



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:37 AM UTC

PDB ID : 2CHT / pdb_00002cht
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

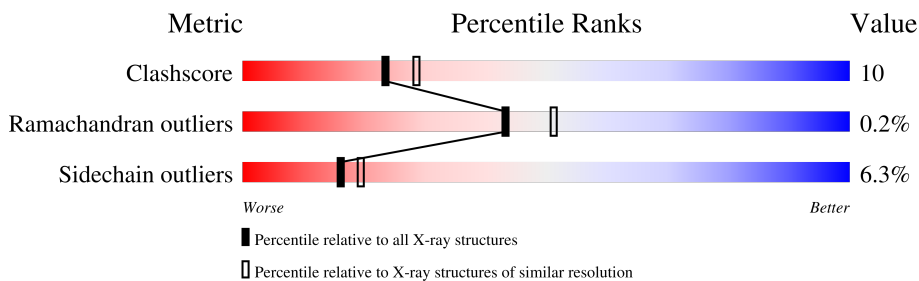
1 Overall quality at a glance i

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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	56% 28% 6% • 10%
1	B	127	54% 32% • • 8%
1	C	127	61% 25% 6% • 7%
1	D	127	59% 29% • 10%
1	E	127	47% 39% 6% • 8%
1	F	127	57% 32% • 7%
1	G	127	61% 25% • • 9%
1	H	127	60% 28% • 9%

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Mol	Chain	Length	Quality of chain
1	I	127	 52% 34% • 10%
1	J	127	 56% 26% 10% 8%
1	K	127	 61% 25% • • 8%
1	L	127	 46% 36% 7% 10%

2 Entry composition [i](#)

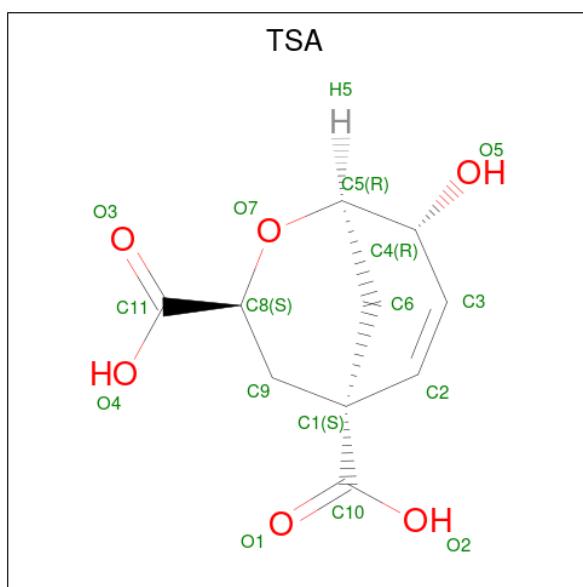
There are 3 unique types of molecules in this entry. The entry contains 15344 atoms, of which 3554 are hydrogens and 0 are deuteriums.

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

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



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

- 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		

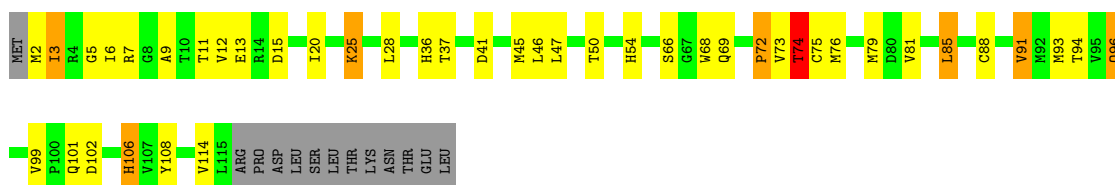
3 Residue-property plots [i](#)

