.58
1:G:30:LYS:O	1:G:34:GLU:HG2	2.03	0.58
1:K:8:GLY:HA2	1:K:107:VAL:O	2.05	0.56
1:C:47:LEU:HG	1:C:91:VAL:HG23	1.88	0.56
1:I:88:CYS:SG	1:I:90:ARG:NH1	2.79	0.55
1:J:118:ASP:HB3	1:L:69:GLN:HE22	1.72	0.55
1:G:101:GLN:HE21	1:I:70:TYR:HB2	1.72	0.55
1:K:77:GLN:HG3	1:L:79:MET:HA	1.87	0.55
1:J:2:MET:HG2	1:J:3:ILE:H	1.71	0.54
1:G:20:ILE:HD12	1:G:55:ALA:HB3	1.89	0.54
1:F:85:LEU:HD23	1:F:88:CYS:SG	2.48	0.54
1:B:45:MET:HB3	1:B:73:VAL:HG12	1.89	0.54
1:K:17:GLU:HG3	1:K:56:VAL:HB	1.88	0.54
1:J:30:LYS:HB3	1:J:107:VAL:HG11	1.90	0.53
1:C:2:MET:HG2	1:C:3:ILE:H	1.74	0.53
1:C:12:VAL:HG12	1:C:23:LYS:HG3	1.90	0.53
1:A:25:LYS:NZ	1:A:25:LYS:HB3	2.23	0.53
1:G:7:ARG:H	1:G:106:HIS:CD2	2.27	0.53
1:H:14:ARG:H	1:H:19:GLU:HG2	1.74	0.52
1:F:8:GLY:HA2	1:F:107:VAL:O	2.11	0.51
1:G:51:PRO:HG2	1:G:80:ASP:HB2	1.92	0.51
1:B:8:GLY:HA2	1:B:107:VAL:O	2.11	0.50
1:D:21:LEU:HD21	1:D:60:LYS:HB3	1.92	0.50
1:H:13:GLU:HG3	1:H:14:ARG:NH1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:GLN:HE21	1:L:70:TYR:HB2	1.76	0.50
1:H:22:GLN:HG2	1:H:23:LYS:NZ	2.27	0.50
1:C:60:LYS:HG3	1:C:63:ARG:HH21	1.77	0.50
1:H:8:GLY:HA2	1:H:107:VAL:O	2.12	0.50
1:B:39:PRO:O	1:C:101:GLN:NE2	2.45	0.50
1:H:74:THR:HA	2:I:208:TSA:H3	1.92	0.50
1:A:7:ARG:H	1:A:106:HIS:CD2	2.29	0.50
1:B:6:ILE:HD12	1:B:93:MET:HE3	1.93	0.50
1:E:45:MET:HB3	1:E:73:VAL:HB	1.94	0.50
1:G:3:ILE:HD11	1:H:2:MET:CE	2.42	0.50
1:A:45:MET:HE3	1:A:73:VAL:CG1	2.41	0.50
1:I:7:ARG:H	1:I:106:HIS:CD2	2.20	0.49
1:B:17:GLU:O	1:B:21:LEU:HG	2.12	0.49
1:C:47:LEU:O	1:C:75:CYS:HA	2.12	0.49
1:F:51:PRO:HG2	1:F:80:ASP:HB2	1.94	0.49
1:I:68:TRP:CE3	1:I:71:VAL:HG21	2.47	0.49
1:L:8:GLY:HA2	1:L:107:VAL:O	2.12	0.49
1:J:30:LYS:O	1:J:34:GLU:HB2	2.12	0.49
1:L:78:GLU:HG2	1:L:90:ARG:NH1	2.27	0.49
1:C:7:ARG:H	1:C:106:HIS:HD2	1.60	0.49
1:C:90:ARG:HD3	2:C:202:TSA:O3	2.12	0.49
1:K:5:GLY:HA3	1:K:92:MET:HE1	1.95	0.49
1:G:48:SER:HB3	1:G:76:MET:HG3	1.95	0.49
1:E:8:GLY:HA2	1:E:107:VAL:O	2.13	0.49
1:J:62:VAL:HG21	1:J:73:VAL:HG11	1.94	0.49
2:D:206:TSA:H3	1:F:74:THR:HA	1.95	0.49
1:B:6:ILE:HD12	1:B:93:MET:CE	2.43	0.48
1:A:85:LEU:HG	1:A:88:CYS:HB2	1.95	0.48
1:A:47:LEU:O	1:A:75:CYS:HA	2.14	0.48
1:G:8:GLY:HA2	1:G:107:VAL:O	2.13	0.48
1:F:110:GLU:O	1:F:113:VAL:HG22	2.13	0.48
