



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:19 PM UTC

PDB ID : 1COM / pdb_00001com
Title : THE MONOFUNCTIONAL CHORISMATE MUTASE FROM BACILLUS SUBTILIS: STRUCTURE DETERMINATION OF CHORISMATE MUTASE AND ITS COMPLEXES WITH A TRANSITION STATE ANALOG AND PREPHENATE, AND IMPLICATIONS ON THE MECHANISM OF ENZY-MATIC REACTION
Authors : Chook, Y.M.; Ke, H.; Lipscomb, W.N.
Deposited on : 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)
Xtriage (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

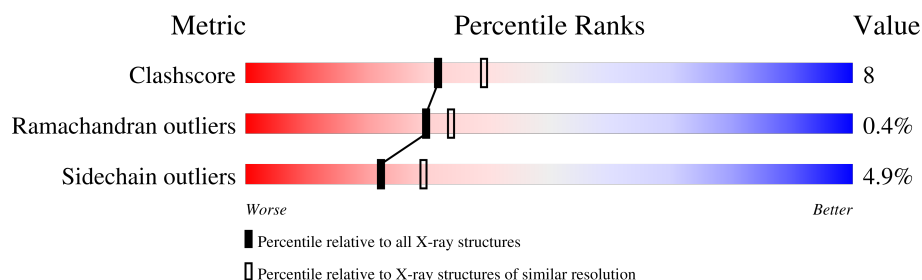
1 Overall quality at a glance

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	65% 20% • 10%
1	B	127	66% 23% • 7%
1	C	127	59% 30% 5% 6%
1	D	127	59% 24% 7% 10%
1	E	127	62% 25% 6% 7%
1	F	127	55% 31% 6% 8%
1	G	127	65% 23% • 10%
1	H	127	65% 21% • 10%

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Mol	Chain	Length	Quality of chain
1	I	127	64%21%5%10%
1	J	127	62%26%••10%
1	K	127	61%28%•9%
1	L	127	63%24%•10%

2 Entry composition

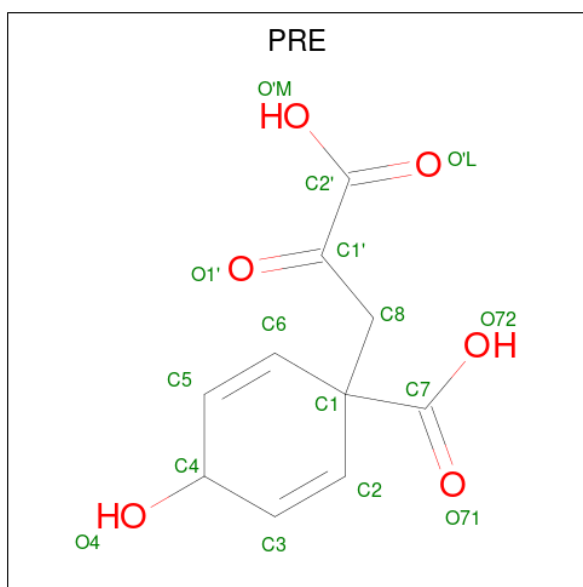
There are 3 unique types of molecules in this entry. The entry contains 15125 atoms, of which 3466 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CHORISMATE MUTASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	B	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	C	119	Total	C	H	N	O	S	0	0	0
			1156	594	211	164	179	8			
1	D	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	E	118	Total	C	H	N	O	S	0	0	0
			1148	591	209	163	177	8			
1	F	117	Total	C	H	N	O	S	0	0	0
			1139	585	208	162	176	8			
1	G	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	H	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	I	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	J	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			
1	K	116	Total	C	H	N	O	S	0	0	0
			1130	581	207	161	173	8			
1	L	114	Total	C	H	N	O	S	0	0	0
			1106	570	201	156	171	8			

- Molecule 2 is PREPHENIC ACID (CCD ID: PRE) (formula: C₁₀H₁₀O₆).



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

- Molecule 3 is water.

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

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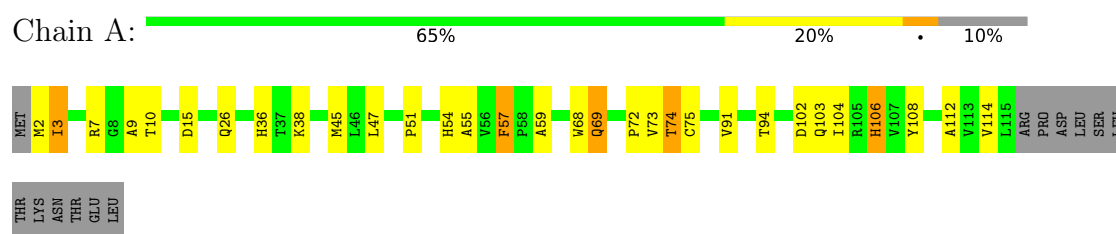
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	37	Total	H	O	0	0
			111	74	37		
3	E	45	Total	H	O	0	0
			135	90	45		
3	F	57	Total	H	O	0	0
			171	114	57		
3	G	33	Total	H	O	0	0
			99	66	33		
3	H	16	Total	H	O	0	0
			48	32	16		
3	I	49	Total	H	O	0	0
			147	98	49		
3	J	36	Total	H	O	0	0
			108	72	36		
3	K	38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

3 Residue-property plots

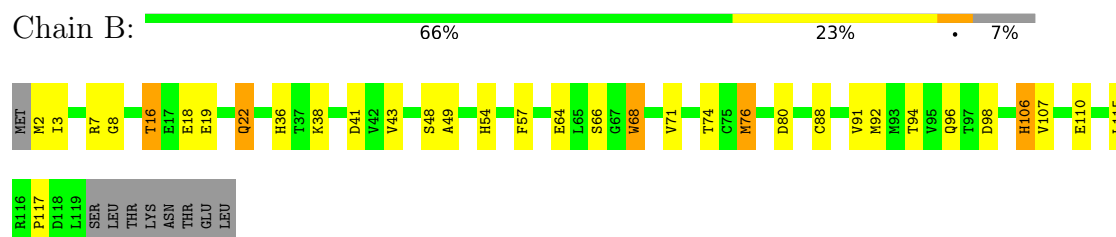
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