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

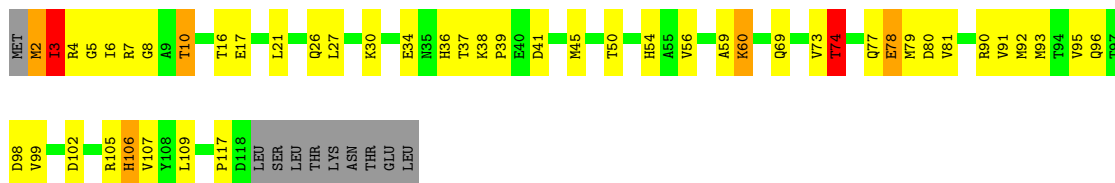
- Molecule 1: CHORISMATE MUTASE

Chain A:  56% 28% 6% • 10%



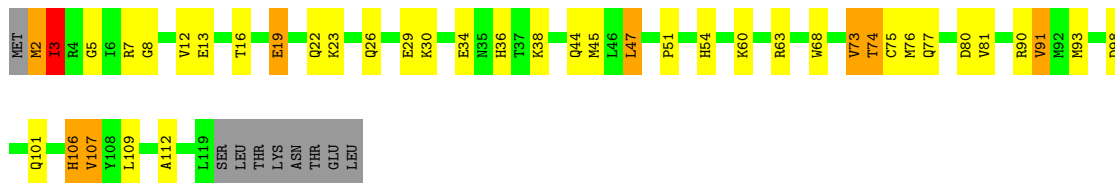
- Molecule 1: CHORISMATE MUTASE

Chain B:  54% 32% • • 8%



- Molecule 1: CHORISMATE MUTASE

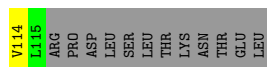
Chain C:  61% 25% 6% • 7%



- Molecule 1: CHORISMATE MUTASE

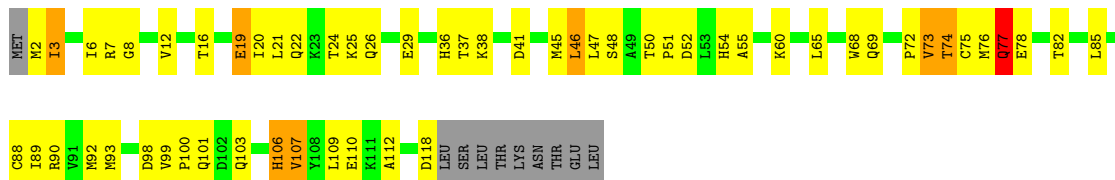
Chain D:  59% 29% • 10%





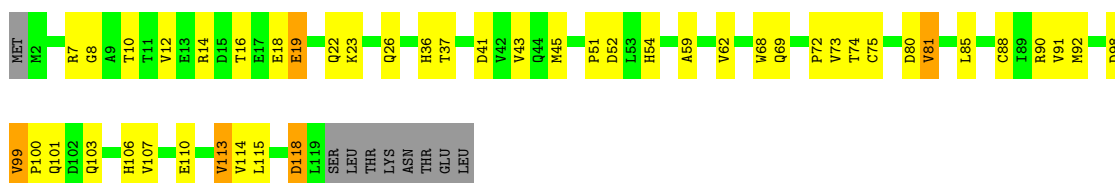
- Molecule 1: CHORISMATE MUTASE

Chain E: 47% 39% 6% • 8%



- Molecule 1: CHORISMATE MUTASE

Chain F: 57% 32% • 7%



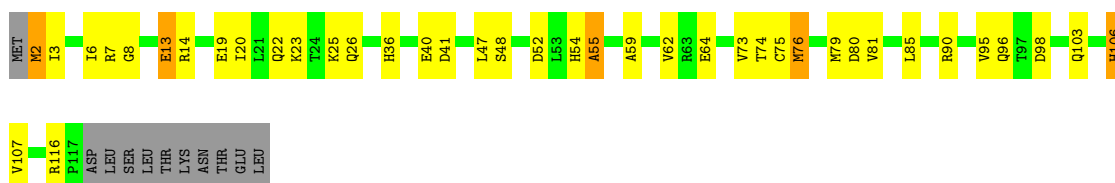
- Molecule 1: CHORISMATE MUTASE

Chain G: 61% 25% • • 9%



- Molecule 1: CHORISMATE MUTASE

Chain H: 60% 28% • 9%



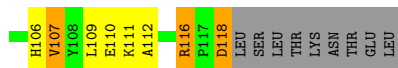
- Molecule 1: CHORISMATE MUTASE

Chain I: 52% 34% • 10%

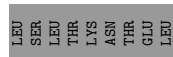




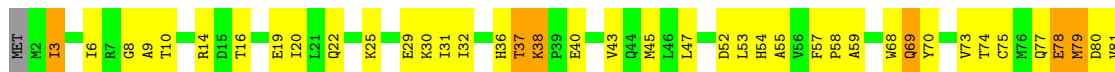
- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



- Molecule 1: CHORISMATE MUTASE



4 Data and refinement statistics

Xtrriage (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	102.40Å 68.30Å 102.80Å 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.	Xtrriage
Total number of atoms	15344	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	0.99	5/917 (0.5%)	1.81	23/1240 (1.9%)
1	B	1.02	4/944 (0.4%)	1.81	21/1277 (1.6%)
1	C	0.95	4/952 (0.4%)	1.74	17/1288 (1.3%)
1	D	1.00	3/917 (0.3%)	1.75	11/1240 (0.9%)
1	E	0.99	4/944 (0.4%)	1.76	24/1277 (1.9%)
1	F	0.99	4/952 (0.4%)	1.82	19/1288 (1.5%)
1	G	0.92	3/928 (0.3%)	1.74	16/1254 (1.3%)
1	H	0.92	3/936 (0.3%)	1.66	13/1266 (1.0%)
1	I	0.97	4/917 (0.4%)	1.72	17/1240 (1.4%)
1	J	1.01	4/944 (0.4%)	1.73	21/1277 (1.6%)
1	K	0.99	5/944 (0.5%)	1.74	17/1277 (1.3%)
1	L	1.03	4/917 (0.4%)	1.81	22/1240 (1.8%)
All	All	0.98	47/11212 (0.4%)	1.76	221/15164 (1.5%)

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

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	54	HIS	CD2-NE2	-7.14	1.30	1.37
1	K	54	HIS	CD2-NE2	-6.98	1.30	1.37
1	B	106	HIS	CD2-NE2	-6.97	1.30	1.37
1	C	54	HIS	CD2-NE2	-6.94	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	106	HIS	CD2-NE2	-6.91	1.30	1.37
1	E	106	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	54	HIS	CD2-NE2	-6.65	1.30	1.37
1	C	36	HIS	CD2-NE2	-6.64	1.30	1.37
1	F	54	HIS	CD2-NE2	-6.60	1.30	1.37
1	H	36	HIS	CD2-NE2	-6.57	1.30	1.37
1	G	106	HIS	CD2-NE2	-6.55	1.30	1.37
1	K	106	HIS	CD2-NE2	-6.55	1.30	1.37
1	K	36	HIS	CD2-NE2	-6.51	1.30	1.37
1	K	20	ILE	CA-CB	6.43	1.62	1.54
1	H	54	HIS	CD2-NE2	-6.37	1.30	1.37
1	L	36	HIS	CD2-NE2	-6.34	1.30	1.37
1	E	36	HIS	CD2-NE2	-6.34	1.30	1.37
1	J	36	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	36	HIS	CD2-NE2	-6.19	1.31	1.37
1	D	106	HIS	CD2-NE2	-6.17	1.31	1.37
1	G	36	HIS	CD2-NE2	-6.16	1.31	1.37
1	E	54	HIS	CD2-NE2	-6.02	1.31	1.37
1	F	106	HIS	CD2-NE2	-6.00	1.31	1.37
1	D	54	HIS	CD2-NE2	-5.96	1.31	1.37
1	F	36	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	106	HIS	CD2-NE2	-5.93	1.31	1.37
1	C	106	HIS	CD2-NE2	-5.93	1.31	1.37
1	L	54	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	91	VAL	CA-CB	5.70	1.64	1.54
1	J	106	HIS	CD2-NE2	-5.65	1.31	1.37
1	L	106	HIS	CD2-NE2	-5.63	1.31	1.37
1	F	54	HIS	CG-ND1	-5.62	1.32	1.38
1	K	54	HIS	CG-ND1	-5.61	1.32	1.38
1	I	36	HIS	CD2-NE2	-5.46	1.31	1.37
1	D	36	HIS	CD2-NE2	-5.45	1.31	1.37
1	L	54	HIS	CG-ND1	-5.44	1.32	1.38
1	H	106	HIS	CD2-NE2	-5.41	1.31	1.37
1	G	54	HIS	CG-ND1	-5.33	1.32	1.38
1	A	36	HIS	CD2-NE2	-5.29	1.32	1.37
1	E	36	HIS	CG-ND1	-5.20	1.32	1.38
1	I	54	HIS	CG-ND1	-5.15	1.32	1.38
1	J	54	HIS	CG-ND1	-5.09	1.32	1.38
1	B	54	HIS	CD2-NE2	-5.08	1.32	1.37
1	J	54	HIS	CD2-NE2	-5.08	1.32	1.37
1	A	54	HIS	CG-ND1	-5.06	1.32	1.38
1	B	37	THR	CA-CB	5.04	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	HIS	CG-ND1	-5.02	1.32	1.38

