



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2017 – 01:10 AM EST

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 : unknown
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (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

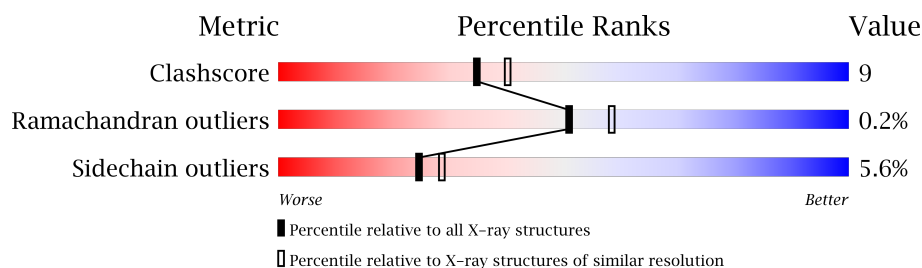
1 Overall quality at a glance

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 ≥ 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	 65% 22% .. 10%
1	B	127	 65% 25% .. 8%
1	C	127	 65% 23% 5% • 7%
1	D	127	 65% 23% • 10%
1	E	127	 60% 27% 6% 8%
1	F	127	 62% 27% • 7%
1	G	127	 66% 21% • 9%

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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

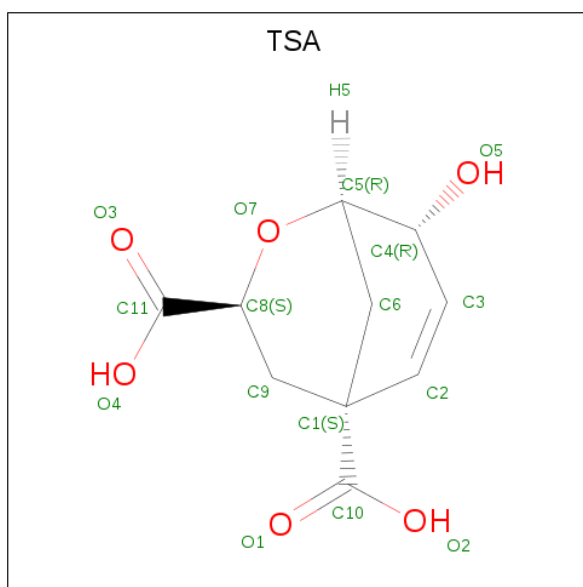
There are 3 unique types of molecules in this entry. The entry contains 15344 atoms, of which 3554 are hydrogens and 0 are deuteriums.

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	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	I	1	Total	C	H	O	0	0
			17	10	1	6		
2	J	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		

- Molecule 3 is water.

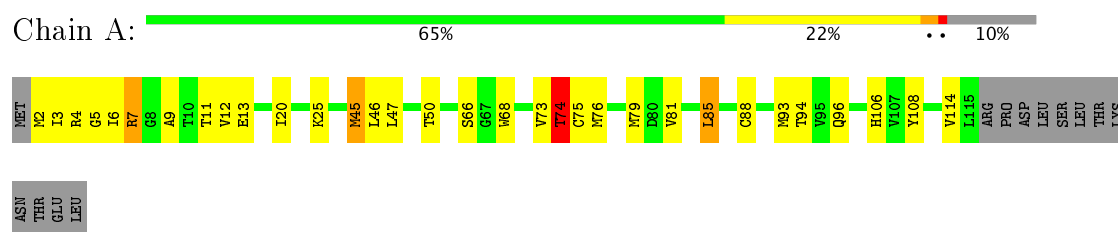
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	49	Total	H	O	0	0
			147	98	49		
3	B	37	Total	H	O	0	0
			111	74	37		
3	C	56	Total	H	O	0	0
			168	112	56		
3	D	53	Total	H	O	0	0
			159	106	53		
3	E	50	Total	H	O	0	0
			150	100	50		
3	F	48	Total	H	O	0	0
			144	96	48		
3	G	42	Total	H	O	0	0
			126	84	42		
3	H	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](#)