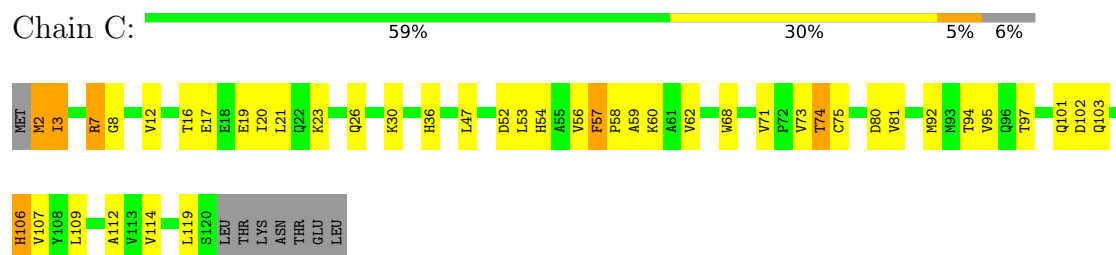
• Molecule 1: CHORISMATE MUTASE



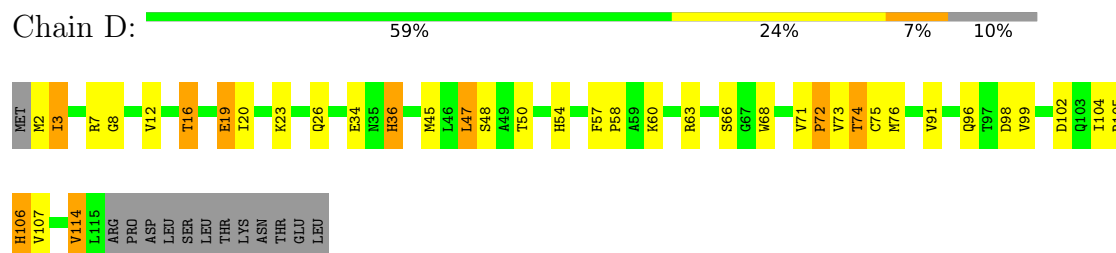
• Molecule 1: CHORISMATE MUTASE



• Molecule 1: CHORISMATE MUTASE

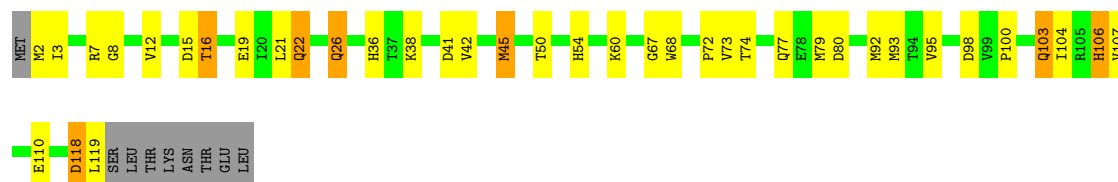


• Molecule 1: CHORISMATE MUTASE



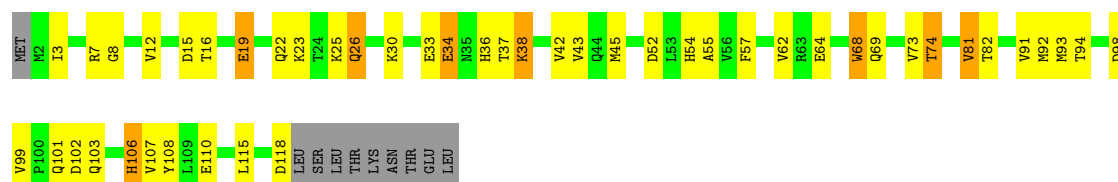
- Molecule 1: CHORISMATE MUTASE

Chain E: 



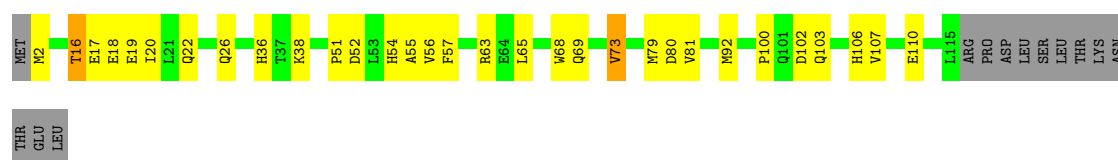
- Molecule 1: CHORISMATE MUTASE

Chain F: 



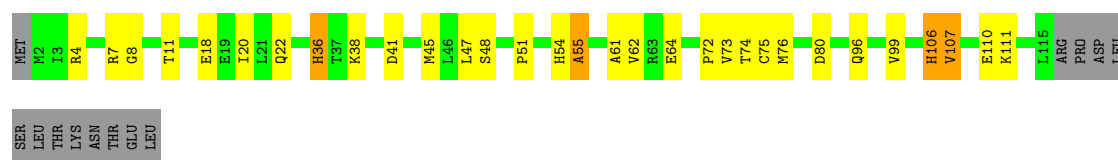
- Molecule 1: CHORISMATE MUTASE

Chain G: 



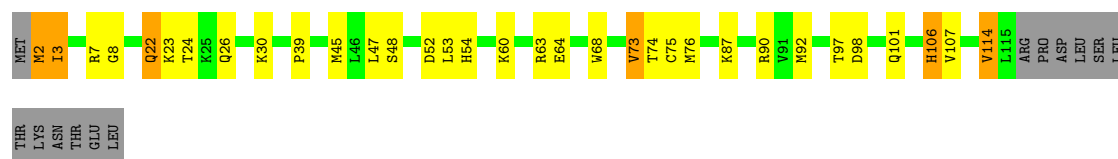
- Molecule 1: CHORISMATE MUTASE

Chain H: 



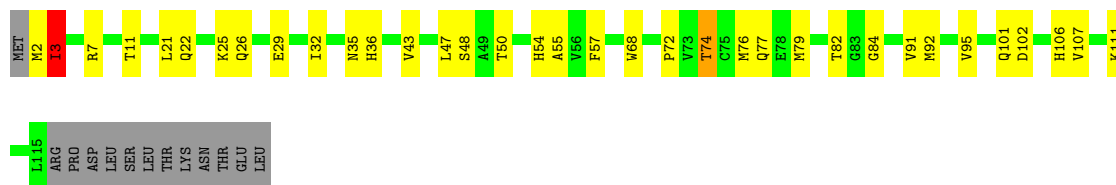
- Molecule 1: CHORISMATE MUTASE

Chain I: 