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	THR	CA-CB-OG1	-12.81	90.39	109.60
1	F	118	ASP	CA-CB-CG	12.17	124.77	112.60
1	B	74	THR	CA-CB-CG2	9.70	126.98	110.50
1	E	98	ASP	CA-CB-CG	9.35	121.95	112.60
1	H	98	ASP	CA-CB-CG	8.84	121.44	112.60
1	K	94	THR	CA-CB-OG1	-8.69	96.56	109.60
1	L	80	ASP	CA-CB-CG	8.43	121.03	112.60
1	L	114	VAL	N-CA-CB	-8.21	97.68	111.23
1	G	115	LEU	N-CA-C	8.01	121.17	111.40
1	D	98	ASP	CA-CB-CG	7.97	120.57	112.60
1	F	69	GLN	OE1-CD-NE2	-7.89	114.71	122.60
1	J	3	ILE	N-CA-C	-7.81	97.23	108.48
1	K	118	ASP	CA-CB-CG	7.81	120.41	112.60
1	H	36	HIS	CB-CG-CD2	-7.75	121.13	131.20
1	E	110	GLU	CB-CA-C	-7.70	107.69	116.54
1	G	69	GLN	N-CA-C	7.69	121.60	111.75
1	K	55	ALA	N-CA-C	7.67	119.72	111.36
1	J	107	VAL	N-CA-C	7.46	118.63	107.51
1	B	98	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	74	THR	CA-CB-OG1	-7.39	98.52	109.60
1	J	69	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	J	118	ASP	CA-CB-CG	7.19	119.79	112.60
1	G	3	ILE	N-CA-C	-7.09	98.18	108.11
1	H	103	GLN	OE1-CD-NE2	-7.02	115.58	122.60
1	E	118	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	102	ASP	CA-CB-CG	6.90	119.50	112.60
1	E	68	TRP	CG-CD2-CE3	6.89	140.79	133.90
1	A	3	ILE	N-CA-C	-6.87	98.45	108.89
1	K	94	THR	CA-CB-CG2	6.87	122.17	110.50
1	G	57	PHE	N-CA-C	-6.83	99.31	109.42
1	F	26	GLN	CA-CB-CG	-6.75	100.59	114.10
1	K	52	ASP	CA-CB-CG	6.71	119.31	112.60
1	C	106	HIS	N-CA-C	-6.68	99.42	110.17
1	J	107	VAL	N-CA-CB	-6.63	103.12	111.41
1	I	3	ILE	N-CA-C	-6.63	98.83	108.11
1	H	41	ASP	N-CA-C	-6.60	105.23	113.28
1	F	36	HIS	CB-CG-CD2	-6.55	122.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	ASP	N-CA-C	-6.52	104.47	112.88
1	B	102	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	74	THR	CA-CB-CG2	6.43	121.43	110.50
1	B	95	VAL	N-CA-C	6.42	117.36	108.12
1	L	36	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	E	22	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	F	52	ASP	CA-CB-CG	6.36	118.96	112.60
1	D	71	VAL	N-CA-C	-6.36	103.16	108.63
1	I	69	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	L	19	GLU	CA-CB-CG	-6.33	101.43	114.10
1	I	79	MET	CA-CB-CG	6.31	126.72	114.10
1	E	52	ASP	CA-CB-CG	6.31	118.91	112.60
1	H	55	ALA	N-CA-C	6.29	118.02	111.03
1	L	79	MET	CA-CB-CG	6.27	126.63	114.10
1	A	41	ASP	CA-CB-CG	6.26	118.86	112.60
1	C	29	GLU	CA-CB-CG	-6.26	101.58	114.10
1	F	99	VAL	CA-C-N	6.22	126.58	119.92
1	F	99	VAL	C-N-CA	6.22	126.58	119.92
1	J	99	VAL	N-CA-C	-6.22	102.85	108.95
1	D	15	ASP	CA-CB-CG	6.21	118.81	112.60
1	E	65	LEU	N-CA-C	-6.17	98.84	108.90
1	I	26	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	72	PRO	CB-CA-C	6.16	117.00	111.40
1	C	5	GLY	O-C-N	-6.15	118.80	123.35
1	J	110	GLU	N-CA-C	6.09	117.57	108.31
1	B	80	ASP	CA-CB-CG	6.08	118.68	112.60
1	D	107	VAL	N-CA-C	6.05	116.32	107.37
1	E	72	PRO	N-CA-CB	6.05	109.60	103.25
1	E	3	ILE	N-CA-C	-6.04	99.42	108.12
1	K	103	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	J	116	ARG	N-CA-C	-6.01	96.54	109.81
1	I	38	LYS	CA-C-N	6.00	125.71	119.05
1	I	38	LYS	C-N-CA	6.00	125.71	119.05
1	K	36	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	G	15	ASP	CA-CB-CG	5.96	118.56	112.60
1	G	22	GLN	CA-CB-CG	5.96	126.01	114.10
1	G	26	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	K	3	ILE	N-CA-C	-5.94	99.91	108.53
1	L	101	GLN	CA-CB-CG	5.94	125.98	114.10
1	G	106	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	B	27	LEU	N-CA-C	-5.93	104.45	111.03
1	F	41	ASP	CA-CB-CG	5.89	118.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	19	GLU	N-CA-CB	-5.89	101.42	110.20
1	F	101	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	F	72	PRO	CB-CA-C	5.85	117.95	111.11
1	G	103	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	B	30	LYS	N-CA-C	-5.83	104.52	111.69
1	L	78	GLU	N-CA-C	-5.82	101.86	110.48
1	K	74	THR	CA-CB-OG1	-5.80	100.89	109.60
1	K	97	THR	O-C-N	5.80	129.63	123.42
1	D	55	ALA	N-CA-C	5.80	119.53	112.23
1	K	110	GLU	CB-CA-C	-5.79	109.89	116.54
1	L	32	ILE	N-CA-CB	-5.78	104.32	110.62
1	C	19	GLU	CA-CB-CG	-5.77	102.55	114.10
1	H	103	GLN	CG-CD-NE2	5.77	125.06	116.40
1	E	103	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	B	41	ASP	CA-CB-CG	5.76	118.36	112.60
1	J	95	VAL	N-CA-C	5.76	117.98	108.99
1	A	101	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	J	57	PHE	CA-C-N	5.76	127.04	119.84
1	J	57	PHE	C-N-CA	5.76	127.04	119.84
1	A	15	ASP	CA-CB-CG	5.75	118.35	112.60
1	J	33	GLU	N-CA-C	-5.75	104.65	111.03
1	B	60	LYS	N-CA-C	-5.74	105.00	112.23
1	C	73	VAL	CB-CA-C	-5.73	101.52	110.69
1	D	2	MET	CA-CB-CG	-5.73	102.64	114.10
1	I	68	TRP	CG-CD2-CE3	5.72	139.62	133.90
1	J	69	GLN	CG-CD-NE2	5.71	124.97	116.40
1	A	99	VAL	CA-C-N	5.71	125.71	119.89
1	A	99	VAL	C-N-CA	5.71	125.71	119.89
1	C	74	THR	CA-CB-CG2	5.69	120.18	110.50
1	L	68	TRP	CG-CD2-CE3	5.67	139.57	133.90
1	C	3	ILE	CB-CA-C	5.66	118.53	110.84
1	A	69	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	E	77	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	C	98	ASP	N-CA-C	-5.64	106.39	113.72
