



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:09 PM GMT

PDB ID : 4KIU
Title : Design and structural analysis of aromatic inhibitors of type II dehydroquinase dehydratase from Mycobacterium tuberculosis - compound 49d [5-[(3-nitrobenzyl)oxy]benzene-1,3-dicarboxylic acid]
Authors : Dias, M.V.B; Howard, N.G.; Blundell, T.L.; Abell, C.
Deposited on : 2013-05-02
Resolution : 2.40 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

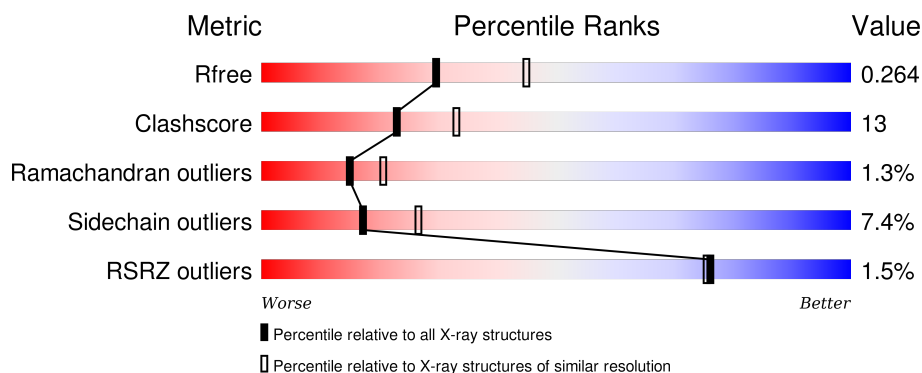
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.
















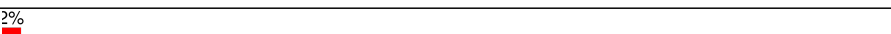





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	153	<div> <div>4%</div> <div>65%</div> <div>23%</div> <div>•</div> <div>8%</div> </div>
1	B	153	<div> <div>%</div> <div>74%</div> <div>17%</div> <div>••</div> <div>8%</div> </div>
1	C	153	<div> <div>76%</div> <div>13%</div> <div>•</div> <div>8%</div> </div>
1	D	153	<div> <div>75%</div> <div>16%</div> <div>•</div> <div>7%</div> </div>
1	E	153	<div> <div>%</div> <div>68%</div> <div>20%</div> <div>••</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	153	
1	G	153	
1	H	153	
1	I	153	
1	J	153	
1	K	153	
1	L	153	
1	M	153	
1	N	153	
1	O	153	
1	P	153	
1	Q	153	
1	R	153	
1	S	153	
1	T	153	
1	U	153	
1	V	153	
1	W	153	
1	X	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KIU	C	201	-	-	-	X
2	KIU	I	201	-	-	X	-
2	KIU	K	201	-	-	X	-
2	KIU	L	201	-	-	-	X
2	KIU	P	201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KIU	Q	201	-	-	-	X
2	KIU	V	201	-	-	X	-
2	KIU	X	201	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26970 atoms, of which 0 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 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	B	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	C	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	D	143	Total	C	N	O	S	0	0	0
			1082	681	198	202	1			
1	E	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	F	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	G	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	H	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	I	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	J	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	K	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	L	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	M	135	Total	C	N	O	S	0	0	0
			1021	644	184	192	1			
1	N	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	O	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	P	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	R	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	S	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	T	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	U	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	V	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	W	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	X	147	Total	C	N	O	S	0	0	0
			1121	707	202	210	2			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
A	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
A	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
A	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
A	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
A	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
B	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
B	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
B	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
B	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
B	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
C	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
C	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
C	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
C	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
C	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
D	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
D	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
D	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
D	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
D	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
E	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
E	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
E	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
E	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
E	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
F	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
F	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
F	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
F	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
F	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
F	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
G	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
G	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
G	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
G	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
G	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
H	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
H	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
H	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
H	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
H	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
H	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
I	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
I	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
I	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
I	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
I	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
J	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
J	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
J	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
J	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
J	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
K	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
K	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
K	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
K	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6

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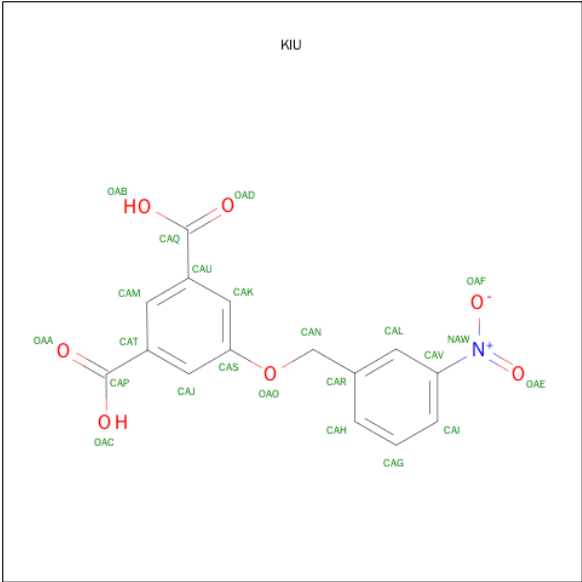
Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
L	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
L	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
L	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
L	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
L	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
M	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
M	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
M	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
M	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
M	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
N	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
N	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
N	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
N	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
N	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
O	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
O	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
O	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
O	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
O	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
P	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
P	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
P	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
P	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
P	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
Q	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
Q	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
Q	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
Q	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
Q	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
R	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
R	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
R	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
R	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
S	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
S	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
S	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
S	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
S	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
T	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
T	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
T	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
T	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
T	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
U	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
U	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
U	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
U	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
U	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
V	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
V	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
V	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
V	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
V	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
W	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
W	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
W	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
W	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
W	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-6	LEU	-	EXPRESSION TAG	UNP P0A4Z6
X	-5	TYR	-	EXPRESSION TAG	UNP P0A4Z6
X	-4	PHE	-	EXPRESSION TAG	UNP P0A4Z6
X	-3	GLN	-	EXPRESSION TAG	UNP P0A4Z6
X	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
X	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6