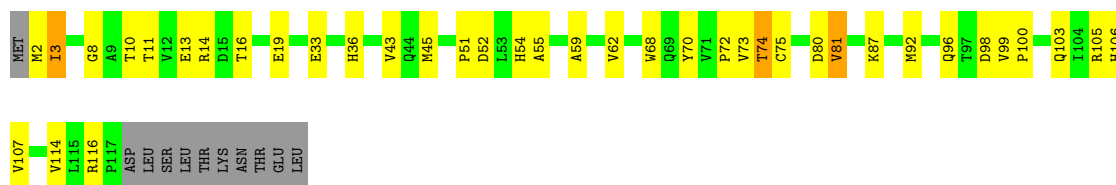
- Molecule 1: CHORISMATE MUTASE

Chain J:  62% 26% .. 10%



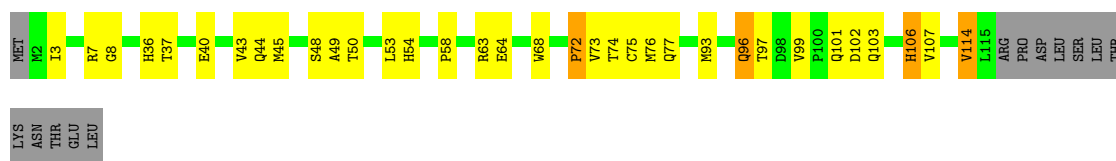
• Molecule 1: CHORISMATE MUTASE

Chain K:  61% 28% • 9%



• Molecule 1: CHORISMATE MUTASE

Chain L:  63% 24% • 10%



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}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15125	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	4/917 (0.4%)	1.75	20/1240 (1.6%)
1	B	1.03	3/952 (0.3%)	1.72	17/1288 (1.3%)
1	C	0.97	4/958 (0.4%)	1.71	13/1296 (1.0%)
1	D	1.04	4/917 (0.4%)	1.77	16/1240 (1.3%)
1	E	1.03	4/952 (0.4%)	1.78	16/1288 (1.2%)
1	F	1.03	4/944 (0.4%)	1.73	20/1277 (1.6%)
1	G	1.01	4/917 (0.4%)	1.71	15/1240 (1.2%)
1	H	0.98	4/917 (0.4%)	1.70	14/1240 (1.1%)
1	I	1.02	3/917 (0.3%)	1.70	13/1240 (1.0%)
1	J	1.01	3/917 (0.3%)	1.73	17/1240 (1.4%)
1	K	1.00	3/936 (0.3%)	1.74	13/1266 (1.0%)
1	L	1.07	4/917 (0.4%)	1.77	19/1240 (1.5%)
All	All	1.02	44/11161 (0.4%)	1.73	193/15095 (1.3%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	54	HIS	CD2-NE2	-7.07	1.30	1.37
1	H	106	HIS	CD2-NE2	-7.06	1.30	1.37
1	D	106	HIS	CD2-NE2	-6.94	1.30	1.37
1	H	54	HIS	CD2-NE2	-6.72	1.30	1.37
1	E	106	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	106	HIS	CD2-NE2	-6.67	1.30	1.37
1	F	106	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	54	HIS	CD2-NE2	-6.58	1.30	1.37
1	E	54	HIS	CD2-NE2	-6.56	1.30	1.37
1	J	36	HIS	CD2-NE2	-6.55	1.30	1.37
1	C	36	HIS	CD2-NE2	-6.53	1.30	1.37
1	L	54	HIS	CD2-NE2	-6.35	1.30	1.37
1	G	54	HIS	CD2-NE2	-6.32	1.30	1.37
1	D	54	HIS	CD2-NE2	-6.29	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.24	1.30	1.37
1	G	36	HIS	CD2-NE2	-6.24	1.30	1.37
1	J	54	HIS	CG-ND1	-6.20	1.31	1.38
1	F	36	HIS	CD2-NE2	-6.20	1.31	1.37
1	K	106	HIS	CD2-NE2	-6.11	1.31	1.37
1	I	106	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	54	HIS	CD2-NE2	-6.03	1.31	1.37
1	J	54	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	36	HIS	CD2-NE2	-5.92	1.31	1.37
1	C	54	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	36	HIS	CD2-NE2	-5.87	1.31	1.37
1	H	36	HIS	CD2-NE2	-5.76	1.31	1.37
1	K	54	HIS	CD2-NE2	-5.73	1.31	1.37
1	C	106	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	104	ILE	CA-CB	5.63	1.60	1.54
1	L	54	HIS	CG-ND1	-5.61	1.32	1.38
1	G	54	HIS	CG-ND1	-5.61	1.32	1.38
1	F	54	HIS	CG-ND1	-5.59	1.32	1.38
1	L	106	HIS	CD2-NE2	-5.56	1.31	1.37
1	K	36	HIS	CD2-NE2	-5.47	1.31	1.37
1	D	54	HIS	CG-ND1	-5.46	1.32	1.38
1	L	36	HIS	CD2-NE2	-5.36	1.31	1.37
1	D	36	HIS	CD2-NE2	-5.33	1.31	1.37
1	F	54	HIS	CD2-NE2	-5.30	1.32	1.37
1	G	106	HIS	CD2-NE2	-5.25	1.32	1.37
1	C	54	HIS	CG-ND1	-5.16	1.32	1.38
1	E	106	HIS	CG-ND1	-5.15	1.32	1.38
1	H	54	HIS	CG-ND1	-5.08	1.32	1.38
1	I	54	HIS	CG-ND1	-5.03	1.32	1.38