1	A	96	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	I	106	HIS	N-CA-C	-5.63	100.53	109.76
1	J	35	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	L	102	ASP	CA-CB-CG	5.63	118.23	112.60
1	I	55	ALA	N-CA-C	5.61	118.11	111.33
1	F	92	MET	CG-SD-CE	-5.57	88.64	100.90
1	I	22	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	G	16	THR	N-CA-C	-5.55	100.73	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	98	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	106	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	B	4	ARG	CB-CG-CD	5.54	124.04	111.30
1	A	106	HIS	CB-CG-ND1	5.53	130.99	122.70
1	I	21	LEU	N-CA-C	5.52	117.73	111.11
1	C	22	GLN	CB-CG-CD	-5.51	103.24	112.60
1	E	101	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	C	74	THR	CA-CB-OG1	-5.49	101.37	109.60
1	D	96	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	K	47	LEU	CD1-CG-CD2	-5.47	98.76	110.80
1	J	36	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	B	10	THR	CA-CB-OG1	-5.45	101.43	109.60
1	F	106	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	L	89	ILE	N-CA-C	-5.44	100.57	108.36
1	H	52	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	96	GLN	CG-CD-NE2	5.42	124.52	116.40
1	L	93	MET	O-C-N	-5.41	117.05	123.22
1	C	68	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	L	54	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	G	57	PHE	CA-C-O	-5.39	115.31	119.46
1	B	38	LYS	CA-C-N	5.37	125.70	119.47
1	B	38	LYS	C-N-CA	5.37	125.70	119.47
1	C	2	MET	CA-CB-CG	-5.37	103.37	114.10
1	E	69	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	B	3	ILE	N-CA-C	-5.36	100.48	108.46
1	E	41	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	37	THR	N-CA-C	5.32	117.94	109.96
1	J	68	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	B	77	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	C	3	ILE	N-CA-CB	-5.30	104.63	110.99
1	E	26	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	K	99	VAL	CA-C-N	5.30	125.24	119.78
1	K	99	VAL	C-N-CA	5.30	125.24	119.78
1	I	69	GLN	CG-CD-NE2	5.30	124.35	116.40
1	L	99	VAL	N-CA-CB	-5.30	104.53	109.99
1	J	38	LYS	CA-C-N	5.29	124.96	119.56
1	J	38	LYS	C-N-CA	5.29	124.96	119.56
1	B	78	GLU	N-CA-C	-5.28	103.05	110.50
1	F	22	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	H	96	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	H	80	ASP	CA-CB-CG	5.26	117.86	112.60
1	L	38	LYS	CA-C-N	5.26	125.31	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	38	LYS	C-N-CA	5.26	125.31	119.32
1	F	54	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	C	3	ILE	N-CA-C	-5.25	100.85	108.36
1	B	26	GLN	CG-CD-NE2	5.24	124.26	116.40
1	I	54	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	J	68	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	F	98	ASP	CA-CB-CG	5.23	117.83	112.60
1	I	69	GLN	N-CA-C	5.22	119.13	112.34
1	A	36	HIS	CA-C-N	5.22	128.26	120.95
1	A	36	HIS	C-N-CA	5.22	128.26	120.95
1	B	59	ALA	N-CA-C	5.22	119.14	112.87
1	D	50	THR	CA-C-N	5.21	126.36	119.84
1	D	50	THR	C-N-CA	5.21	126.36	119.84
1	F	115	LEU	N-CA-C	5.21	119.69	112.45
1	I	52	ASP	CA-CB-CG	5.21	117.81	112.60
1	H	26	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	D	96	GLN	CG-CD-NE2	5.20	124.20	116.40
1	F	68	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	F	81	VAL	CA-CB-CG2	-5.19	101.58	110.40
1	A	68	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	E	36	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	H	85	LEU	N-CA-C	-5.16	101.56	109.76
1	J	10	THR	CA-CB-OG1	-5.16	101.86	109.60
1	D	86	LYS	CA-CB-CG	5.16	124.41	114.10
1	L	10	THR	CA-CB-OG1	-5.16	101.87	109.60
1	K	35	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	54	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	E	46	LEU	N-CA-C	-5.14	100.66	109.24
1	L	68	TRP	CE2-CD2-CG	-5.14	101.04	107.20
1	G	38	LYS	CA-C-N	5.13	124.58	119.24
1	G	38	LYS	C-N-CA	5.13	124.58	119.24
1	L	3	ILE	N-CA-C	-5.13	101.09	108.53
1	E	68	TRP	CB-CG-CD1	-5.13	119.21	126.90
1	L	69	GLN	CB-CG-CD	5.13	121.32	112.60
1	B	26	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	C	54	HIS	CB-CG-CD2	-5.11	124.55	131.20
1	E	55	ALA	N-CA-C	5.11	116.93	111.36
1	G	106	HIS	CB-CG-ND1	5.11	130.37	122.70
1	H	54	HIS	CB-CG-CD2	-5.10	124.56	131.20
1	I	68	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	H	13	GLU	N-CA-CB	-5.10	102.59	110.13
1	A	68	TRP	N-CA-C	5.09	119.44	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	HIS	CB-CG-CD2	-5.09	124.59	131.20
1	C	22	GLN	N-CA-C	5.08	116.90	111.36
1	L	22	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	L	102	ASP	N-CA-C	5.08	119.16	112.92
1	B	99	VAL	N-CA-C	-5.08	104.30	109.02
1	G	107	VAL	N-CA-C	5.07	115.16	107.80
1	E	26	GLN	CG-CD-NE2	5.07	124.01	116.40
1	J	82	THR	N-CA-C	-5.07	102.36	109.96
1	F	81	VAL	CA-CB-CG1	5.06	119.00	110.40
1	E	38	LYS	N-CA-C	-5.06	102.69	110.32
1	A	28	LEU	CA-C-O	-5.04	115.53	120.82
1	K	72	PRO	CB-CA-C	5.03	117.55	111.46
1	K	94	THR	N-CA-CB	-5.03	102.68	110.57
1	A	68	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	E	107	VAL	N-CA-CB	-5.01	105.15	111.46
1	I	40	GLU	CB-CG-CD	5.01	121.11	112.60