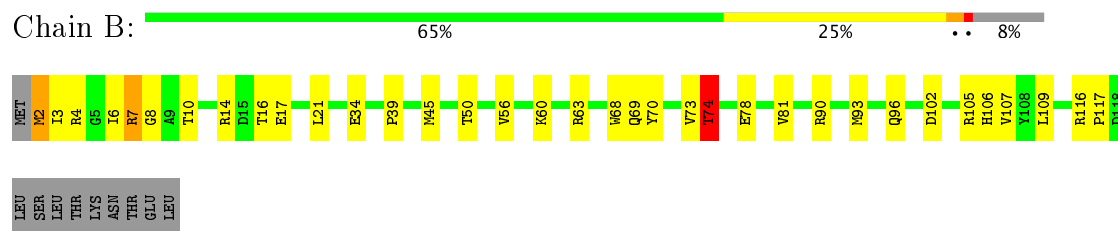
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

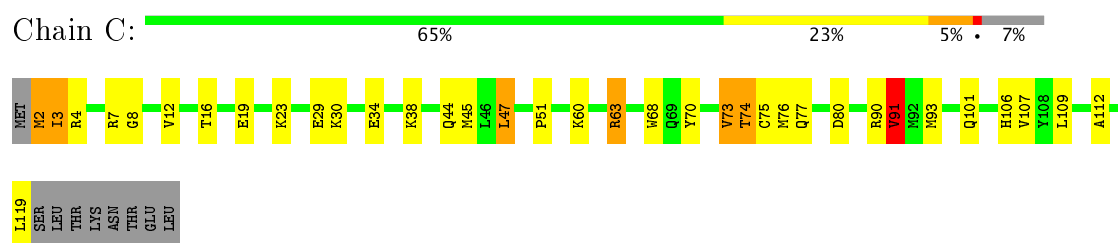
• Molecule 1: CHORISMATE MUTASE



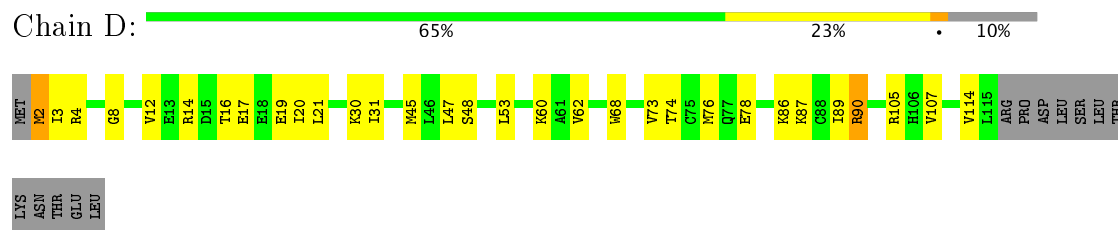
• Molecule 1: CHORISMATE MUTASE



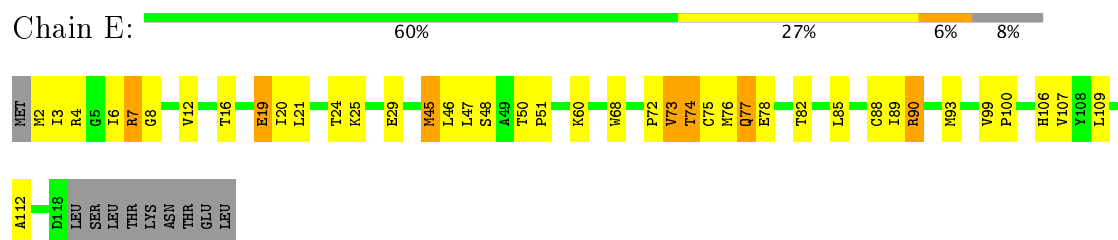
• Molecule 1: CHORISMATE MUTASE