- Molecule 2 is 5-[(3-NITROBENZYL)OXY]BENZENE-1,3-DICARBOXYLIC ACID (three-letter code: KIU) (formula: C₁₅H₁₁NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	15	1	7		
2	B	1	Total	C	N	O	0	0
			23	15	1	7		
2	C	1	Total	C	N	O	0	0
			23	15	1	7		
2	D	1	Total	C	N	O	0	0
			23	15	1	7		
2	E	1	Total	C	N	O	0	0
			23	15	1	7		
2	F	1	Total	C	N	O	0	0
			23	15	1	7		
2	G	1	Total	C	N	O	0	0
			23	15	1	7		
2	H	1	Total	C	N	O	0	0
			23	15	1	7		
2	I	1	Total	C	N	O	0	0
			23	15	1	7		
2	J	1	Total	C	N	O	0	0
			23	15	1	7		
2	K	1	Total	C	N	O	0	0
			23	15	1	7		
2	L	1	Total	C	N	O	0	0
			23	15	1	7		
2	N	1	Total	C	N	O	0	0
			23	15	1	7		
2	O	1	Total	C	N	O	0	0
			23	15	1	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	P	1	Total	C	N	O	0	0
			23	15	1	7		
2	Q	1	Total	C	N	O	0	0
			23	15	1	7		
2	R	1	Total	C	N	O	0	0
			23	15	1	7		
2	T	1	Total	C	N	O	0	0
			23	15	1	7		
2	U	1	Total	C	N	O	0	0
			23	15	1	7		
2	V	1	Total	C	N	O	0	0
			23	15	1	7		
2	W	1	Total	C	N	O	0	0
			23	15	1	7		
2	X	1	Total	C	N	O	0	0
			23	15	1	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	34	Total	O	0	0
			34	34		
3	C	44	Total	O	0	0
			44	44		
3	D	40	Total	O	0	0
			40	40		
3	E	38	Total	O	0	0
			38	38		
3	F	48	Total	O	0	0
			48	48		
3	G	33	Total	O	0	0
			33	33		
3	H	34	Total	O	0	0
			34	34		
3	I	41	Total	O	0	0
			41	41		
3	J	41	Total	O	0	0
			41	41		
3	K	28	Total	O	0	0
			28	28		

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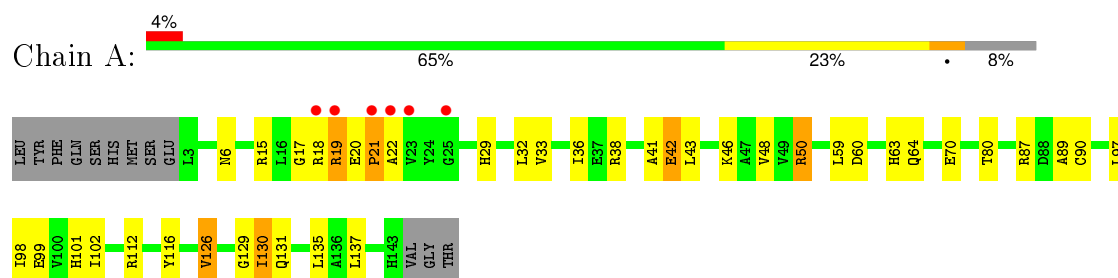
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	27	Total 27	O 27	0	0
3	M	29	Total 29	O 29	0	0
3	N	19	Total 19	O 19	0	0
3	O	36	Total 36	O 36	0	0
3	P	26	Total 26	O 26	0	0
3	Q	19	Total 19	O 19	0	0
3	R	26	Total 26	O 26	0	0
3	S	28	Total 28	O 28	0	0
3	T	37	Total 37	O 37	0	0
3	U	33	Total 33	O 33	0	0
3	V	24	Total 24	O 24	0	0
3	W	16	Total 16	O 16	0	0
3	X	31	Total 31	O 31	0	0

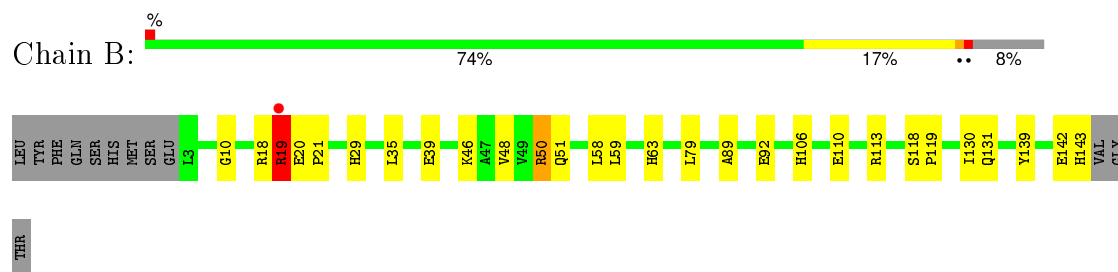
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

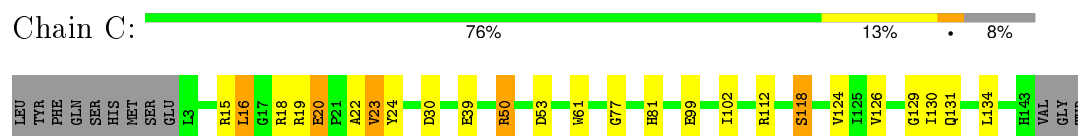
- Molecule 1: 3-dehydroquinate dehydratase



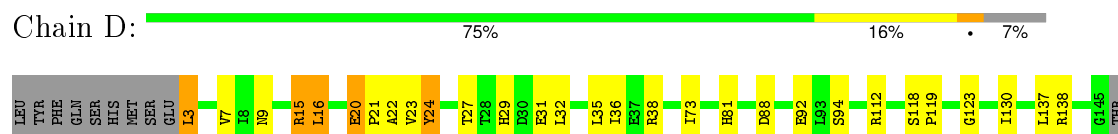
- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase