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 [i](#)

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	19	0
1	B	931	208	960	17	0
1	C	939	209	971	21	0
1	D	905	201	936	20	0
1	E	931	208	960	26	0
1	F	939	209	971	19	0
1	G	916	207	949	20	0
1	H	923	207	956	20	0
1	I	905	201	936	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	931	208	960	28	0
1	K	931	208	960	17	0
1	L	905	201	936	27	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
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	233	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 10.

All (233) 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
1:A:72:PRO:HB2	1:B:92:MET:HE1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:74:THR:HA	2:F:205:TSA:H3	1.74	0.67
1:G:3:ILE:HG21	1:H:3:ILE:HD11	1.77	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:C:45:MET:HE2	1:C:93:MET:HG3	1.79	0.64
1:I:51:PRO:HG3	1:I:80:ASP:HB2	1.79	0.64
1:B:7:ARG:H	1:B:106:HIS:HD2	1.44	0.63
1:E:12:VAL:HG11	1:E:20:ILE:HA	1.80	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:J:45:MET:HE2	1:J:93:MET:HE2	1.82	0.62
1:A:45:MET:HE3	1:A:73:VAL:HG12	1.79	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	1.82	0.62
1:B:6:ILE:HD12	1:B:93:MET:HE3	1.83	0.60
1:E:7:ARG:H	1:E:106:HIS:CD2	2.17	0.60
1:H:7:ARG:H	1:H:106:HIS:HD2	1.50	0.60
1:C:2:MET:HE3	1:C:3:ILE:O	2.02	0.60
1:G:3:ILE:HD11	1:H:2:MET:HE1	1.84	0.60
1:F:16:THR:HG23	1:F:19:GLU:H	1.67	0.59
1:B:2:MET:HE2	1:B:3:ILE:H	1.66	0.59
1:D:72:PRO:HB3	1:E:92:MET:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HG11	1:A:20:ILE:HA	1.84	0.59
1:I:30:LYS:HB3	1:I:107:VAL:HG11	1.83	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:E:37:THR:HG21	1:E:93:MET:HE3	1.87	0.56
1:C:47:LEU:HG	1:C:91:VAL:HG23	1.88	0.56
1:K:8:GLY:HA2	1:K:107:VAL:O	2.05	0.56
1:I:88:CYS:SG	1:I:90:ARG:NH1	2.79	0.55
1:K:2:MET:HE3	1:K:4:ARG:NH1	2.22	0.55
1:G:101:GLN:HE21	1:I:70:TYR:HB2	1.72	0.55
1:J:118:ASP:HB3	1:L:69:GLN:HE22	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:B:45:MET:HB3	1:B:73:VAL:HG12	1.89	0.54
1:F:85:LEU:HD23	1:F:88:CYS:SG	2.48	0.54
1:G:20:ILE:HD12	1:G:55:ALA:HB3	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:H:2:MET:HA	1:H:2:MET:HE2	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:D:92:MET:HE3	1:D:92:MET:HA	1.91	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
1:J:101:GLN:HE21	1:L:70:TYR:HB2	1.76	0.50
1:C:60:LYS:HG3	1:C:63:ARG:HH21	1.77	0.50
1:H:22:GLN:HG2	1:H:23:LYS:NZ	2.27	0.50
1:K:72:PRO:HB2	1:L:92:MET:HE1	1.93	0.50
1:B:39:PRO:O	1:C:101:GLN:NE2	2.45	0.50
1:H:8:GLY:HA2	1:H:107:VAL:O	2.12	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:E:45:MET:HB3	1:E:73:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:ILE:HD11	1:H:2:MET:CE	2.42	0.50
1:B:17:GLU:O	1:B:21:LEU:HG	2.12	0.49
1:I:7:ARG:H	1:I:106:HIS:CD2	2.20	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:E:8:GLY:HA2	1:E:107:VAL:O	2.13	0.49
1:G:48:SER:HB3	1:G:76:MET:HG3	1.95	0.49
1:I:45:MET:HE2	1:I:93:MET:HG3	1.94	0.49
2:D:206:TSA:H3	1:F:74:THR:HA	1.95	0.49
1:J:62:VAL:HG21	1:J:73:VAL:HG11	1.94	0.49
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:L:37:THR:HG21	1:L:93:MET:HE3	1.95	0.48
1:C:109:LEU:O	1:C:112:ALA:HB3	2.13	0.48
1:F:110:GLU:O	1:F:113:VAL:HG22	2.13	0.48
1:G:8:GLY:HA2	1:G:107:VAL:O	2.13	0.48
1:A:45:MET:HE3	1:A:73:VAL:CG1	2.42	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:H:79:MET:HG3	1:H:81:VAL:HG23	1.96	0.47
1:I:4:ARG:HG3	1:I:97:THR:CG2	2.43	0.47
1:J:38:LYS:HA	1:J:38:LYS:HD3	1.75	0.47
1:G:45:MET:HE3	1:G:73:VAL:CG1	2.45	0.47
1:G:45:MET:SD	1:G:93:MET:HE3	2.55	0.47
1:B:6:ILE:HD12	1:B:93:MET:CE	2.43	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
1:D:8:GLY:HA3	1:D:31:ILE:HD11	1.97	0.46
1:F:12:VAL:HB	1:F:19:GLU:HG2	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:A:6:ILE:HD12	1:A:93:MET:CE	2.46	0.46
1:B:5:GLY:HA3	1:B:92:MET:HE2	1.98	0.46
1:I:48:SER:HA	1:I:76:MET:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:109:LEU:O	1:J:112:ALA:HB3	2.16	0.46
1:J:46:LEU:HB3	1:J:76:MET:HE2	1.98	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:J:47:LEU:O	1:J:75:CYS:HA	2.15	0.45
1:K:47:LEU:O	1:K:75:CYS:HA	2.16	0.45
1:A:3:ILE:HA	1:A:96:GLN:HA	1.99	0.45
1:I:39:PRO:HG3	1:I:68:TRP:NE1	2.30	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:D:72:PRO:CB	1:E:92:MET:HE1	2.47	0.44
1:K:5:GLY:HA3	1:K:92:MET:HE1	1.99	0.44
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:HD2	1:L:30:LYS:HA	1.77	0.44
1:C:30:LYS:O	1:C:34:GLU:HG2	2.17	0.44
1:G:3:ILE:HA	1:G:95:VAL:O	2.18	0.44
1:I:105:ARG:HA	1:I:105:ARG:HD3	1.79	0.44
1:J:44:GLN:NE2	1:K:92:MET:HE2	2.32	0.44
1:L:47:LEU:O	1:L:75:CYS:HA	2.17	0.44
1:B:79:MET:HE2	1:B:81:VAL:CG2	2.48	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:HD2	1:G:30:LYS:HA	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:B:34:GLU:HB3	1:B:105:ARG:HD3	1.99	0.43
1:J:51:PRO:HB3	1:J:77:GLN:NE2	2.33	0.43
1:K:43:VAL:CG1	1:L:3:ILE:HG13	2.49	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
1:H:20:ILE:HD12	1:H:55:ALA:HB3	1.99	0.43
1:K:59:ALA:HB1	1:K:73:VAL:HG21	2.00	0.43
1:L:6:ILE:HG21	1:L:31:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:MET:HG2	1:C:3:ILE:N	2.33	0.43
1:I:12:VAL:HB	1:I:19:GLU:CG	2.43	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: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:45:MET:O	1:E:73:VAL:HA	2.20	0.42
1:E:51:PRO:HB3	1:E:77:GLN:OE1	2.19	0.42
1:B:10:THR:HA	1:B:109:LEU:O	2.19	0.42
1:H:6:ILE:HD11	1:H:95:VAL:HG21	2.01	0.42
1:J:23:LYS:HD3	1:J:26:GLN:NE2	2.35	0.42
1:J:93:MET:HE3	1:J:93:MET:HB2	1.79	0.42
1:B:78:GLU:HG2	1:B:90:ARG:NH1	2.35	0.42
1:J:38:LYS:HB3	1:J:40:GLU:OE2	2.20	0.42
1:L:79:MET:HG3	1:L:81:VAL:HG23	2.02	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:E:109:LEU:O	1:E:112:ALA:HB3	2.20	0.41
1:H:25:LYS:HD3	1:H:64:GLU:OE1	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:C:51:PRO:HG3	1:C:80:ASP:HB2	2.03	0.41
1:J:68:TRP:CD1	1:J:68:TRP:N	2.88	0.41
1:K:116:ARG:HH11	1:K:116:ARG:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:N	1:A:106:HIS:HD2	2.18	0.41
1:D:30:LYS:HB3	1:D:107:VAL:HG11	2.02	0.41
1:L:108:TYR:O	1:L:113:VAL:HG12	2.20	0.41
1:E:24:THR:OG1	1:E:89:ILE:HD13	2.20	0.41
1:E:25:LYS:O	1:E:29:GLU:HG3	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: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:A:94:THR:OG1	1:C:44:GLN:NE2	2.53	0.40
1:J:30:LYS:HD2	1:J:30:LYS:HA	1.98	0.40
1:L:9:ALA:HB3	1:L:108:TYR:CD1	2.55	0.40
1:E:46:LEU:CD2	1:E:74:THR:HG22	2.52	0.40
1:E:99:VAL:HA	1:E:100:PRO:HD2	1.68	0.40
1:I:85:LEU:HD21	1:I:112:ALA:HA	2.03	0.40
1:K:43:VAL:HG11	1:L:3:ILE:HG13	2.03	0.40
1:L:14:ARG:NH2	1:L:16:THR:HG21	2.35	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
1:J:101:GLN:OE1	1:L:40:GLU:HA	2.22	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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	14	14
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%)	14	14
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%)	14	14
All	All	1367/1524 (90%)	1284 (94%)	80 (6%)	3 (0%)	43	51