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	102	ASP	CA-CB-CG	11.38	123.98	112.60
1	H	36	HIS	CA-CB-CG	11.13	124.93	113.80
1	B	74	THR	CA-CB-OG1	-9.14	95.89	109.60
1	K	103	GLN	OE1-CD-NE2	-8.74	113.86	122.60
1	B	41	ASP	CA-CB-CG	8.61	121.21	112.60
1	H	41	ASP	CA-CB-CG	8.49	121.09	112.60
1	A	26	GLN	OE1-CD-NE2	-8.48	114.12	122.60
1	L	101	GLN	OE1-CD-NE2	-8.30	114.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	114	VAL	N-CA-CB	-8.26	97.61	111.23
1	D	102	ASP	CA-CB-CG	8.00	120.60	112.60
1	K	55	ALA	N-CA-C	7.92	119.69	111.14
1	J	102	ASP	CA-CB-CG	7.90	120.50	112.60
1	K	3	ILE	N-CA-C	-7.75	97.32	108.48
1	F	98	ASP	CA-CB-CG	7.73	120.33	112.60
1	J	82	THR	N-CA-C	-7.61	98.40	109.59
1	E	118	ASP	CA-CB-CG	7.60	120.20	112.60
1	E	22	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	K	74	THR	CA-CB-OG1	-7.51	98.33	109.60
1	L	77	GLN	CA-CB-CG	-7.51	99.07	114.10
1	G	110	GLU	CB-CA-C	-7.46	107.96	116.54
1	A	55	ALA	N-CA-C	7.38	120.20	111.71
1	A	26	GLN	CA-CB-CG	7.33	128.75	114.10
1	F	55	ALA	N-CA-C	7.30	121.29	112.38
1	A	26	GLN	CG-CD-NE2	7.29	127.33	116.40
1	I	3	ILE	N-CA-C	-7.27	97.93	108.11
1	G	22	GLN	CA-CB-CG	7.24	128.58	114.10
1	B	74	THR	CA-CB-CG2	7.21	122.75	110.50
1	H	55	ALA	N-CA-C	7.19	120.18	111.40
1	C	52	ASP	CA-CB-CG	7.17	119.77	112.60
1	F	118	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	38	LYS	N-CA-C	-6.87	99.94	110.32
1	F	22	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	F	26	GLN	OE1-CD-NE2	-6.82	115.78	122.60
1	F	38	LYS	N-CA-C	-6.80	101.55	110.39
1	K	36	HIS	CB-CG-CD2	-6.77	122.39	131.20
1	K	103	GLN	CG-CD-NE2	6.73	126.49	116.40
1	G	102	ASP	CA-CB-CG	6.71	119.31	112.60
1	F	115	LEU	N-CA-C	6.65	118.52	111.28
1	K	52	ASP	CA-CB-CG	6.60	119.20	112.60
1	J	101	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	H	99	VAL	N-CA-C	-6.58	102.90	109.02
1	F	102	ASP	CA-CB-CG	6.53	119.13	112.60
1	C	101	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	B	22	GLN	OE1-CD-NE2	-6.45	116.16	122.60
1	H	36	HIS	N-CA-CB	-6.42	102.44	112.13
1	K	74	THR	CA-CB-CG2	6.41	121.40	110.50
1	F	33	GLU	CA-CB-CG	6.40	126.91	114.10
1	I	2	MET	CG-SD-CE	-6.37	86.89	100.90
1	D	72	PRO	CB-CA-C	6.34	118.52	111.11
1	H	38	LYS	N-CA-C	-6.31	100.79	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	43	VAL	N-CA-C	-6.30	104.37	110.42
1	C	57	PHE	CA-C-N	6.30	126.78	119.47
1	C	57	PHE	C-N-CA	6.30	126.78	119.47
1	J	55	ALA	N-CA-C	6.27	118.20	111.36
1	I	101	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	I	114	VAL	N-CA-CB	-6.21	100.99	111.23
1	B	36	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	G	107	VAL	N-CA-C	6.16	117.17	108.36
1	J	79	MET	CA-CB-CG	6.15	126.40	114.10
1	B	54	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	B	115	LEU	N-CA-C	6.11	117.74	111.14
1	E	45	MET	CG-SD-CE	-6.09	87.50	100.90
1	G	52	ASP	CA-CB-CG	6.06	118.66	112.60
1	F	110	GLU	CB-CA-C	-6.06	109.61	116.63
1	I	97	THR	CA-C-O	6.05	127.76	121.10
1	E	54	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	H	74	THR	CA-CB-OG1	-6.00	100.60	109.60
1	A	94	THR	CA-CB-OG1	-6.00	100.61	109.60
1	L	72	PRO	CB-CA-C	5.96	118.09	111.11
1	J	3	ILE	N-CA-C	-5.92	99.64	108.46
1	A	36	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	H	106	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	D	71	VAL	N-CA-C	-5.89	103.56	108.63
1	L	50	THR	CA-C-N	5.88	125.58	119.82
1	L	50	THR	C-N-CA	5.88	125.58	119.82
1	D	114	VAL	N-CA-CB	-5.86	101.56	111.23
1	I	98	ASP	N-CA-CB	-5.82	102.58	110.67
1	G	73	VAL	CB-CA-C	-5.82	101.54	110.50
1	A	51	PRO	N-CA-C	5.81	121.18	114.03
1	B	98	ASP	CA-CB-CG	5.79	118.39	112.60
1	L	97	THR	O-C-N	5.77	129.59	123.42
1	G	54	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	G	107	VAL	N-CA-CB	-5.75	104.09	110.99
1	L	106	HIS	CB-CG-ND1	5.75	131.32	122.70
1	K	36	HIS	CB-CG-ND1	5.74	131.31	122.70
1	A	103	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	B	68	TRP	CG-CD2-CE3	5.68	139.59	133.90
1	B	38	LYS	CA-C-N	5.68	125.79	119.32
1	B	38	LYS	C-N-CA	5.68	125.79	119.32
1	E	110	GLU	CB-CA-C	-5.68	110.05	116.63
1	D	34	GLU	CA-CB-CG	-5.67	102.77	114.10
1	B	106	HIS	CA-CB-CG	-5.65	108.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	I	54	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	D	99	VAL	N-CA-C	-5.64	102.81	108.96
1	H	107	VAL	O-C-N	-5.64	116.50	123.10
1	L	106	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	15	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	102	ASP	CA-CB-CG	5.63	118.23	112.60
1	F	81	VAL	N-CA-CB	-5.62	103.60	111.25
1	E	104	ILE	N-CA-C	-5.61	100.50	108.58
1	F	101	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	E	68	TRP	CG-CD2-CE3	5.57	139.47	133.90
1	G	69	GLN	N-CA-C	5.56	119.55	112.87
1	E	26	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	I	26	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	E	103	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	F	34	GLU	N-CA-C	5.54	116.99	111.07
1	F	15	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	98	ASP	CA-CB-CG	5.51	118.11	112.60
1	K	68	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	F	108	TYR	N-CA-C	-5.50	99.32	108.34
1	C	36	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	G	65	LEU	N-CA-C	-5.48	99.59	108.52
1	E	98	ASP	CA-CB-CG	5.46	118.06	112.60
1	E	68	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	J	36	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	C	80	ASP	CA-CB-CG	5.45	118.05	112.60
1	J	26	GLN	CG-CD-NE2	5.44	124.56	116.40
1	J	84	GLY	N-CA-C	-5.44	105.32	112.82
1	A	69	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	D	26	GLN	OE1-CD-NE2	-5.42	117.19	122.60
1	B	68	TRP	CE2-CD2-CG	-5.41	100.70	107.20
1	A	57	PHE	CA-C-N	5.41	125.49	119.32
1	A	57	PHE	C-N-CA	5.41	125.49	119.32
1	B	80	ASP	CA-CB-CG	5.41	118.01	112.60
1	J	68	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	A	54	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	G	36	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	I	24	THR	CA-CB-OG1	-5.38	101.53	109.60
1	B	110	GLU	CB-CA-C	-5.37	110.40	116.63
1	L	74	THR	CA-CB-CG2	5.37	119.62	110.50
1	F	52	ASP	CA-CB-CG	5.34	117.94	112.60
1	H	74	THR	CA-CB-CG2	5.32	119.55	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	CA-CB-CG	-5.32	108.48	113.80
1	J	77	GLN	CA-CB-CG	-5.32	103.47	114.10
1	I	22	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	C	119	LEU	N-CA-C	-5.30	96.63	107.70
1	H	99	VAL	CA-C-N	5.29	125.23	119.78
1	H	99	VAL	C-N-CA	5.29	125.23	119.78
1	G	107	VAL	O-C-N	-5.29	117.16	123.03
1	L	97	THR	CA-C-O	5.28	126.88	121.23
1	F	99	VAL	CA-C-N	5.27	125.56	119.92
1	F	99	VAL	C-N-CA	5.27	125.56	119.92
1	F	68	TRP	CG-CD2-CE3	5.27	139.17	133.90
1	C	26	GLN	CG-CD-NE2	5.27	124.30	116.40
1	C	7	ARG	NE-CZ-NH2	-5.26	114.46	119.20
1	E	41	ASP	CA-CB-CG	5.26	117.86	112.60
1	L	96	GLN	N-CA-C	-5.26	101.39	109.76
1	J	107	VAL	N-CA-C	5.26	115.66	107.99
1	J	68	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	K	81	VAL	CA-CB-CG2	-5.25	101.47	110.40
1	E	15	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	68	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	B	64	GLU	CA-CB-CG	-5.23	103.63	114.10
1	H	41	ASP	N-CA-C	-5.22	106.91	113.28
1	I	52	ASP	CA-CB-CG	5.21	117.81	112.60
1	K	72	PRO	CB-CA-C	5.21	117.20	111.11
1	D	104	ILE	O-C-N	-5.20	116.95	122.61
1	D	3	ILE	N-CA-C	-5.18	100.90	108.99
1	A	114	VAL	N-CA-CB	-5.16	102.71	111.23
1	K	10	THR	CA-CB-OG1	-5.16	101.86	109.60
1	L	103	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	J	32	ILE	N-CA-CB	-5.15	104.52	110.55
1	C	103	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	L	36	HIS	N-CA-C	-5.15	104.79	111.74
1	C	94	THR	O-C-N	-5.14	117.22	123.13
1	C	102	ASP	CA-CB-CG	5.13	117.73	112.60
1	L	99	VAL	CA-C-N	5.13	125.06	119.78
1	L	99	VAL	C-N-CA	5.13	125.06	119.78
1	E	80	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	38	LYS	N-CA-C	-5.12	102.59	110.32
1	E	77	GLN	CA-CB-CG	-5.12	103.87	114.10
1	D	106	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	I	74	THR	CA-CB-OG1	-5.10	101.94	109.60
1	D	19	GLU	CA-CB-CG	5.10	124.30	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	35	ASN	CA-CB-CG	-5.10	107.50	112.60
1	G	68	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	L	114	VAL	CB-CA-C	5.09	119.64	111.29
1	J	101	GLN	CG-CD-NE2	5.09	124.04	116.40
1	I	106	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	L	68	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	D	68	TRP	CG-CD2-CE3	5.05	138.95	133.90
1	A	3	ILE	N-CA-C	-5.05	101.21	108.48
1	G	26	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	G	68	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	38	LYS	CA-C-N	5.02	124.46	119.24
1	A	38	LYS	C-N-CA	5.02	124.46	119.24
1	H	110	GLU	CB-CA-C	-5.02	110.77	116.54
1	D	57	PHE	CA-C-N	5.02	125.04	119.32
1	D	57	PHE	C-N-CA	5.02	125.04	119.32
1	F	103	GLN	CA-CB-CG	-5.01	104.08	114.10
1	D	105	ARG	NE-CZ-NH2	-5.01	114.69	119.20

There are no chirality outliers.