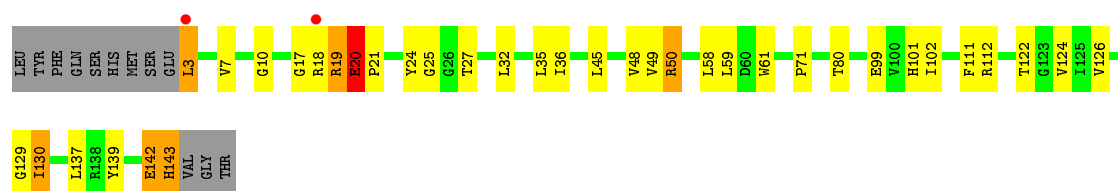


- Molecule 1: 3-dehydroquinate dehydratase



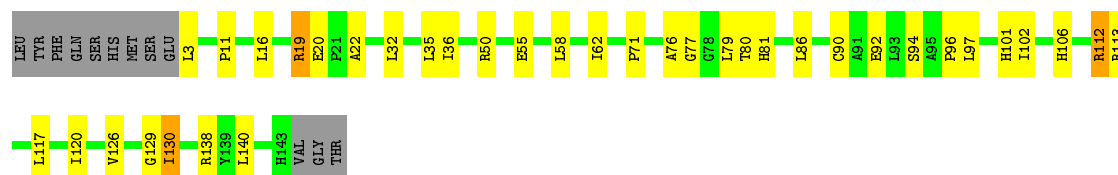
- Molecule 1: 3-dehydroquinate dehydratase





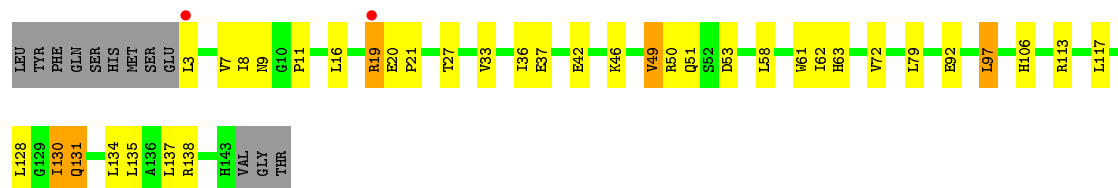
- Molecule 1: 3-dehydroquinatase dehydratase

Chain F: 68% 22% 8%



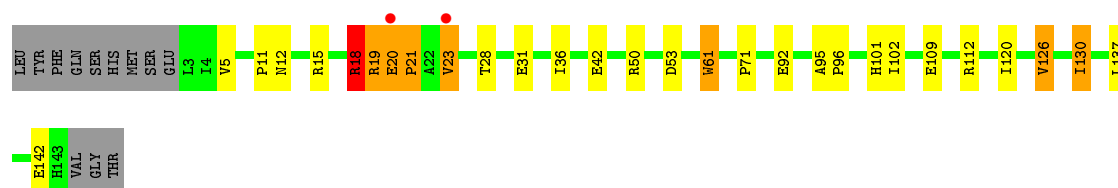
- Molecule 1: 3-dehydroquinatase dehydratase

Chain G: 68% 21% 8%



- Molecule 1: 3-dehydroquinatase dehydratase

Chain H: 73% 14% 5% 8%



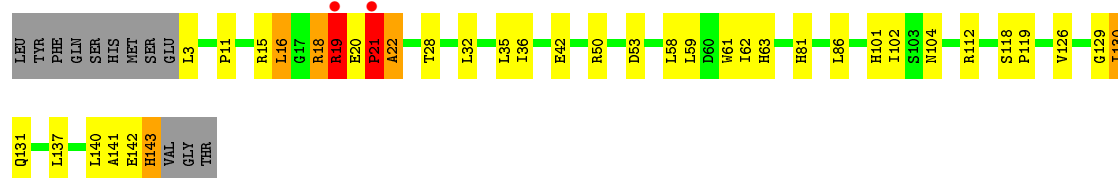
- Molecule 1: 3-dehydroquinatase dehydratase

Chain I: 65% 23% 8%

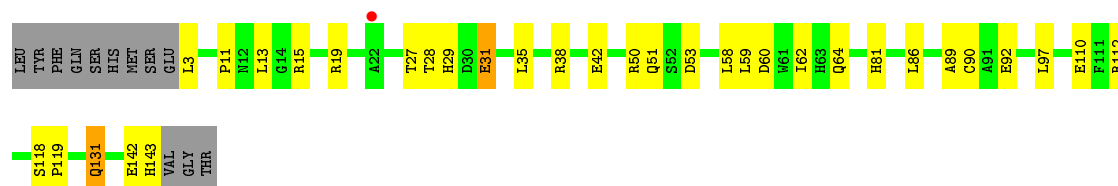


- Molecule 1: 3-dehydroquinatase dehydratase

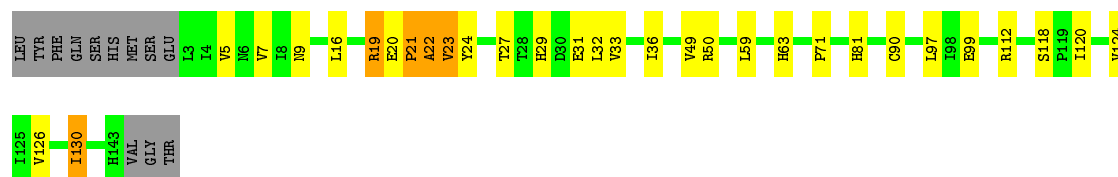
Chain J: 67% 20% 8%



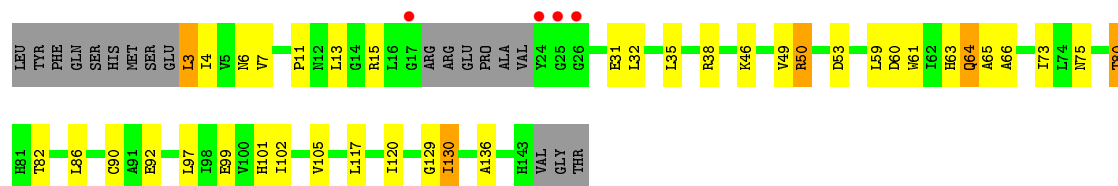
- Molecule 1: 3-dehydroquinate dehydratase