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 [i](#)

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%)	93 (90%)	10 (10%)	8	8
1	B	106/116 (91%)	99 (93%)	7 (7%)	15	18
1	C	107/116 (92%)	95 (89%)	12 (11%)	6	5
1	D	103/116 (89%)	99 (96%)	4 (4%)	28	39
1	E	106/116 (91%)	100 (94%)	6 (6%)	18	23
1	F	107/116 (92%)	100 (94%)	7 (6%)	15	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	104/116 (90%)	97 (93%)	7 (7%)	15	17
1	H	105/116 (90%)	102 (97%)	3 (3%)	37	51
1	I	103/116 (89%)	99 (96%)	4 (4%)	28	39
1	J	106/116 (91%)	99 (93%)	7 (7%)	15	18
1	K	106/116 (91%)	98 (92%)	8 (8%)	12	14
1	L	103/116 (89%)	99 (96%)	4 (4%)	28	39
All	All	1259/1392 (90%)	1180 (94%)	79 (6%)	16	19

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	13	GLU
1	A	25	LYS
1	A	50	THR
1	A	66	SER
1	A	74	THR
1	A	76	MET
1	A	85	LEU
1	A	91	VAL
1	A	114	VAL
1	B	2	MET
1	B	3	ILE
1	B	16	THR
1	B	50	THR
1	B	69	GLN
1	B	74	THR
1	B	91	VAL
1	C	3	ILE
1	C	13	GLU
1	C	26	GLN
1	C	38	LYS
1	C	47	LEU
1	C	73	VAL
1	C	74	THR
1	C	76	MET
1	C	77	GLN
1	C	81	VAL
1	C	91	VAL
1	C	107	VAL

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Mol	Chain	Res	Type
1	D	13	GLU
1	D	17	GLU
1	D	91	VAL
1	D	114	VAL
1	E	2	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	37	THR
1	F	81	VAL
1	F	91	VAL
1	F	113	VAL
1	F	114	VAL
1	G	2	MET
1	G	3	ILE
1	G	10	THR
1	G	16	THR
1	G	34	GLU
1	G	40	GLU
1	G	105	ARG
1	H	2	MET
1	H	40	GLU
1	H	76	MET
1	I	4	ARG
1	I	69	GLN
1	I	91	VAL
1	I	98	ASP
1	J	26	GLN
1	J	34	GLU
1	J	40	GLU
1	J	52	ASP
1	J	76	MET
1	J	77	GLN
1	J	111	LYS
1	K	2	MET
1	K	18	GLU
1	K	19	GLU
1	K	31	ILE