1:C:109:LEU:O	1:C:112:ALA:HB3	2.13	0.48
1:C:16:THR:CG2	1:C:19:GLU:HB2	2.44	0.48
1:J:3:ILE:HA	1:J:95:VAL:O	2.14	0.48
1:K:46:LEU:HD23	1:K:74:THR:HG22	1.94	0.48
1:I:4:ARG:HG3	1:I:97:THR:CG2	2.43	0.47
1:B:2:MET:HE2	1:B:3:ILE:H	1.80	0.47
1:H:79:MET:HG3	1:H:81:VAL:HG23	1.96	0.47
1:J:38:LYS:HA	1:J:38:LYS:HD3	1.75	0.47
1:D:48:SER:HB3	1:D:76:MET:HG3	1.95	0.47
1:C:7:ARG:N	1:C:106:HIS:HD2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:VAL:HB	1:F:19:GLU:HG2	1.97	0.46
1:D:8:GLY:HA3	1:D:31:ILE:HD11	1.97	0.46
1:J:51:PRO:HG3	1:J:80:ASP:HB2	1.96	0.46
1:A:5:GLY:HA2	1:A:93:MET:O	2.15	0.46
1:G:3:ILE:HD11	1:H:2:MET:HE1	1.98	0.46
1:A:6:ILE:HD12	1:A:93:MET:CE	2.46	0.46
1:G:68:TRP:CZ3	1:G:93:MET:HE1	2.51	0.46
1:I:48:SER:HA	1:I:76:MET:O	2.15	0.46
1:J:109:LEU:O	1:J:112:ALA:HB3	2.16	0.46
1:J:3:ILE:HG22	1:L:43:VAL:CG1	2.46	0.46
1:C:60:LYS:HA	1:C:63:ARG:NE	2.31	0.46
1:E:47:LEU:O	1:E:75:CYS:HA	2.15	0.46
1:K:47:LEU:O	1:K:75:CYS:HA	2.16	0.45
1:J:47:LEU:O	1:J:75:CYS:HA	2.15	0.45
1:I:39:PRO:HG3	1:I:68:TRP:NE1	2.30	0.45
1:A:3:ILE:HA	1:A:96:GLN:HA	1.99	0.45
1:A:79:MET:HG3	1:A:81:VAL:HG23	1.99	0.45
1:E:16:THR:HB	1:E:19:GLU:HB3	1.98	0.45
1:I:59:ALA:HB2	1:I:75:CYS:SG	2.57	0.45
1:A:11:THR:HG21	1:A:85:LEU:HD11	1.99	0.45
1:H:59:ALA:HB2	1:H:75:CYS:SG	2.57	0.45
1:J:20:ILE:HD12	1:J:55:ALA:HB3	1.98	0.45
1:E:46:LEU:HA	1:E:74:THR:O	2.17	0.44
1:L:59:ALA:HB2	1:L:75:CYS:SG	2.58	0.44
1:L:30:LYS:HA	1:L:30:LYS:HD2	1.77	0.44
1:G:3:ILE:HA	1:G:95:VAL:O	2.18	0.44
1:C:30:LYS:O	1:C:34:GLU:HG2	2.17	0.44
1:I:105:ARG:HA	1:I:105:ARG:HD3	1.79	0.44
1:L:47:LEU:O	1:L:75:CYS:HA	2.17	0.44
1:E:78:GLU:HG2	1:E:90:ARG:NH1	2.33	0.44
1:J:63:ARG:HH21	1:J:69:GLN:HG3	1.82	0.44
1:G:30:LYS:HA	1:G:30:LYS:HD2	1.77	0.43
1:K:99:VAL:HA	1:K:100:PRO:HD3	1.88	0.43
1:C:8:GLY:HA2	1:C:107:VAL:O	2.18	0.43
1:F:7:ARG:NH2	1:F:90:ARG:HB3	2.33	0.43
1:K:43:VAL:CG1	1:L:3:ILE:HG13	2.49	0.43
1:J:51:PRO:HB3	1:J:77:GLN:NE2	2.33	0.43
1:B:34:GLU:HB3	1:B:105:ARG:HD3	1.99	0.43
1:A:46:LEU:HA	1:A:74:THR:O	2.17	0.43
1:I:47:LEU:O	1:I:75:CYS:HA	2.18	0.43
1:G:3:ILE:HG22	1:I:43:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ILE:HD12	1:H:55:ALA:HB3	1.99	0.43
1:L:6:ILE:HG21	1:L:31:ILE:HG23	2.00	0.43