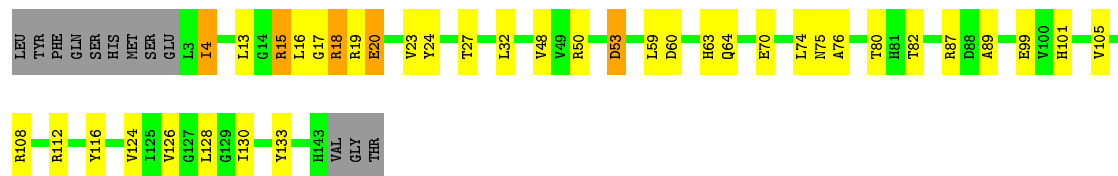
- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase

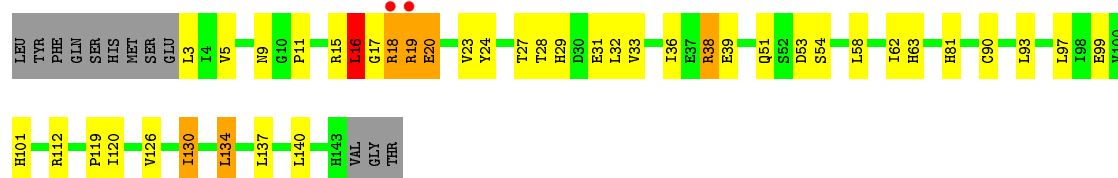


- Molecule 1: 3-dehydroquinate dehydratase

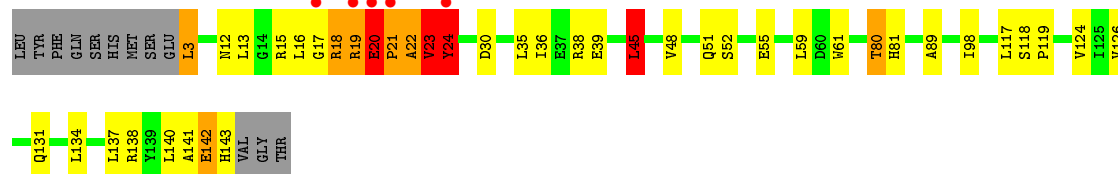


- Molecule 1: 3-dehydroquinate dehydratase

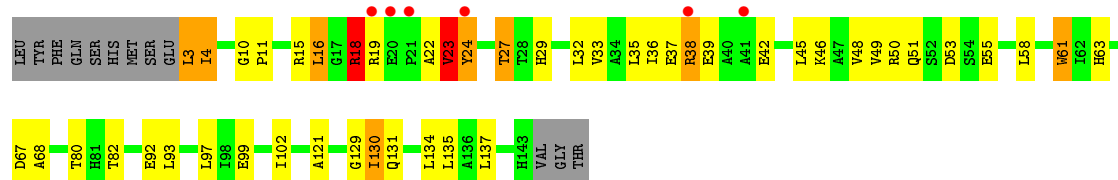




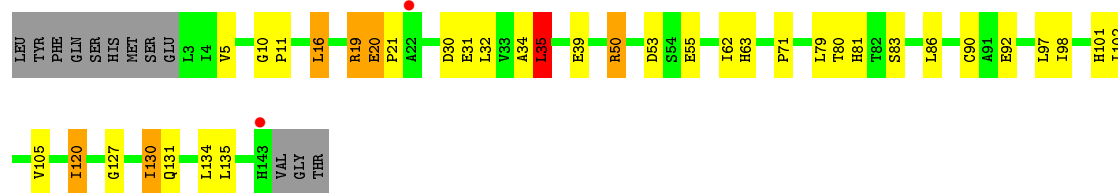
- Molecule 1: 3-dehydroquinatase dehydratase



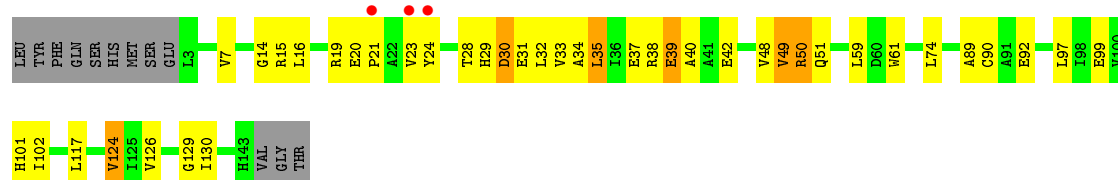
- Molecule 1: 3-dehydroquinatase dehydratase



- Molecule 1: 3-dehydroquinatase dehydratase



- Molecule 1: 3-dehydroquinatase dehydratase

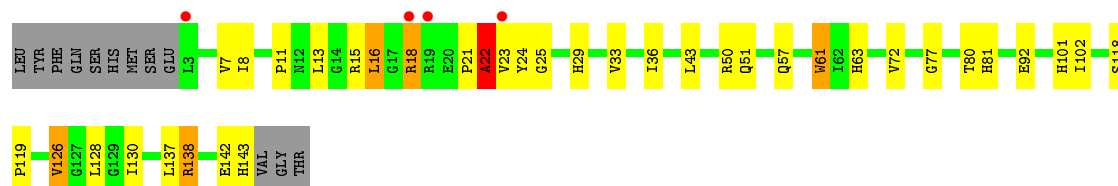


- Molecule 1: 3-dehydroquinatase dehydratase

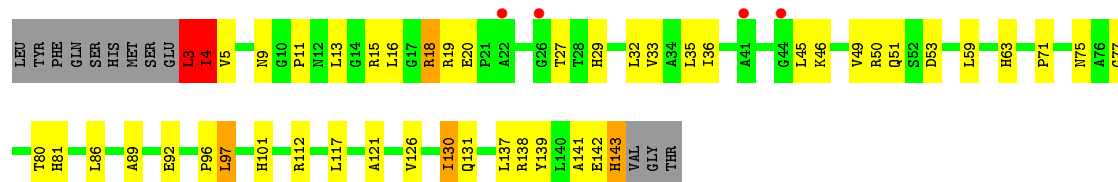




- Molecule 1: 3-dehydroquinatase dehydratase



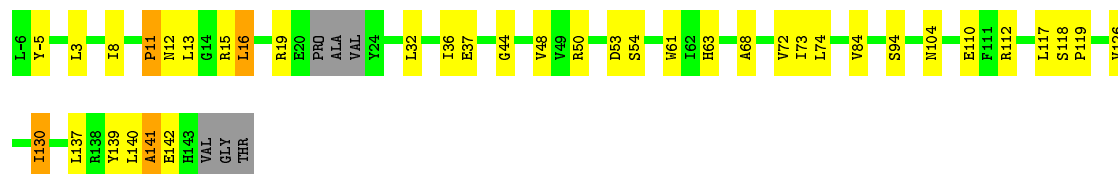
- Molecule 1: 3-dehydroquinatase dehydratase