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Mol	Chain	Res	Type
1	K	63	ARG
1	K	74	THR
1	K	94	THR
1	K	98	ASP
1	L	37	THR
1	L	38	LYS
1	L	52	ASP
1	L	114	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) 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	106	HIS
1	C	44	GLN
1	C	96	GLN
1	C	103	GLN
1	C	106	HIS
1	D	22	GLN
1	D	77	GLN
1	D	96	GLN
1	D	106	HIS
1	E	44	GLN
1	E	69	GLN
1	E	101	GLN
1	E	103	GLN
1	E	106	HIS
1	F	36	HIS
1	F	106	HIS
1	G	22	GLN
1	G	101	GLN
1	G	106	HIS
1	H	26	GLN
1	H	44	GLN
1	H	101	GLN
1	H	103	GLN
1	H	106	HIS
1	I	26	GLN
1	I	44	GLN

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Mol	Chain	Res	Type
1	I	106	HIS
1	J	26	GLN
1	J	44	GLN
1	J	77	GLN
1	J	101	GLN
1	J	106	HIS
1	K	22	GLN
1	K	44	GLN
1	K	77	GLN
1	K	96	GLN
1	K	101	GLN
1	K	103	GLN
1	K	106	HIS
1	L	77	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 oligosaccharides 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	H	207	-	16,17,17	1.25	2 (12%)	16,26,26	1.52	3 (18%)
2	TSA	A	203	-	16,17,17	1.30	2 (12%)	16,26,26	1.49	2 (12%)
2	TSA	E	204	-	16,17,17	1.17	2 (12%)	16,26,26	1.62	5 (31%)
2	TSA	I	208	-	16,17,17	1.26	2 (12%)	16,26,26	1.40	3 (18%)
2	TSA	G	209	-	16,17,17	1.18	2 (12%)	16,26,26	1.34	3 (18%)
2	TSA	K	210	-	16,17,17	1.46	3 (18%)	16,26,26	1.73	3 (18%)
2	TSA	B	201	-	16,17,17	1.35	4 (25%)	16,26,26	1.73	5 (31%)
2	TSA	J	212	-	16,17,17	1.24	2 (12%)	16,26,26	1.38	2 (12%)
2	TSA	D	206	-	16,17,17	1.24	3 (18%)	16,26,26	1.62	4 (25%)
2	TSA	F	205	-	16,17,17	1.10	1 (6%)	16,26,26	1.72	4 (25%)
2	TSA	L	211	-	16,17,17	1.20	2 (12%)	16,26,26	1.71	5 (31%)
2	TSA	C	202	-	16,17,17	1.24	3 (18%)	16,26,26	1.53	2 (12%)

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	H	207	-	-	6/10/34/34	1/3/2/2
2	TSA	A	203	-	-	6/10/34/34	1/3/2/2
2	TSA	E	204	-	-	3/10/34/34	1/3/2/2
2	TSA	I	208	-	-	6/10/34/34	1/3/2/2
2	TSA	G	209	-	-	5/10/34/34	1/3/2/2
2	TSA	K	210	-	-	6/10/34/34	1/3/2/2
2	TSA	B	201	-	-	4/10/34/34	1/3/2/2
2	TSA	J	212	-	-	6/10/34/34	1/3/2/2
2	TSA	D	206	-	-	5/10/34/34	1/3/2/2
2	TSA	F	205	-	-	5/10/34/34	1/3/2/2
2	TSA	L	211	-	-	5/10/34/34	1/3/2/2
2	TSA	C	202	-	-	5/10/34/34	1/3/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	210	TSA	C8-C11	3.56	1.56	1.52
2	A	203	TSA	C8-C11	2.75	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	210	TSA	C3-C2	2.58	1.36	1.32
2	H	207	TSA	C3-C2	2.56	1.36	1.32
2	B	201	TSA	O5-C4	-2.48	1.39	1.43
2	L	211	TSA	C3-C2	2.46	1.36	1.32
2	I	208	TSA	O4-C11	-2.45	1.22	1.30
2	C	202	TSA	O4-C11	-2.44	1.22	1.30
2	I	208	TSA	C3-C2	2.43	1.36	1.32
2	J	212	TSA	C3-C2	2.38	1.35	1.32
2	E	204	TSA	O4-C11	-2.34	1.23	1.30
2	C	202	TSA	O2-C10	-2.34	1.22	1.30
2	G	209	TSA	C3-C2	2.32	1.35	1.32
2	B	201	TSA	O4-C11	-2.31	1.23	1.30
2	B	201	TSA	C8-C11	2.30	1.55	1.52
2	D	206	TSA	O4-C11	-2.29	1.23	1.30
2	E	204	TSA	C3-C2	2.23	1.35	1.32
2	H	207	TSA	O4-C11	-2.19	1.23	1.30
2	J	212	TSA	O4-C11	-2.17	1.23	1.30
2	C	202	TSA	C3-C2	2.16	1.35	1.32
2	G	209	TSA	O4-C11	-2.16	1.23	1.30
2	B	201	TSA	C3-C2	2.16	1.35	1.32
2	A	203	TSA	C3-C2	2.15	1.35	1.32
2	L	211	TSA	O4-C11	-2.14	1.23	1.30
2	F	205	TSA	O4-C11	-2.12	1.23	1.30
2	K	210	TSA	O4-C11	-2.12	1.23	1.30
2	D	206	TSA	C3-C2	2.10	1.35	1.32
2	D	206	TSA	O5-C4	-2.05	1.39	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	202	TSA	O7-C8-C9	3.63	115.10	109.95
2	K	210	TSA	O7-C8-C11	3.56	114.43	107.72
2	F	205	TSA	O7-C8-C11	3.50	114.33	107.72
2	K	210	TSA	C9-C1-C10	-3.39	101.84	109.84
2	E	204	TSA	C9-C1-C10	-3.16	102.39	109.84
2	I	208	TSA	O7-C8-C9	3.08	114.32	109.95
2	B	201	TSA	C9-C1-C10	-2.91	102.98	109.84
2	K	210	TSA	O4-C11-C8	2.91	120.27	112.71
2	D	206	TSA	O4-C11-C8	2.88	120.21	112.71
2	B	201	TSA	O7-C8-C11	2.87	113.14	107.72
2	F	205	TSA	O4-C11-C8	2.85	120.14	112.71
2	E	204	TSA	O7-C8-C9	2.85	114.00	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	211	TSA	O7-C8-C11	2.78	112.97	107.72
2	L	211	TSA	O4-C11-C8	2.75	119.87	112.71
2	A	203	TSA	C9-C8-C11	2.74	116.19	112.05
2	H	207	TSA	O4-C11-C8	2.72	119.78	112.71
2	E	204	TSA	O4-C11-C8	2.66	119.62	112.71
2	B	201	TSA	O4-C11-C8	2.62	119.52	112.71
2	L	211	TSA	O5-C4-C5	-2.60	105.44	110.94
2	D	206	TSA	C9-C1-C10	-2.51	103.92	109.84
2	J	212	TSA	O7-C8-C11	2.51	112.45	107.72
2	H	207	TSA	C9-C1-C10	-2.50	103.95	109.84
2	A	203	TSA	O4-C11-C8	2.44	119.05	112.71
2	J	212	TSA	O4-C11-C8	2.43	119.03	112.71
2	H	207	TSA	O7-C8-C11	2.39	112.23	107.72
2	D	206	TSA	O7-C8-C11	2.39	112.22	107.72
2	F	205	TSA	O7-C8-C9	2.38	113.33	109.95
2	C	202	TSA	O4-C11-C8	2.33	118.78	112.71
2	L	211	TSA	O7-C8-C9	2.28	113.19	109.95
2	G	209	TSA	O7-C8-C11	2.28	112.02	107.72
2	B	201	TSA	C5-C4-C3	2.27	114.20	108.83
2	B	201	TSA	O5-C4-C3	-2.21	104.81	109.93
2	F	205	TSA	O3-C11-C8	-2.19	118.11	122.85
2	G	209	TSA	O4-C11-C8	2.14	118.27	112.71
2	E	204	TSA	C6-C1-C10	2.14	114.87	109.84
2	L	211	TSA	O3-C11-C8	-2.12	118.27	122.85
2	G	209	TSA	O7-C8-C9	2.10	112.93	109.95
2	E	204	TSA	O3-C11-C8	-2.10	118.31	122.85
2	D	206	TSA	C5-C4-C3	2.10	113.78	108.83
2	I	208	TSA	O4-C11-C8	2.07	118.09	112.71
2	I	208	TSA	C5-C4-C3	2.01	113.58	108.83