There are no planarity outliers.

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	12	0
1	B	939	209	971	15	0
1	C	945	211	976	28	0
1	D	905	201	936	20	2
1	E	939	209	971	22	1
1	F	931	208	960	22	1
1	G	905	201	936	8	0
1	H	905	201	936	15	1
1	I	905	201	936	13	0
1	J	905	201	936	14	0
1	K	923	207	956	17	1
1	L	905	201	936	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	16	1	8	4	0
2	B	16	1	8	2	0
2	C	16	1	8	1	0
2	D	16	1	8	3	0
2	E	16	1	8	1	0
2	F	16	1	8	1	0
2	G	16	1	8	0	0
2	H	16	1	8	1	0
2	K	16	1	8	2	0
3	A	36	72	0	0	0
3	B	42	84	0	0	0
3	C	44	88	0	0	0
3	D	37	74	0	0	1
3	E	45	90	0	0	1
3	F	57	114	0	0	0
3	G	33	66	0	0	0
3	H	16	32	0	0	0
3	I	49	98	0	0	0
3	J	36	72	0	0	0
3	K	38	76	0	1	0
3	L	70	140	0	0	3
All	All	11659	3466	11458	183	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (183) 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:A:72:PRO:HB2	1:B:92:MET:HE1	1.47	0.97
1:H:45:MET:HB3	1:H:73:VAL:HG12	1.58	0.84
1:G:100:PRO:HG2	1:G:103:GLN:HG3	1.61	0.82
1:D:72:PRO:HB2	1:E:92:MET:HE1	1.62	0.82
1:B:7:ARG:H	1:B:106:HIS:HD2	1.34	0.76
1:E:45:MET:HE3	1:E:93:MET:HG3	1.69	0.75
1:F:7:ARG:H	1:F:106:HIS:HD2	1.31	0.74
1:D:7:ARG:H	1:D:106:HIS:HD2	1.33	0.74
1:D:3:ILE:HD13	1:E:3:ILE:HD11	1.70	0.74
1:C:7:ARG:H	1:C:106:HIS:HD2	1.36	0.73
1:E:74:THR:HA	2:F:225:PRE:H5	1.71	0.70
2:A:223:PRE:H5	1:C:74:THR:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:ARG:H	1:H:106:HIS:HD2	1.37	0.70
1:E:7:ARG:H	1:E:106:HIS:HD2	1.39	0.69
1:F:62:VAL:HG21	1:F:73:VAL:HG11	1.75	0.68
1:D:45:MET:HB3	1:D:73:VAL:HG12	1.75	0.68
1:H:11:THR:HG21	1:H:111:LYS:HB2	1.75	0.68
1:L:7:ARG:H	1:L:106:HIS:HD2	1.42	0.68
1:D:60:LYS:HA	1:D:63:ARG:NH1	2.09	0.67
1:I:7:ARG:H	1:I:106:HIS:HD2	1.44	0.66
1:H:62:VAL:HG21	1:H:73:VAL:HG11	1.78	0.66
1:D:74:THR:HA	2:E:224:PRE:H5	1.78	0.65
1:J:11:THR:HG21	1:J:111:LYS:HB2	1.77	0.65
1:K:14:ARG:HH21	1:K:16:THR:HG21	1.63	0.64
1:G:20:ILE:HD12	1:G:55:ALA:HB3	1.79	0.64
1:B:16:THR:HG23	1:B:19:GLU:HB2	1.81	0.63
1:D:16:THR:HG23	1:D:19:GLU:HB3	1.81	0.62
1:F:92:MET:HA	1:F:92:MET:HE3	1.82	0.61
1:J:2:MET:HG2	1:J:3:ILE:H	1.66	0.61
1:K:3:ILE:HD13	1:K:96:GLN:HA	1.82	0.61
1:C:20:ILE:HD11	1:C:53:LEU:HD22	1.84	0.60
1:G:16:THR:HG23	1:G:19:GLU:HB2	1.83	0.60
1:J:92:MET:HE1	1:L:72:PRO:HB2	1.84	0.59
1:A:3:ILE:HD11	1:C:3:ILE:HG21	1.82	0.59
1:A:45:MET:HB3	1:A:73:VAL:HG12	1.84	0.59
1:L:8:GLY:HA2	1:L:107:VAL:O	2.03	0.59
1:H:72:PRO:HB2	1:I:92:MET:HE1	1.84	0.59
1:A:7:ARG:H	1:A:106:HIS:HD2	1.48	0.59
1:C:12:VAL:HG12	1:C:23:LYS:HG3	1.85	0.58
1:K:51:PRO:HG3	1:K:80:ASP:HB2	1.84	0.58
1:C:62:VAL:HG21	1:C:73:VAL:HG11	1.83	0.58
1:H:8:GLY:HA2	1:H:107:VAL:O	2.04	0.58
1:K:59:ALA:HB2	1:K:75:CYS:SG	2.43	0.58
2:D:226:PRE:H5	1:F:74:THR:HA	1.85	0.58
1:E:45:MET:HB3	1:E:73:VAL:HG12	1.85	0.58
2:D:226:PRE:H3	1:F:57:PHE:CD1	2.39	0.57
1:L:45:MET:HB3	1:L:73:VAL:HG12	1.86	0.57
1:I:8:GLY:HA2	1:I:107:VAL:O	2.04	0.57
1:L:49:ALA:HB1	1:L:53:LEU:HD12	1.86	0.57
1:G:51:PRO:HG3	1:G:80:ASP:HB2	1.87	0.56
1:E:16:THR:HG22	1:E:19:GLU:CB	2.36	0.55
1:F:8:GLY:HA2	1:F:107:VAL:O	2.07	0.55
1:A:7:ARG:H	1:A:106:HIS:CD2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LYS:HA	1:D:63:ARG:HH11	1.71	0.55
1:K:92:MET:HE3	1:K:92:MET:HA	1.88	0.55
1:E:12:VAL:HB	1:E:19:GLU:HG3	1.89	0.55
1:H:7:ARG:H	1:H:106:HIS:CD2	2.22	0.55
1:I:60:LYS:HA	1:I:63:ARG:HD3	1.89	0.54
2:D:226:PRE:H3	1:F:57:PHE:CG	2.43	0.54
1:C:2:MET:HE2	1:C:3:ILE:H	1.73	0.54
1:G:57:PHE:CG	2:H:227:PRE:H3	2.43	0.54
1:F:12:VAL:HG12	1:F:23:LYS:HG3	1.90	0.54
1:C:16:THR:HG23	1:C:19:GLU:H	1.72	0.54
1:D:3:ILE:HD11	1:F:3:ILE:HG21	1.89	0.54
1:J:74:THR:HA	2:K:230:PRE:H5	1.91	0.53
1:L:3:ILE:HD13	1:L:96:GLN:HA	1.91	0.53
1:J:92:MET:HE3	1:J:92:MET:HA	1.91	0.52
1:K:62:VAL:HG21	1:K:73:VAL:HG11	1.91	0.52
1:E:21:LEU:HD11	1:E:60:LYS:HD3	1.90	0.52
1:B:3:ILE:HD12	1:B:94:THR:CG2	2.39	0.52
2:A:223:PRE:H3	1:C:57:PHE:CE1	2.45	0.52
1:B:96:GLN:HB2	1:C:2:MET:SD	2.50	0.52
1:E:45:MET:HE1	1:E:93:MET:HE2	1.92	0.52
1:D:47:LEU:O	1:D:75:CYS:HA	2.10	0.51
1:B:96:GLN:HB2	1:C:2:MET:CE	2.41	0.51
1:C:2:MET:N	1:C:97:THR:O	2.43	0.51
1:G:92:MET:HA	1:G:92:MET:HE3	1.93	0.51
1:J:7:ARG:H	1:J:106:HIS:CD2	2.28	0.51
1:D:7:ARG:H	1:D:106:HIS:CD2	2.21	0.51
1:D:2:MET:HE3	1:F:43:VAL:HG22	1.91	0.51
1:J:7:ARG:HG2	1:J:92:MET:HE1	1.93	0.51
1:B:8:GLY:HA2	1:B:107:VAL:O	2.12	0.50
1:L:48:SER:HB3	1:L:76:MET:HE3	1.94	0.50
1:E:8:GLY:HA2	1:E:107:VAL:O	2.12	0.49
1:B:48:SER:HA	1:B:76:MET:O	2.12	0.49
1:H:4:ARG:HH11	1:H:4:ARG:HG2	1.77	0.49
1:K:16:THR:HG23	1:K:19:GLU:H	1.78	0.49
1:A:57:PHE:CD1	2:B:221:PRE:H3	2.47	0.49
1:C:47:LEU:O	1:C:75:CYS:HA	2.12	0.49
1:D:2:MET:HG2	1:D:3:ILE:H	1.78	0.49
1:H:20:ILE:HD12	1:H:55:ALA:HB3	1.94	0.49
1:H:61:ALA:HA	1:H:64:GLU:HG2	1.96	0.48
1:K:16:THR:HG22	1:K:19:GLU:HB2	1.95	0.48
1:H:18:GLU:O	1:H:22:GLN:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:GLY:HA2	1:C:107:VAL:O	2.15	0.47
1:E:16:THR:HG22	1:E:19:GLU:HB3	1.96	0.47
1:L:45:MET:O	1:L:73:VAL:HA	2.14	0.47