1:K:59:ALA:HB1	1:K:73:VAL:HG21	2.00	0.43
1:I:12:VAL:HB	1:I:19:GLU:CG	2.43	0.43
1:C:2:MET:HG2	1:C:3:ILE:N	2.33	0.43
1:B:56:VAL:HG21	1:B:60:LYS:HD2	2.01	0.43
1:L:20:ILE:HD12	1:L:55:ALA:HB3	2.01	0.43
1:J:3:ILE:HG22	1:L:43:VAL:HG11	2.00	0.43
1:H:7:ARG:NH2	1:H:90:ARG:HG2	2.34	0.43
1:I:11:THR:HG22	1:I:88:CYS:HB2	1.99	0.43
1:D:78:GLU:HG2	1:D:90:ARG:HH21	1.84	0.42
1:D:3:ILE:HD12	1:F:43:VAL:HG11	2.01	0.42
1:E:46:LEU:HD23	1:E:74:THR:HG22	2.01	0.42
1:F:16:THR:HG22	1:F:19:GLU:HB2	2.01	0.42
1:E:45:MET:O	1:E:73:VAL:HA	2.20	0.42
1:C:16:THR:HG22	1:C:19:GLU:HB2	2.01	0.42
1:D:20:ILE:HG23	1:D:89:ILE:CD1	2.50	0.42
1:E:51:PRO:HB3	1:E:77:GLN:OE1	2.19	0.42
1:J:23:LYS:HD3	1:J:26:GLN:NE2	2.35	0.42
1:H:6:ILE:HD11	1:H:95:VAL:HG21	2.01	0.42
1:B:10:THR:HA	1:B:109:LEU:O	2.19	0.42
1:L:79:MET:HG3	1:L:81:VAL:HG23	2.02	0.42
1:J:38:LYS:HB3	1:J:40:GLU:OE2	2.20	0.42
1:B:78:GLU:HG2	1:B:90:ARG:NH1	2.35	0.42
1:G:74:THR:HB	1:H:7:ARG:HD3	2.02	0.42
1:J:79:MET:HA	1:L:77:GLN:HG3	2.01	0.42
1:L:25:LYS:O	1:L:29:GLU:HG3	2.20	0.42
1:F:14:ARG:NH2	1:F:16:THR:HG21	2.33	0.42
1:F:99:VAL:HA	1:F:100:PRO:HD3	1.89	0.42
1:H:62:VAL:HG21	1:H:73:VAL:HG11	2.02	0.42
1:I:2:MET:HG2	1:I:3:ILE:N	2.31	0.42
1:H:47:LEU:O	1:H:75:CYS:HA	2.19	0.42
1:A:45:MET:HB3	1:A:73:VAL:HG12	2.01	0.41
1:H:25:LYS:HD3	1:H:64:GLU:OE1	2.20	0.41
1:E:109:LEU:O	1:E:112:ALA:HB3	2.20	0.41
1:A:9:ALA:HB3	1:A:108:TYR:CD1	2.56	0.41
1:E:48:SER:HA	1:E:76:MET:O	2.21	0.41
1:E:21:LEU:HD21	1:E:60:LYS:HB3	2.03	0.41
1:D:16:THR:HG23	1:D:19:GLU:CB	2.51	0.41
1:F:10:THR:O	1:F:88:CYS:HA	2.21	0.41
1:J:68:TRP:N	1:J:68:TRP:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:116:ARG:HH11	1:K:116:ARG:HA	1.85	0.41
1:C:51:PRO:HG3	1:C:80:ASP:HB2	2.03	0.41
1:A:7:ARG:N	1:A:106:HIS:HD2	2.18	0.41
1:L:108:TYR:O	1:L:113:VAL:HG12	2.20	0.41
1:D:30:LYS:HB3	1:D:107:VAL:HG11	2.02	0.41
1:E:24:THR:OG1	1:E:89:ILE:HD13	2.20	0.41
1:F:59:ALA:HB2	1:F:75:CYS:SG	2.61	0.41
1:I:111:LYS:O	1:I:114:VAL:HG12	2.21	0.41
1:L:57:PHE:HA	1:L:58:PRO:HD3	1.96	0.41
1:E:25:LYS:O	1:E:29:GLU:HG3	2.20	0.41
1:G:30:LYS:CG	1:G:107:VAL:HG11	2.51	0.41
1:G:43:VAL:HB	1:G:94:THR:HB	2.02	0.41
1:G:112:ALA:HB1	1:G:115:LEU:HD12	2.03	0.40
1:J:30:LYS:HA	1:J:30:LYS:HD2	1.98	0.40