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	203	TSA	C6-C1-C10-O2
2	I	208	TSA	C6-C1-C10-O2
2	J	212	TSA	C6-C1-C10-O2
2	K	210	TSA	C6-C1-C10-O2
2	L	211	TSA	C6-C1-C10-O2
2	C	202	TSA	C6-C1-C10-O1
2	D	206	TSA	C6-C1-C10-O1
2	G	209	TSA	C6-C1-C10-O1

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Mol	Chain	Res	Type	Atoms
2	I	208	TSA	C6-C1-C10-O1
2	K	210	TSA	C6-C1-C10-O1
2	L	211	TSA	C6-C1-C10-O1
2	L	211	TSA	C2-C1-C10-O2
2	K	210	TSA	C2-C1-C10-O2
2	A	203	TSA	C2-C1-C10-O2
2	D	206	TSA	C2-C1-C10-O2
2	E	204	TSA	C2-C1-C10-O2
2	F	205	TSA	C2-C1-C10-O2
2	G	209	TSA	C2-C1-C10-O2
2	H	207	TSA	C6-C1-C10-O2
2	B	201	TSA	C2-C1-C10-O2
2	C	202	TSA	C2-C1-C10-O2
2	H	207	TSA	C2-C1-C10-O2
2	I	208	TSA	C2-C1-C10-O2
2	J	212	TSA	C2-C1-C10-O2
2	A	203	TSA	C6-C1-C10-O1
2	A	203	TSA	C9-C1-C10-O1
2	H	207	TSA	C6-C1-C10-O1
2	J	212	TSA	C6-C1-C10-O1
2	A	203	TSA	C2-C1-C10-O1
2	B	201	TSA	C2-C1-C10-O1
2	C	202	TSA	C2-C1-C10-O1
2	D	206	TSA	C2-C1-C10-O1
2	E	204	TSA	C2-C1-C10-O1
2	F	205	TSA	C2-C1-C10-O1
2	G	209	TSA	C2-C1-C10-O1
2	H	207	TSA	C2-C1-C10-O1
2	I	208	TSA	C2-C1-C10-O1
2	J	212	TSA	C2-C1-C10-O1
2	K	210	TSA	C2-C1-C10-O1
2	L	211	TSA	C2-C1-C10-O1
2	A	203	TSA	C9-C1-C10-O2
2	B	201	TSA	C6-C1-C10-O2
2	B	201	TSA	C9-C1-C10-O2
2	C	202	TSA	C6-C1-C10-O2
2	C	202	TSA	C9-C1-C10-O2
2	D	206	TSA	C6-C1-C10-O2
2	D	206	TSA	C9-C1-C10-O2
2	E	204	TSA	C9-C1-C10-O2
2	F	205	TSA	C6-C1-C10-O2
2	F	205	TSA	C9-C1-C10-O2

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Mol	Chain	Res	Type	Atoms
2	G	209	TSA	C6-C1-C10-O2
2	G	209	TSA	C9-C1-C10-O2
2	H	207	TSA	C9-C1-C10-O2
2	I	208	TSA	C9-C1-C10-O2
2	J	212	TSA	C9-C1-C10-O2
2	K	210	TSA	C9-C1-C10-O2
2	F	205	TSA	C6-C1-C10-O1
2	H	207	TSA	C9-C1-C10-O1
2	I	208	TSA	C9-C1-C10-O1
2	J	212	TSA	C9-C1-C10-O1
2	K	210	TSA	C9-C1-C10-O1
2	L	211	TSA	C9-C1-C10-O1

All (12) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	211	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	F	205	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	I	208	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	C	202	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	J	212	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	D	206	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	K	210	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	A	203	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	G	209	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	B	201	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	H	207	TSA	C1-C2-C3-C4-C5-C8-C9-O7
2	E	204	TSA	C1-C2-C3-C4-C5-C8-C9-O7

11 monomers are involved in 12 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	202	TSA	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.