1:G:17:GLU:HG3	1:G:56:VAL:HB	1.95	0.47
1:A:74:THR:HA	2:B:221:PRE:H5	1.96	0.47
1:D:12:VAL:HG11	1:D:20:ILE:HA	1.96	0.46
1:A:7:ARG:N	1:A:106:HIS:HD2	2.13	0.46
1:K:8:GLY:HA2	1:K:107:VAL:O	2.15	0.46
1:A:9:ALA:HB3	1:A:108:TYR:HD1	1.80	0.46
1:J:72:PRO:HB3	1:K:92:MET:HE1	1.97	0.46
1:C:7:ARG:N	1:C:106:HIS:HD2	2.11	0.46
1:H:51:PRO:HG3	1:H:80:ASP:HB2	1.97	0.46
1:E:16:THR:HG22	1:E:19:GLU:HB2	1.98	0.46
1:E:42:VAL:HG22	1:E:95:VAL:HG12	1.98	0.46
1:K:11:THR:HA	1:K:87:LYS:O	2.16	0.46
1:K:45:MET:HB3	1:K:73:VAL:HG12	1.97	0.46
1:B:57:PHE:CG	2:C:222:PRE:H3	2.51	0.46
1:E:100:PRO:HG2	1:E:103:GLN:HB2	1.97	0.46
1:A:47:LEU:O	1:A:75:CYS:HA	2.16	0.46
1:C:92:MET:HE3	1:C:92:MET:HA	1.98	0.46
1:J:3:ILE:HA	1:J:95:VAL:O	2.16	0.45
1:B:68:TRP:CE3	1:B:71:VAL:HG21	2.51	0.45
1:E:45:MET:O	1:E:73:VAL:HA	2.16	0.45
1:J:47:LEU:HD23	1:J:91:VAL:HB	1.99	0.45
1:K:105:ARG:HA	3:K:676:HOH:O	2.15	0.45
1:C:59:ALA:HB2	1:C:75:CYS:SG	2.57	0.45
1:C:47:LEU:HD13	1:C:58:PRO:HB2	1.98	0.45
1:G:79:MET:HE2	1:G:81:VAL:CG2	2.47	0.45
1:C:21:LEU:HD21	1:C:60:LYS:HB3	1.98	0.45
1:E:7:ARG:H	1:E:106:HIS:CD2	2.26	0.45
1:F:42:VAL:HG21	1:F:68:TRP:CH2	2.52	0.45
1:F:42:VAL:HG21	1:F:68:TRP:CZ3	2.52	0.45
1:F:23:LYS:HA	1:F:26:GLN:HE21	1.81	0.44
1:L:58:PRO:HD2	1:L:75:CYS:SG	2.56	0.44
1:E:21:LEU:HD21	1:E:60:LYS:HB3	2.00	0.44
1:D:12:VAL:HB	1:D:19:GLU:HG3	1.99	0.44
1:D:48:SER:HB3	1:D:76:MET:HE3	2.00	0.44
1:F:30:LYS:O	1:F:34:GLU:HG2	2.18	0.44
1:E:16:THR:HG22	1:E:19:GLU:H	1.83	0.44
1:L:48:SER:HA	1:L:76:MET:O	2.18	0.44
1:F:45:MET:HG3	1:F:93:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:VAL:HB	1:F:19:GLU:HG2	1.99	0.43
1:D:58:PRO:HD2	1:E:79:MET:SD	2.58	0.43
1:C:68:TRP:CE3	1:C:71:VAL:HG21	2.54	0.43
1:I:30:LYS:HB3	1:I:107:VAL:HG11	1.99	0.43
1:K:99:VAL:HA	1:K:100:PRO:HD3	1.89	0.43
2:A:223:PRE:H3	1:C:57:PHE:CD1	2.53	0.43
1:B:16:THR:CG2	1:B:19:GLU:HB2	2.46	0.43
1:C:7:ARG:H	1:C:106:HIS:CD2	2.25	0.43
1:B:43:VAL:HG11	1:C:3:ILE:HG22	2.00	0.43
1:K:43:VAL:HG22	1:L:3:ILE:O	2.18	0.43
1:B:3:ILE:HD12	1:B:94:THR:HG22	2.01	0.43
1:J:2:MET:HE3	1:L:43:VAL:HG22	2.01	0.43
1:H:4:ARG:HG2	1:H:4:ARG:NH1	2.34	0.42
1:D:3:ILE:HG12	1:F:3:ILE:HG12	2.01	0.42
1:J:48:SER:HB3	1:J:76:MET:HE3	2.01	0.42
1:C:17:GLU:HG3	1:C:56:VAL:HB	2.01	0.42
1:E:72:PRO:HB2	1:F:92:MET:HE1	2.02	0.42
1:F:16:THR:HG23	1:F:19:GLU:HB3	2.01	0.42
1:I:48:SER:HA	1:I:76:MET:O	2.20	0.42
1:D:12:VAL:HG12	1:D:23:LYS:HG3	2.00	0.42
1:C:3:ILE:HA	1:C:95:VAL:O	2.20	0.42
1:C:109:LEU:O	1:C:112:ALA:HB3	2.20	0.42
1:E:22:GLN:O	1:E:26:GLN:HG3	2.20	0.42
1:K:16:THR:CG2	1:K:19:GLU:HB2	2.50	0.42
1:A:59:ALA:HB2	1:A:75:CYS:SG	2.60	0.41
1:H:47:LEU:O	1:H:75:CYS:HA	2.20	0.41
1:I:22:GLN:OE1	1:I:23:LYS:HE3	2.19	0.41
1:J:57:PHE:CG	2:K:230:PRE:H3	2.55	0.41
1:A:108:TYR:HB3	1:A:112:ALA:O	2.20	0.41
1:B:16:THR:HG23	1:B:19:GLU:CB	2.49	0.41
1:L:7:ARG:N	1:L:106:HIS:HD2	2.15	0.41
1:K:14:ARG:NH2	1:K:16:THR:HG21	2.31	0.41
2:A:223:PRE:H2	1:C:57:PHE:CD2	2.55	0.41
1:I:53:LEU:HD21	1:I:87:LYS:HG2	2.01	0.41
1:B:49:ALA:HA	1:B:88:CYS:O	2.21	0.41
1:C:30:LYS:HD2	1:C:30:LYS:HA	1.89	0.41
1:L:37:THR:HG21	1:L:93:MET:HE3	2.03	0.41
1:I:2:MET:HE3	1:I:3:ILE:O	2.21	0.41
1:D:8:GLY:HA2	1:D:107:VAL:O	2.21	0.41
1:F:23:LYS:HA	1:F:23:LYS:HD3	1.89	0.41
1:F:25:LYS:HE2	1:F:25:LYS:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:VAL:HB	1:F:94:THR:HB	2.03	0.41
1:I:47:LEU:O	1:I:75:CYS:HA	2.21	0.40
1:I:48:SER:OG	1:I:90:ARG:HB2	2.20	0.40
1:J:25:LYS:O	1:J:29:GLU:HG3	2.21	0.40
1:H:48:SER:HA	1:H:76:MET:O	2.21	0.40
1:I:45:MET:O	1:I:73:VAL:HA	2.20	0.40
1:I:39:PRO:HG3	1:I:68:TRP:NE1	2.36	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
1	B	116/127 (91%)	111 (96%)	4 (3%)	1 (1%)	14	14
1	C	117/127 (92%)	110 (94%)	7 (6%)	0	100	100
1	D	112/127 (88%)	105 (94%)	5 (4%)	2 (2%)	6	4
1	E	116/127 (91%)	112 (97%)	3 (3%)	1 (1%)	14	14
1	F	115/127 (91%)	111 (96%)	4 (4%)	0	100	100
1	G	112/127 (88%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	112/127 (88%)	108 (96%)	4 (4%)	0	100	100
1	I	112/127 (88%)	107 (96%)	5 (4%)	0	100	100
1	J	112/127 (88%)	110 (98%)	2 (2%)	0	100	100
1	K	114/127 (90%)	112 (98%)	2 (2%)	0	100	100
1	L	112/127 (88%)	108 (96%)	3 (3%)	1 (1%)	14	14
All	All	1362/1524 (89%)	1311 (96%)	46 (3%)	5 (0%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	118	ASP
1	L	44	GLN
1	B	117	PRO
1	D	66	SER
1	D	114	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/116 (89%)	98 (95%)	5 (5%)	22	29
1	B	107/116 (92%)	100 (94%)	7 (6%)	15	18
1	C	108/116 (93%)	103 (95%)	5 (5%)	24	32
1	D	103/116 (89%)	98 (95%)	5 (5%)	22	29
1	E	107/116 (92%)	103 (96%)	4 (4%)	30	41
1	F	106/116 (91%)	98 (92%)	8 (8%)	12	14
1	G	103/116 (89%)	97 (94%)	6 (6%)	18	22
1	H	103/116 (89%)	102 (99%)	1 (1%)	68	81
1	I	103/116 (89%)	100 (97%)	3 (3%)	37	51
1	J	103/116 (89%)	98 (95%)	5 (5%)	22	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	105/116 (90%)	97 (92%)	8 (8%)	12	14
1	L	103/116 (89%)	99 (96%)	4 (4%)	28	39
All	All	1254/1392 (90%)	1193 (95%)	61 (5%)	22	29