- Molecule 1: 3-dehydroquinatase dehydratase



- Molecule 1: 3-dehydroquinatase dehydratase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.41Å 139.15Å 143.29Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	45.28 – 2.40 45.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (45.28-2.40) 95.0 (45.28-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.190 , 0.265 0.190 , 0.264	Depositor DCC
R_{free} test set	6962 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 139255 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26970	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.74	0/1089	0.88	0/1483
1	B	0.76	0/1089	0.87	0/1483
1	C	0.77	0/1089	0.87	0/1483
1	D	0.83	0/1100	0.93	3/1498 (0.2%)
1	E	0.76	1/1089 (0.1%)	0.87	2/1483 (0.1%)
1	F	0.73	0/1089	0.82	0/1483
1	G	0.76	1/1089 (0.1%)	0.93	2/1483 (0.1%)
1	H	0.78	1/1089 (0.1%)	0.86	1/1483 (0.1%)
1	I	0.78	0/1089	0.89	1/1483 (0.1%)
1	J	0.81	1/1089 (0.1%)	0.93	2/1483 (0.1%)
1	K	0.71	0/1083	0.85	0/1476
1	L	0.76	0/1089	0.97	0/1483
1	M	0.71	0/1037	0.83	0/1411
1	N	0.67	0/1089	0.79	1/1483 (0.1%)
1	O	0.76	0/1089	0.91	2/1483 (0.1%)
1	P	0.69	1/1089 (0.1%)	0.86	2/1483 (0.1%)
1	Q	0.66	1/1089 (0.1%)	0.84	2/1483 (0.1%)
1	R	0.68	0/1083	0.82	0/1476
1	S	0.69	1/1089 (0.1%)	0.83	0/1483
1	T	0.77	0/1089	0.86	0/1483
1	U	0.73	1/1089 (0.1%)	0.84	0/1483
1	V	0.76	0/1089	0.87	2/1483 (0.1%)
1	W	0.64	0/1089	0.83	0/1483
1	X	0.74	1/1140 (0.1%)	0.86	0/1549
All	All	0.74	9/26134 (0.0%)	0.87	20/35587 (0.1%)

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	D	0	2
1	E	0	1
1	I	0	1
1	O	0	1
1	P	0	2
1	Q	0	1
1	U	0	1
1	W	0	1
All	All	0	10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	61	TRP	CD2-CE2	6.42	1.49	1.41
1	H	61	TRP	CD2-CE2	5.88	1.48	1.41
1	S	61	TRP	CD2-CE2	5.72	1.48	1.41
1	G	61	TRP	CD2-CE2	5.45	1.47	1.41
1	E	61	TRP	CD2-CE2	5.43	1.47	1.41
1	J	61	TRP	CD2-CE2	5.35	1.47	1.41
1	P	61	TRP	CD2-CE2	5.20	1.47	1.41
1	X	61	TRP	CD2-CE2	5.18	1.47	1.41
1	Q	61	TRP	CD2-CE2	5.06	1.47	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	LEU	CB-CG-CD1	-7.04	99.03	111.00
1	H	53	ASP	CB-CG-OD1	6.84	124.46	118.30
1	V	20	GLU	N-CA-C	-6.27	94.06	111.00
1	I	24	TYR	N-CA-C	6.26	127.90	111.00
1	P	45	LEU	CA-CB-CG	5.99	129.08	115.30
1	Q	23	VAL	N-CA-C	5.83	126.73	111.00
1	G	3	LEU	CA-CB-CG	5.77	128.57	115.30
1	Q	23	VAL	C-N-CA	5.76	136.09	121.70
1	V	3	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	15	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	24	TYR	N-CA-C	5.66	126.29	111.00
1	P	24	TYR	N-CA-C	5.54	125.96	111.00
1	D	3	LEU	CA-CB-CG	5.50	127.94	115.30
1	J	21	PRO	C-N-CA	5.43	135.26	121.70
1	N	53	ASP	CB-CG-OD1	5.40	123.16	118.30
1	E	59	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	E	3	LEU	CA-CB-CG	5.34	127.58	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	18	ARG	N-CA-C	5.27	125.23	111.00
1	J	50	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	O	134	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	22	ALA	Peptide
1	D	24	TYR	Peptide
1	E	20	GLU	Peptide
1	I	24	TYR	Peptide
1	O	16	LEU	Peptide
1	P	142	GLU	Peptide
1	P	24	TYR	Peptide
1	Q	22	ALA	Peptide
1	U	22	ALA	Peptide
1	W	20	GLU	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	1071	0	1079	39	0
1	B	1071	0	1079	17	0
1	C	1071	0	1079	23	0
1	D	1082	0	1091	25	0
1	E	1071	0	1079	23	0
1	F	1071	0	1079	24	0
1	G	1071	0	1079	26	0
1	H	1071	0	1079	23	0
1	I	1071	0	1079	34	0
1	J	1071	0	1079	32	0
1	K	1065	0	1068	29	0
1	L	1071	0	1079	26	0
1	M	1021	0	1025	33	0
1	N	1071	0	1079	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1071	0	1079	39	0
1	P	1071	0	1079	38	0
1	Q	1071	0	1079	32	0
1	R	1065	0	1068	34	0
1	S	1071	0	1079	24	0
1	T	1071	0	1079	32	0
1	U	1071	0	1079	29	0
1	V	1071	0	1079	60	0
1	W	1071	0	1079	44	0
1	X	1121	0	1114	30	0
2	A	23	0	9	2	0
2	B	23	0	9	2	0
2	C	23	0	9	6	0
2	D	23	0	9	3	0
2	E	23	0	9	2	0
2	F	23	0	9	6	0
2	G	23	0	9	2	0
2	H	23	0	9	4	0
2	I	23	0	9	7	0
2	J	23	0	9	6	0
2	K	23	0	9	8	0
2	L	23	0	9	4	0
2	N	23	0	9	5	0
2	O	23	0	9	3	0
2	P	23	0	9	7	0
2	Q	23	0	9	2	0
2	R	23	0	9	4	0
2	T	23	0	9	6	0
2	U	23	0	9	4	0
2	V	23	0	9	16	0
2	W	23	0	9	6	0
2	X	23	0	9	5	0
3	A	29	0	0	0	0
3	B	34	0	0	0	0
3	C	44	0	0	0	0
3	D	40	0	0	0	0
3	E	38	0	0	1	0
3	F	48	0	0	1	0
3	G	33	0	0	2	0
3	H	34	0	0	0	0
3	I	41	0	0	1	0
3	J	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	28	0	0	0	0
3	L	27	0	0	2	0
3	M	29	0	0	0	0
3	N	19	0	0	0	0
3	O	36	0	0	0	0
3	P	26	0	0	1	0
3	Q	19	0	0	1	0
3	R	26	0	0	0	0
3	S	28	0	0	1	0
3	T	37	0	0	0	0
3	U	33	0	0	1	0
3	V	24	0	0	0	0
3	W	16	0	0	0	0
3	X	31	0	0	0	0
All	All	26970	0	26065	704	0