1:L:9:ALA:HB3	1:L:108:TYR:CD1	2.55	0.40
1:A:94:THR:OG1	1:C:44:GLN:NE2	2.53	0.40
1:K:43:VAL:HG11	1:L:3:ILE:HG13	2.03	0.40
1:E:46:LEU:CD2	1:E:74:THR:HG22	2.52	0.40
1:L:14:ARG:NH2	1:L:16:THR:HG21	2.35	0.40
1:I:85:LEU:HD21	1:I:112:ALA:HA	2.03	0.40
1:E:99:VAL:HA	1:E:100:PRO:HD2	1.68	0.40
1:J:101:GLN:OE1	1:L:40:GLU:HA	2.22	0.40
1:H:48:SER:HA	1:H:76:MET:O	2.21	0.40
1:I:8:GLY:HA3	1:I:31:ILE:HD11	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:L:86:LYS:HZ2	3:F:228:HOH:H2[1_556]	1.26	0.34
1:L:96:GLN:O	3:D:272:HOH:H1[2_746]	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%)	107 (96%)	5 (4%)	0	100	100
1	B	115/127 (91%)	108 (94%)	6 (5%)	1 (1%)	21	19
1	C	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
1	D	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
1	E	115/127 (91%)	108 (94%)	7 (6%)	0	100	100
1	F	116/127 (91%)	108 (93%)	7 (6%)	1 (1%)	21	19
1	G	113/127 (89%)	105 (93%)	8 (7%)	0	100	100
1	H	114/127 (90%)	107 (94%)	7 (6%)	0	100	100
1	I	112/127 (88%)	105 (94%)	7 (6%)	0	100	100
1	J	115/127 (91%)	108 (94%)	7 (6%)	0	100	100
1	K	115/127 (91%)	112 (97%)	3 (3%)	0	100	100
1	L	112/127 (88%)	104 (93%)	7 (6%)	1 (1%)	21	19
All	All	1367/1524 (90%)	1284 (94%)	80 (6%)	3 (0%)	52	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	118	ASP
1	L	101	GLN
1	B	117	PRO

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%)	94 (91%)	9 (9%)	13	12
1	B	106/116 (91%)	100 (94%)	6 (6%)	25	29
1	C	107/116 (92%)	98 (92%)	9 (8%)	14	13
1	D	103/116 (89%)	100 (97%)	3 (3%)	50	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	106/116 (91%)	99 (93%)	7 (7%)	21	22
1	F	107/116 (92%)	100 (94%)	7 (6%)	21	23
1	G	104/116 (90%)	98 (94%)	6 (6%)	25	28
1	H	105/116 (90%)	103 (98%)	2 (2%)	65	77
1	I	103/116 (89%)	100 (97%)	3 (3%)	50	62
1	J	106/116 (91%)	99 (93%)	7 (7%)	21	22
1	K	106/116 (91%)	98 (92%)	8 (8%)	17	17
1	L	103/116 (89%)	100 (97%)	3 (3%)	50	62
All	All	1259/1392 (90%)	1189 (94%)	70 (6%)	26	29

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	13	GLU
1	A	45	MET
1	A	50	THR
1	A	66	SER
1	A	74	THR
1	A	76	MET
1	A	85	LEU
1	A	114	VAL
1	B	2	MET
1	B	16	THR
1	B	50	THR
1	B	63	ARG
1	B	69	GLN
1	B	74	THR
1	C	3	ILE
1	C	38	LYS
1	C	47	LEU
1	C	63	ARG
1	C	73	VAL