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	10	THR
1	A	69	GLN
1	A	74	THR
1	A	91	VAL
1	B	2	MET
1	B	16	THR
1	B	18	GLU
1	B	22	GLN
1	B	66	SER
1	B	76	MET
1	B	91	VAL
1	C	2	MET
1	C	3	ILE
1	C	74	THR
1	C	81	VAL
1	C	114	VAL
1	D	16	THR
1	D	47	LEU
1	D	50	THR
1	D	74	THR
1	D	91	VAL
1	E	2	MET
1	E	16	THR
1	E	50	THR
1	E	119	LEU
1	F	19	GLU
1	F	37	THR
1	F	64	GLU
1	F	69	GLN
1	F	74	THR
1	F	81	VAL
1	F	82	THR
1	F	91	VAL

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Mol	Chain	Res	Type
1	G	2	MET
1	G	16	THR
1	G	18	GLU
1	G	38	LYS
1	G	63	ARG
1	G	73	VAL
1	H	96	GLN
1	I	64	GLU
1	I	73	VAL
1	I	114	VAL
1	J	3	ILE
1	J	21	LEU
1	J	22	GLN
1	J	50	THR
1	J	74	THR
1	K	2	MET
1	K	13	GLU
1	K	33	GLU
1	K	74	THR
1	K	81	VAL
1	K	98	ASP
1	K	114	VAL
1	K	116	ARG
1	L	40	GLU
1	L	63	ARG
1	L	64	GLU
1	L	114	VAL

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

Mol	Chain	Res	Type
1	A	36	HIS
1	A	77	GLN
1	A	106	HIS
1	B	44	GLN
1	B	69	GLN
1	B	101	GLN
1	B	106	HIS
1	C	26	GLN
1	C	44	GLN
1	C	77	GLN
1	C	101	GLN