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 13.

All (704) 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)
2:I:201:KIU:NAW	2:I:201:KIU:OAF	1.56	1.37
2:I:201:KIU:NAW	2:I:201:KIU:OAE	1.60	1.35
2:T:201:KIU:OAE	2:T:201:KIU:NAW	1.61	1.33
2:J:201:KIU:OAF	2:J:201:KIU:NAW	1.61	1.32
2:B:201:KIU:OAF	2:B:201:KIU:NAW	1.62	1.31
2:Q:201:KIU:NAW	2:Q:201:KIU:OAE	1.63	1.31
2:P:201:KIU:NAW	2:P:201:KIU:OAF	1.60	1.30
2:P:201:KIU:OAE	2:P:201:KIU:NAW	1.61	1.30
2:B:201:KIU:OAE	2:B:201:KIU:NAW	1.68	1.25
2:T:201:KIU:OAF	2:T:201:KIU:NAW	1.71	1.23
2:C:201:KIU:NAW	2:C:201:KIU:OAF	1.71	1.23
2:G:201:KIU:OAF	2:G:201:KIU:NAW	1.72	1.22
1:U:92:GLU:HB3	1:V:19:ARG:NH1	1.55	1.20
2:H:201:KIU:NAW	2:H:201:KIU:OAF	1.72	1.20
2:H:201:KIU:OAE	2:H:201:KIU:NAW	1.73	1.19
2:G:201:KIU:NAW	2:G:201:KIU:OAE	1.78	1.16
2:J:201:KIU:NAW	2:J:201:KIU:OAE	1.79	1.15
1:W:15:ARG:HG2	1:W:15:ARG:HH11	1.11	1.14
1:M:3:LEU:HB3	1:M:4:ILE:HD12	1.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:18:ARG:HD2	1:V:18:ARG:H	1.04	1.11
1:P:19:ARG:HH11	1:P:19:ARG:HG2	1.02	1.11
1:K:81:HIS:NE2	2:K:201:KIU:OAD	1.83	1.10
1:P:17:GLY:HA3	1:P:18:ARG:HB2	1.27	1.09
1:N:15:ARG:HG2	1:N:15:ARG:HH11	1.08	1.08
1:J:18:ARG:HH11	1:J:18:ARG:HG2	1.02	1.07
1:V:19:ARG:HE	2:V:201:KIU:CAI	1.68	1.07
1:R:50:ARG:HG3	1:R:50:ARG:HH11	1.18	1.05
1:O:38:ARG:HG2	1:O:38:ARG:HH11	1.18	1.05
1:N:17:GLY:HA3	1:N:18:ARG:HB2	1.39	1.04
1:C:112:ARG:HD3	2:C:201:KIU:OAD	1.58	1.04
1:B:92:GLU:OE1	1:C:19:ARG:HG3	1.58	1.04
1:C:81:HIS:NE2	2:C:201:KIU:OAB	1.93	1.02
1:O:112:ARG:HD3	2:O:201:KIU:OAC	1.59	1.01
1:I:21:PRO:HG2	1:X:44:GLY:HA2	1.42	1.00
1:R:34:ALA:O	1:R:35:LEU:HB2	1.58	1.00
1:V:19:ARG:HE	2:V:201:KIU:H11	1.27	0.98
1:I:112:ARG:NH1	2:I:201:KIU:OAD	1.95	0.98
1:N:17:GLY:HA3	1:N:18:ARG:CB	1.93	0.98
1:J:18:ARG:NH1	1:J:18:ARG:HG2	1.75	0.95
1:V:19:ARG:CG	2:V:201:KIU:OAE	2.15	0.95
1:P:18:ARG:HG3	1:P:19:ARG:HH12	1.32	0.94
1:V:18:ARG:HD2	1:V:18:ARG:N	1.84	0.93
1:U:92:GLU:HB3	1:V:19:ARG:HH12	1.35	0.92
1:S:99:GLU:HB3	1:S:124:VAL:HG13	1.52	0.92
1:P:20:GLU:H	1:P:21:PRO:HA	1.33	0.91
1:I:81:HIS:NE2	2:I:201:KIU:OAB	2.04	0.91
1:R:105:VAL:HG12	2:R:201:KIU:OAB	1.71	0.91
1:V:18:ARG:HG3	1:V:18:ARG:HH11	1.32	0.90
1:P:19:ARG:NH1	1:P:19:ARG:HG2	1.81	0.90
1:W:138:ARG:CG	1:W:138:ARG:HH11	1.85	0.89
1:V:18:ARG:CD	1:V:18:ARG:H	1.80	0.89
1:S:32:LEU:HD13	1:S:130:ILE:HG23	1.52	0.89
1:U:92:GLU:HB3	1:V:19:ARG:HH11	1.36	0.87
1:R:92:GLU:HG3	1:S:19:ARG:HG3	1.56	0.87
1:D:32:LEU:HD13	1:D:130:ILE:HD12	1.57	0.86
1:N:13:LEU:HD23	2:N:201:KIU:H10	1.57	0.86
1:J:21:PRO:HB2	1:J:22:ALA:HB2	1.56	0.85
1:X:141:ALA:C	1:X:142:GLU:OE1	2.15	0.85
1:R:50:ARG:NH1	1:R:50:ARG:HG3	1.80	0.85
1:X:19:ARG:HD3	2:X:201:KIU:OAE	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:ARG:HG3	1:P:19:ARG:NH1	1.92	0.84