1	C	74	THR
1	C	76	MET
1	C	77	GLN
1	C	91	VAL
1	D	17	GLU
1	D	47	LEU

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Mol	Chain	Res	Type
1	D	114	VAL
1	E	2	MET
1	E	45	MET
1	E	50	THR
1	E	73	VAL
1	E	74	THR
1	E	77	GLN
1	E	82	THR
1	F	18	GLU
1	F	19	GLU
1	F	36	HIS
1	F	37	THR
1	F	52	ASP
1	F	113	VAL
1	F	114	VAL
1	G	2	MET
1	G	10	THR
1	G	16	THR
1	G	34	GLU
1	G	44	GLN
1	G	105	ARG
1	H	2	MET
1	H	76	MET
1	I	4	ARG
1	I	69	GLN
1	I	98	ASP
1	J	26	GLN
1	J	34	GLU
1	J	52	ASP
1	J	76	MET
1	J	77	GLN
1	J	105	ARG
1	J	111	LYS
1	K	2	MET
1	K	18	GLU
1	K	19	GLU
1	K	63	ARG
1	K	74	THR
1	K	94	THR
1	K	98	ASP
1	K	118	ASP
1	L	38	LYS

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Mol	Chain	Res	Type
1	L	52	ASP
1	L	114	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	101	GLN
1	A	103	GLN
1	A	106	HIS
1	B	44	GLN
1	B	101	GLN
1	B	106	HIS
1	C	44	GLN
1	C	69	GLN
1	C	101	GLN
1	C	106	HIS
1	D	44	GLN
1	D	106	HIS
1	E	44	GLN
1	E	77	GLN
1	E	106	HIS
1	F	44	GLN
1	F	106	HIS
1	G	44	GLN
1	G	101	GLN
1	G	106	HIS
1	H	44	GLN
1	H	103	GLN
1	H	106	HIS
1	I	44	GLN
1	I	106	HIS
1	J	26	GLN
1	J	44	GLN
1	J	77	GLN
1	J	103	GLN
1	J	106	HIS
1	K	22	GLN
1	K	44	GLN
1	K	96	GLN
1	K	106	HIS
1	L	44	GLN

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Mol	Chain	Res	Type
1	L	106	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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	TSA	A	203	-	11,17,17	1.20	1 (9%)	7,26,26	2.36	2 (28%)
2	TSA	B	201	-	11,17,17	1.29	2 (18%)	7,26,26	2.14	2 (28%)
2	TSA	C	202	-	11,17,17	1.16	0	7,26,26	2.52	2 (28%)
2	TSA	D	206	-	11,17,17	1.19	1 (9%)	7,26,26	2.38	1 (14%)
2	TSA	E	204	-	11,17,17	1.20	1 (9%)	7,26,26	2.13	2 (28%)
2	TSA	F	205	-	11,17,17	1.12	1 (9%)	7,26,26	2.37	2 (28%)
2	TSA	G	209	-	11,17,17	1.19	1 (9%)	7,26,26	2.07	2 (28%)
2	TSA	H	207	-	11,17,17	1.27	2 (18%)	7,26,26	2.35	1 (14%)
2	TSA	I	208	-	11,17,17	1.33	2 (18%)	7,26,26	2.29	2 (28%)
2	TSA	J	212	-	11,17,17	1.22	1 (9%)	7,26,26	2.28	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TSA	K	210	-	11,17,17	1.23	2 (18%)	7,26,26	2.32	2 (28%)
2	TSA	L	211	-	11,17,17	1.18	2 (18%)	7,26,26	2.45	2 (28%)

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	TSA	A	203	-	-	0/0/34/34	0/0/2/2