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Mol	Chain	Res	Type
1	C	106	HIS
1	D	96	GLN
1	D	101	GLN
1	D	106	HIS
1	E	36	HIS
1	E	106	HIS
1	F	26	GLN
1	F	101	GLN
1	F	103	GLN
1	F	106	HIS
1	G	22	GLN
1	G	44	GLN
1	G	101	GLN
1	H	26	GLN
1	H	96	GLN
1	H	101	GLN
1	H	106	HIS
1	I	101	GLN
1	I	106	HIS
1	J	96	GLN
1	J	106	HIS
1	K	101	GLN
1	L	22	GLN
1	L	26	GLN
1	L	101	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PRE	F	225	-	16,16,16	1.50	1 (6%)	14,23,23	1.85	4 (28%)
2	PRE	K	230	-	16,16,16	1.59	4 (25%)	14,23,23	1.65	3 (21%)
2	PRE	C	222	-	16,16,16	1.69	5 (31%)	14,23,23	1.63	2 (14%)
2	PRE	D	226	-	16,16,16	1.61	3 (18%)	14,23,23	1.64	5 (35%)
2	PRE	E	224	-	16,16,16	1.52	3 (18%)	14,23,23	1.84	5 (35%)
2	PRE	B	221	-	16,16,16	1.43	2 (12%)	14,23,23	1.56	2 (14%)
2	PRE	A	223	-	16,16,16	1.62	3 (18%)	14,23,23	1.75	4 (28%)
2	PRE	H	227	-	16,16,16	1.65	3 (18%)	14,23,23	2.02	5 (35%)
2	PRE	G	229	-	16,16,16	1.50	2 (12%)	14,23,23	1.68	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PRE	F	225	-	-	5/15/27/27	0/1/1/1
2	PRE	K	230	-	-	2/15/27/27	0/1/1/1
2	PRE	C	222	-	-	1/15/27/27	0/1/1/1
2	PRE	D	226	-	-	2/15/27/27	0/1/1/1
2	PRE	E	224	-	-	0/15/27/27	0/1/1/1
2	PRE	B	221	-	-	5/15/27/27	0/1/1/1
2	PRE	A	223	-	-	0/15/27/27	0/1/1/1
2	PRE	H	227	-	-	4/15/27/27	0/1/1/1
2	PRE	G	229	-	-	3/15/27/27	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	229	PRE	C8-C1'	2.97	1.54	1.51
2	D	226	PRE	C5-C6	2.92	1.36	1.32
2	A	223	PRE	C5-C6	2.82	1.36	1.32
2	C	222	PRE	C8-C1'	2.73	1.54	1.51
2	B	221	PRE	O'M-C2'	-2.72	1.23	1.30
2	C	222	PRE	O'M-C2'	-2.69	1.23	1.30
2	A	223	PRE	C8-C1'	2.66	1.54	1.51
2	E	224	PRE	C5-C6	2.66	1.36	1.32
2	K	230	PRE	O'M-C2'	-2.64	1.23	1.30
2	D	226	PRE	C8-C1'	2.63	1.54	1.51
2	H	227	PRE	O'M-C2'	-2.61	1.23	1.30
2	C	222	PRE	C1-C7	2.58	1.56	1.53
2	H	227	PRE	C3-C2	2.57	1.36	1.32
2	F	225	PRE	O'M-C2'	-2.53	1.23	1.30
2	E	224	PRE	O'M-C2'	-2.46	1.23	1.30
2	H	227	PRE	C5-C6	2.43	1.36	1.32
2	K	230	PRE	C5-C6	2.42	1.36	1.32
2	D	226	PRE	O'M-C2'	-2.39	1.24	1.30
2	G	229	PRE	O'M-C2'	-2.39	1.24	1.30
2	A	223	PRE	O'M-C2'	-2.29	1.24	1.30
2	E	224	PRE	C3-C2	2.26	1.35	1.32
2	K	230	PRE	C3-C2	2.21	1.35	1.32
2	K	230	PRE	C1-C7	2.18	1.55	1.53
2	B	221	PRE	C3-C2	2.15	1.35	1.32
2	C	222	PRE	C3-C2	2.06	1.35	1.32
2	C	222	PRE	C5-C6	2.01	1.35	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	227	PRE	C4-C5-C6	-4.76	119.49	123.40
2	F	225	PRE	O'L-C2'-C1'	-3.68	117.23	121.81
2	A	223	PRE	C4-C3-C2	-3.59	120.44	123.40
2	G	229	PRE	C4-C5-C6	-3.32	120.67	123.40
2	F	225	PRE	C4-C3-C2	-3.31	120.67	123.40
2	K	230	PRE	O'L-C2'-C1'	-3.22	117.81	121.81
2	E	224	PRE	O72-C7-C1	3.11	120.69	114.86
2	C	222	PRE	O72-C7-C1	2.96	120.40	114.86
2	A	223	PRE	O72-C7-C1	2.83	120.16	114.86
2	H	227	PRE	O1'-C1'-C8	-2.68	116.26	121.76
2	B	221	PRE	C4-C3-C2	-2.65	121.22	123.40
2	G	229	PRE	O72-C7-C1	2.65	119.82	114.86
2	E	224	PRE	O'L-C2'-C1'	-2.57	118.61	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	230	PRE	O72-C7-C1	2.50	119.54	114.86
2	K	230	PRE	O'M-C2'-C1'	2.49	120.48	113.59
2	D	226	PRE	O72-C7-C1	2.47	119.49	114.86
2	B	221	PRE	O1'-C1'-C2'	2.46	123.17	119.67
2	D	226	PRE	C4-C3-C2	-2.43	121.40	123.40
2	E	224	PRE	C4-C3-C2	-2.34	121.48	123.40
2	F	225	PRE	O'M-C2'-C1'	2.32	120.03	113.59
2	F	225	PRE	O72-C7-C1	2.27	119.11	114.86
2	C	222	PRE	O'L-C2'-C1'	-2.26	119.00	121.81
2	E	224	PRE	O'M-C2'-C1'	2.24	119.80	113.59
2	D	226	PRE	C4-C5-C6	-2.24	121.56	123.40
2	D	226	PRE	O1'-C1'-C2'	2.21	122.83	119.67
2	D	226	PRE	O'M-C2'-C1'	2.17	119.60	113.59
2	H	227	PRE	O1'-C1'-C2'	2.17	122.76	119.67
2	E	224	PRE	O71-C7-C1	-2.15	118.64	121.96
2	H	227	PRE	C4-C3-C2	-2.14	121.64	123.40
2	H	227	PRE	O72-C7-C1	2.12	118.82	114.86
2	A	223	PRE	O'M-C2'-C1'	2.08	119.36	113.59
2	A	223	PRE	O'L-C2'-C1'	-2.00	119.32	121.81

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	221	PRE	C2'-C1'-C8-C1
2	B	221	PRE	C8-C1'-C2'-O'L
2	B	221	PRE	C8-C1'-C2'-O'M
2	F	225	PRE	C6-C1-C7-O72
2	F	225	PRE	C8-C1'-C2'-O'M
2	G	229	PRE	C2'-C1'-C8-C1
2	G	229	PRE	C8-C1'-C2'-O'M
2	H	227	PRE	C2'-C1'-C8-C1
2	H	227	PRE	C8-C1'-C2'-O'M
2	K	230	PRE	C8-C1'-C2'-O'M
2	F	225	PRE	C8-C1'-C2'-O'L
2	G	229	PRE	C8-C1'-C2'-O'L
2	H	227	PRE	C8-C1'-C2'-O'L
2	K	230	PRE	C8-C1'-C2'-O'L
2	H	227	PRE	C7-C1-C8-C1'
2	D	226	PRE	O1'-C1'-C8-C1
2	B	221	PRE	O1'-C1'-C2'-O'M
2	D	226	PRE	O1'-C1'-C2'-O'M

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Mol	Chain	Res	Type	Atoms
2	F	225	PRE	O1'-C1'-C2'-O'M
2	B	221	PRE	O1'-C1'-C2'-O'L
2	C	222	PRE	C6-C1-C7-O71
2	F	225	PRE	C6-C1-C7-O71

There are no ring outliers.

8 monomers are involved in 15 short contacts:

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