1:V:81:HIS:NE2	2:V:201:KIU:OAC	2.10	0.84
1:E:32:LEU:HD13	1:E:130:ILE:HD13	1.58	0.83
1:X:142:GLU:N	1:X:142:GLU:OE1	2.09	0.83
1:W:112:ARG:NH1	2:W:201:KIU:OAB	2.11	0.83
1:P:17:GLY:CA	1:P:18:ARG:HB2	2.08	0.83
1:P:17:GLY:HA3	1:P:18:ARG:CB	2.09	0.82
1:W:15:ARG:HG2	1:W:15:ARG:NH1	1.92	0.82
1:V:19:ARG:HG3	2:V:201:KIU:OAE	1.78	0.81
1:N:15:ARG:CG	1:N:15:ARG:HH11	1.89	0.81
1:B:18:ARG:O	1:B:19:ARG:HB2	1.78	0.81
1:D:112:ARG:HD3	2:D:201:KIU:OAD	1.80	0.81
1:V:32:LEU:HD13	1:V:130:ILE:HG13	1.62	0.81
1:W:15:ARG:CG	1:W:15:ARG:HH11	1.93	0.81
1:M:63:HIS:CG	1:W:15:ARG:HD2	2.17	0.80
1:Q:97:LEU:HD23	1:Q:121:ALA:HA	1.62	0.80
1:A:48:VAL:HG12	1:A:50:ARG:HD2	1.64	0.80
1:D:81:HIS:NE2	2:D:201:KIU:OAB	2.14	0.79
1:N:15:ARG:HG2	1:N:15:ARG:NH1	1.87	0.79
1:T:16:LEU:HD23	2:T:201:KIU:H10	1.64	0.78
1:W:36:ILE:HG22	1:W:37:GLU:H	1.44	0.78
1:P:20:GLU:N	1:P:21:PRO:HA	1.99	0.78
1:X:112:ARG:HD3	2:X:201:KIU:OAD	1.84	0.78
1:K:112:ARG:HD3	2:K:201:KIU:OAB	1.83	0.78
1:F:112:ARG:NH1	2:F:201:KIU:OAA	2.16	0.78
1:P:48:VAL:HA	3:P:304:HOH:O	1.83	0.78
1:W:19:ARG:HD2	2:W:201:KIU:H11	1.64	0.77
1:J:18:ARG:HH11	1:J:18:ARG:CG	1.90	0.77
1:R:34:ALA:O	1:R:35:LEU:CB	2.31	0.77
1:W:19:ARG:HB3	2:W:201:KIU:OAF	1.85	0.77
1:X:48:VAL:HG12	1:X:50:ARG:HD2	1.66	0.76
1:O:32:LEU:HD13	1:O:130:ILE:HG12	1.67	0.76
1:V:19:ARG:NE	2:V:201:KIU:H11	1.98	0.76
1:W:36:ILE:O	1:W:38:ARG:N	2.18	0.76
1:V:18:ARG:CG	1:V:18:ARG:HH11	1.99	0.76
1:C:18:ARG:O	1:C:19:ARG:HD2	1.87	0.75
1:N:13:LEU:CD2	2:N:201:KIU:H10	2.17	0.75
1:W:138:ARG:HG3	1:W:138:ARG:HH11	1.50	0.74
1:M:63:HIS:CD2	1:W:15:ARG:HD2	2.23	0.74
1:X:16:LEU:HD12	2:X:201:KIU:OAF	1.88	0.74
1:O:18:ARG:NH2	1:O:28:THR:HB	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:102:ILE:HG23	1:Q:129:GLY:HA2	1.68	0.73
1:A:19:ARG:HH21	1:A:19:ARG:HG2	1.53	0.73
1:C:20:GLU:HG3	1:C:24:TYR:HD1	1.53	0.72
1:A:18:ARG:CB	1:A:19:ARG:HB2	2.20	0.72
1:D:15:ARG:HD2	1:G:63:HIS:CG	2.24	0.72
1:B:59:LEU:CD2	1:B:89:ALA:HB2	2.20	0.72
1:Q:38:ARG:NH1	1:Q:38:ARG:HB3	2.04	0.72
1:T:19:ARG:HG3	1:V:92:GLU:CG	2.20	0.71
1:L:21:PRO:N	1:L:22:ALA:HB3	2.05	0.71
1:B:59:LEU:HD22	1:B:89:ALA:HB2	1.72	0.71
1:E:99:GLU:HB3	1:E:124:VAL:HG13	1.72	0.71
1:U:43:LEU:HD21	1:U:138:ARG:HD2	1.71	0.71
1:H:112:ARG:NH1	2:H:201:KIU:OAA	2.23	0.71
1:K:59:LEU:HD23	1:K:86:LEU:HD12	1.72	0.71
1:A:18:ARG:HB3	1:A:19:ARG:HG2	1.74	0.70
1:O:23:VAL:HG22	1:O:24:TYR:CE1	2.26	0.70
1:O:23:VAL:HG22	1:O:24:TYR:CD1	2.27	0.70
1:L:32:LEU:HD13	1:L:130:ILE:HG13	1.71	0.70
1:R:50:ARG:CG	1:R:50:ARG:HH11	1.99	0.69
1:R:32:LEU:HD13	1:R:130:ILE:HG13	1.73	0.69
1:H:18:ARG:HH11	1:H:18:ARG:HG2	1.57	0.69
1:U:21:PRO:HG2	3:U:322:HOH:O	1.91	0.69
1:H:101:HIS:HB2	1:H:126:VAL:HG22	1.74	0.69
1:K:19:ARG:NE	2:K:201:KIU:H11	2.08	0.68
1:A:18:ARG:N	1:A:19:ARG:O	2.25	0.68