2	TSA	B	201	-	-	0/0/34/34	0/0/2/2
2	TSA	C	202	-	-	0/0/34/34	0/0/2/2
2	TSA	D	206	-	-	0/0/34/34	0/0/2/2
2	TSA	E	204	-	-	0/0/34/34	0/0/2/2
2	TSA	F	205	-	-	0/0/34/34	0/0/2/2
2	TSA	G	209	-	-	0/0/34/34	0/0/2/2
2	TSA	H	207	-	-	0/0/34/34	0/0/2/2
2	TSA	I	208	-	-	0/0/34/34	0/0/2/2
2	TSA	J	212	-	-	0/0/34/34	0/0/2/2
2	TSA	K	210	-	-	0/0/34/34	0/0/2/2
2	TSA	L	211	-	-	0/0/34/34	0/0/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	TSA	O5-C4	-2.17	1.39	1.43
2	K	210	TSA	C1-C10	2.01	1.54	1.50
2	J	212	TSA	C3-C2	2.04	1.35	1.32
2	G	209	TSA	C1-C10	2.04	1.54	1.50
2	I	208	TSA	C3-C2	2.09	1.36	1.32
2	A	203	TSA	C1-C10	2.09	1.54	1.50
2	L	211	TSA	C1-C10	2.10	1.54	1.50
2	L	211	TSA	C3-C2	2.11	1.36	1.32
2	D	206	TSA	C1-C10	2.15	1.54	1.50
2	H	207	TSA	C3-C2	2.20	1.36	1.32
2	F	205	TSA	C1-C10	2.20	1.54	1.50
2	K	210	TSA	C3-C2	2.21	1.36	1.32
2	E	204	TSA	C1-C10	2.29	1.54	1.50
2	B	201	TSA	C1-C10	2.40	1.55	1.50
2	I	208	TSA	C1-C10	2.41	1.55	1.50
2	H	207	TSA	C1-C10	2.53	1.55	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	210	TSA	O7-C5-C6	-2.24	106.90	109.81
2	B	201	TSA	O5-C4-C3	-2.22	104.81	110.00
2	A	203	TSA	O7-C5-C6	-2.11	107.07	109.81
2	G	209	TSA	O7-C8-C9	2.34	112.93	109.62
2	L	211	TSA	O7-C8-C9	2.53	113.19	109.62
2	F	205	TSA	O7-C8-C9	2.62	113.33	109.62
2	E	204	TSA	O7-C8-C9	3.09	114.00	109.62
2	I	208	TSA	O7-C8-C9	3.32	114.32	109.62
2	C	202	TSA	O7-C8-C9	3.87	115.10	109.62
2	E	204	TSA	C5-O7-C8	4.23	120.84	112.28
2	I	208	TSA	C5-O7-C8	4.49	121.36	112.28
2	B	201	TSA	C5-O7-C8	4.51	121.41	112.28
2	G	209	TSA	C5-O7-C8	4.67	121.73	112.28
2	C	202	TSA	C5-O7-C8	4.85	122.09	112.28
2	A	203	TSA	C5-O7-C8	5.00	122.40	112.28
2	J	212	TSA	C5-O7-C8	5.03	122.46	112.28
2	D	206	TSA	C5-O7-C8	5.20	122.79	112.28
2	F	205	TSA	C5-O7-C8	5.27	122.93	112.28
2	K	210	TSA	C5-O7-C8	5.34	123.08	112.28
2	L	211	TSA	C5-O7-C8	5.51	123.43	112.28
2	H	207	TSA	C5-O7-C8	5.64	123.69	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	TSA	1	0
2	C	202	TSA	2	0
2	D	206	TSA	1	0
2	E	204	TSA	1	0
2	F	205	TSA	1	0
2	G	209	TSA	1	0
2	H	207	TSA	1	0
2	I	208	TSA	1	0
2	J	212	TSA	1	0
2	K	210	TSA	1	0
2	L	211	TSA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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