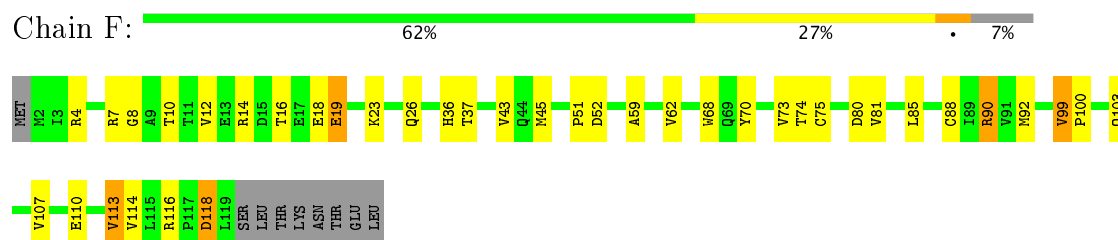
• Molecule 1: CHORISMATE MUTASE



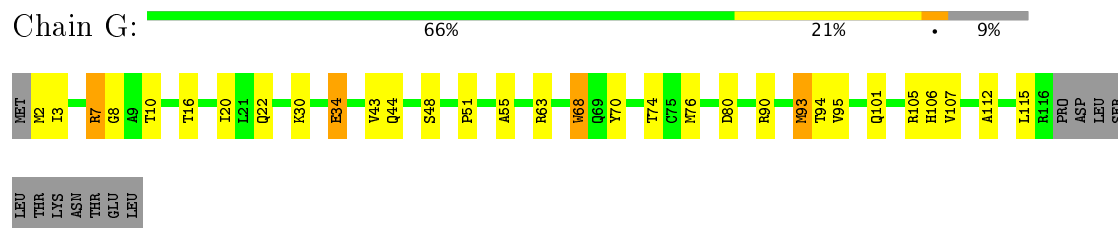
- Molecule 1: CHORISMATE MUTASE



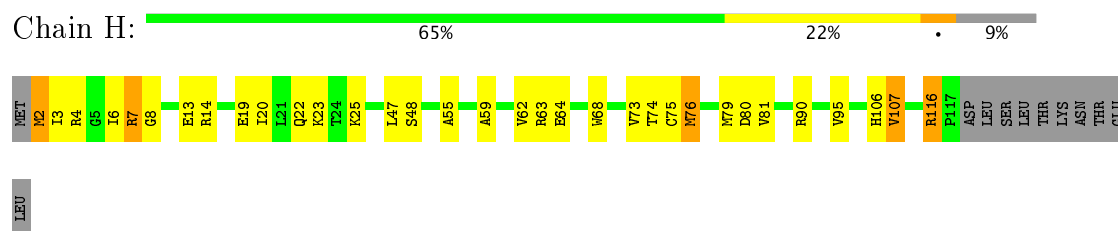
- Molecule 1: CHORISMATE MUTASE



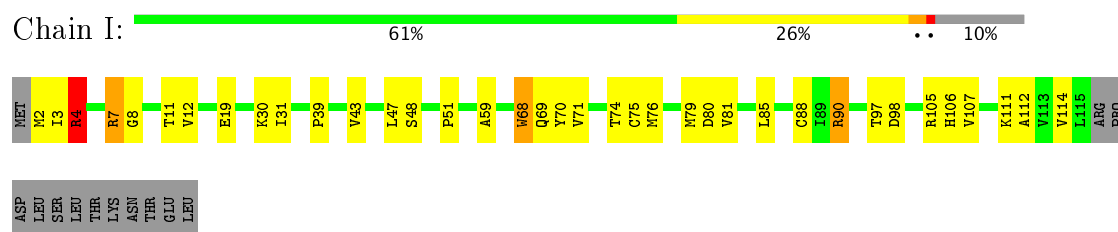
- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE

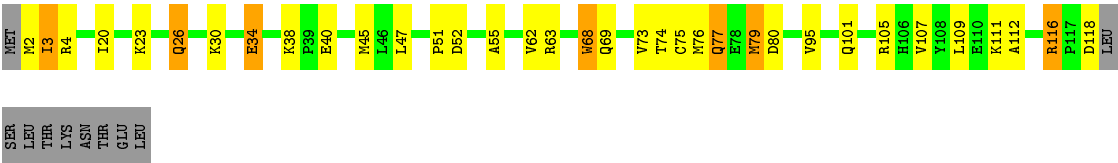


- Molecule 1: CHORISMATE MUTASE

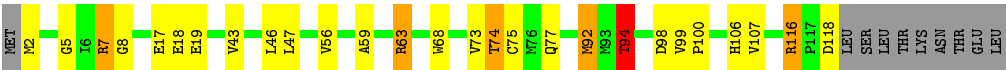


- Molecule 1: CHORISMATE MUTASE

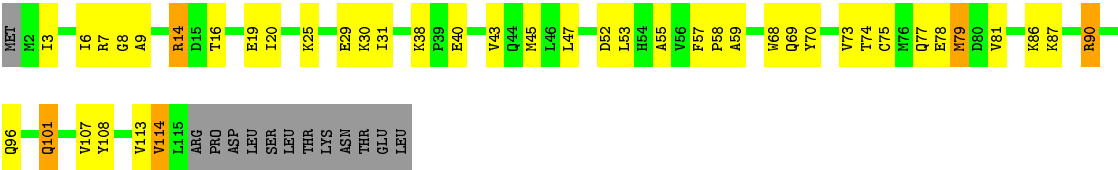




• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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.

The worst 5 of 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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

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%)	20	18
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%)	20	18
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%)	20	18
All	All	1367/1524 (90%)	1284 (94%)	80 (6%)	3 (0%)	51	58

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%)	12	12
1	B	106/116 (91%)	100 (94%)	6 (6%)	24	28
1	C	107/116 (92%)	98 (92%)	9 (8%)	13	12
1	D	103/116 (89%)	100 (97%)	3 (3%)	48	60
1	E	106/116 (91%)	99 (93%)	7 (7%)	19	21
1	F	107/116 (92%)	100 (94%)	7 (6%)	20	22
1	G	104/116 (90%)	98 (94%)	6 (6%)	23	27
1	H	105/116 (90%)	103 (98%)	2 (2%)	62	76
1	I	103/116 (89%)	100 (97%)	3 (3%)	48	60
1	J	106/116 (91%)	99 (93%)	7 (7%)	19	21
1	K	106/116 (91%)	98 (92%)	8 (8%)	16	16
1	L	103/116 (89%)	100 (97%)	3 (3%)	48	60
All	All	1259/1392 (90%)	1189 (94%)	70 (6%)	25	29

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	74	THR
1	F	113	VAL
1	K	94	THR
1	E	77	GLN
1	F	19	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	44	GLN
1	G	106	HIS
1	K	106	HIS
1	F	106	HIS
1	G	44	GLN

5.3.3 RNA ⓘ

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](#)

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	1.21	1 (9%)	7,26,26	2.49	2 (28%)
2	TSA	B	201	-	11,17,17	1.31	2 (18%)	7,26,26	2.18	3 (42%)
2	TSA	C	202	-	11,17,17	1.13	0	7,26,26	2.56	2 (28%)
2	TSA	D	206	-	11,17,17	1.19	1 (9%)	7,26,26	2.36	1 (14%)
2	TSA	E	204	-	11,17,17	1.20	1 (9%)	7,26,26	2.20	2 (28%)
2	TSA	F	205	-	11,17,17	1.11	1 (9%)	7,26,26	2.43	2 (28%)
2	TSA	G	209	-	11,17,17	1.18	2 (18%)	7,26,26	2.15	2 (28%)
2	TSA	H	207	-	11,17,17	1.28	2 (18%)	7,26,26	2.51	2 (28%)
2	TSA	I	208	-	11,17,17	1.32	2 (18%)	7,26,26	2.37	2 (28%)
2	TSA	J	212	-	11,17,17	1.21	1 (9%)	7,26,26	2.31	2 (28%)
2	TSA	K	210	-	11,17,17	1.22	2 (18%)	7,26,26	2.36	2 (28%)
2	TSA	L	211	-	11,17,17	1.17	2 (18%)	7,26,26	2.65	3 (42%)

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

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	TSA	O5-C4	-2.25	1.39	1.43
2	K	210	TSA	C1-C10	2.02	1.54	1.50
2	G	209	TSA	C3-C2	2.06	1.35	1.32
2	G	209	TSA	C1-C10	2.06	1.54	1.50
2	A	203	TSA	C1-C10	2.11	1.54	1.50

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	211	TSA	O5-C4-C5	-2.86	105.44	110.94
2	K	210	TSA	O7-C5-C6	-2.41	106.90	109.83
2	A	203	TSA	O7-C5-C6	-2.28	107.07	109.83
2	B	201	TSA	O5-C4-C3	-2.22	104.81	110.00
2	J	212	TSA	O7-C5-C6	-2.09	107.30	109.83

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 ⓘ

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.