1:V:18:ARG:NH1	1:V:18:ARG:HG3	2.08	0.68
1:G:33:VAL:HG22	1:G:49:VAL:HG22	1.75	0.68
1:S:102:ILE:HG23	1:S:129:GLY:HA2	1.75	0.68
1:M:63:HIS:CD2	1:W:15:ARG:CD	2.77	0.67
1:K:90:CYS:HB3	1:K:97:LEU:HD22	1.74	0.67
1:W:102:ILE:HG23	1:W:129:GLY:HA2	1.75	0.67
1:M:31:GLU:O	1:M:35:LEU:HB2	1.94	0.67
1:U:22:ALA:HA	1:U:25:GLY:HA3	1.74	0.67
1:P:21:PRO:O	1:P:22:ALA:CB	2.42	0.67
1:P:17:GLY:CA	1:P:18:ARG:CB	2.68	0.67
1:W:64:GLN:HE21	1:W:64:GLN:HA	1.58	0.67
1:J:21:PRO:CB	1:J:22:ALA:HB2	2.23	0.67
1:G:27:THR:OG1	1:G:130:ILE:HD13	1.95	0.67
1:M:60:ASP:OD1	1:M:64:GLN:NE2	2.28	0.67
1:S:7:VAL:HB	1:S:49:VAL:HB	1.77	0.66
1:L:22:ALA:HB1	3:L:326:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ARG:CD	1:I:138:ARG:HD3	2.25	0.66
1:O:81:HIS:NE2	2:O:201:KIU:OAA	2.29	0.66
1:P:19:ARG:HH11	1:P:19:ARG:CG	1.92	0.66
1:V:19:ARG:CD	2:V:201:KIU:OAE	2.43	0.66
1:V:131:GLN:HE22	1:X:139:TYR:HA	1.61	0.66
1:I:18:ARG:O	1:I:19:ARG:HB2	1.97	0.65
1:C:102:ILE:HG23	1:C:129:GLY:HA2	1.78	0.65
1:E:20:GLU:HG3	1:E:21:PRO:HD3	1.77	0.65
1:A:63:HIS:CG	1:K:15:ARG:HD2	2.32	0.65
1:A:63:HIS:CD2	1:K:15:ARG:HD2	2.32	0.64
1:V:59:LEU:CD2	1:V:89:ALA:HB2	2.27	0.64
1:E:3:LEU:N	3:E:306:HOH:O	2.29	0.64
1:W:81:HIS:NE2	2:W:201:KIU:OAD	2.29	0.64
1:Q:29:HIS:CE1	1:Q:51:GLN:HB2	2.33	0.63
1:F:58:LEU:O	1:F:62:ILE:HG12	1.97	0.63
1:D:27:THR:HG23	1:D:31:GLU:HB3	1.80	0.63
1:W:138:ARG:HG2	1:W:138:ARG:HH11	1.60	0.63
1:X:19:ARG:NH2	2:X:201:KIU:H11	2.14	0.63
1:K:27:THR:HG23	1:K:31:GLU:HG3	1.80	0.63
1:H:15:ARG:HD2	1:J:63:HIS:CG	2.34	0.63
1:K:81:HIS:HE2	2:K:201:KIU:CAQ	2.04	0.63
1:T:102:ILE:HG23	1:T:129:GLY:HA2	1.81	0.62
1:S:31:GLU:O	1:S:35:LEU:HB2	1.98	0.62
1:N:23:VAL:HG22	1:N:24:TYR:CD2	2.34	0.62
1:S:48:VAL:HG12	1:S:50:ARG:HD2	1.80	0.62
1:O:90:CYS:HB2	1:O:120:ILE:HD11	1.81	0.62
1:L:5:VAL:HG22	1:L:71:PRO:HG2	1.81	0.62
1:R:105:VAL:CG1	2:R:201:KIU:OAB	2.45	0.61
1:M:32:LEU:HD13	1:M:130:ILE:HD12	1.83	0.61
1:Q:11:PRO:HA	1:Q:53:ASP:OD1	2.00	0.61
1:Q:32:LEU:HD13	1:Q:130:ILE:HG13	1.81	0.61
1:O:19:ARG:O	1:O:20:GLU:HB2	2.01	0.61
1:A:18:ARG:HB3	1:A:19:ARG:HB2	1.81	0.60
1:O:38:ARG:HG2	1:O:38:ARG:NH1	1.97	0.60
1:A:20:GLU:C	1:A:22:ALA:HB3	2.22	0.60
1:D:15:ARG:HD2	1:G:63:HIS:CD2	2.37	0.60
1:I:15:ARG:O	1:I:18:ARG:HG2	2.01	0.60
1:A:18:ARG:HB3	1:A:19:ARG:CG	2.31	0.60
1:H:92:GLU:HG2	1:I:19:ARG:HH21	1.66	0.60
1:H:28:THR:OG1	1:H:31:GLU:HG3	2.02	0.60
1:M:82:THR:CG2	1:X:84:VAL:HG23	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:22:ALA:HA	1:P:23:VAL:C	2.22	0.60
1:N:15:ARG:HD2	1:Q:92:GLU:OE1	2.02	0.59
1:C:99:GLU:OE1	1:C:118:SER:OG	2.18	0.59
1:I:32:LEU:HD13	1:I:130:ILE:HG13	1.84	0.59
1:J:16:LEU:O	1:J:28:THR:HA	2.01	0.59
1:R:92:GLU:HG2	1:R:92:GLU:O	2.01	0.59
1:A:29:HIS:O	1:A:33:VAL:HG23	2.01	0.59
1:H:18:ARG:NH1	1:H:18:ARG:HG2	2.16	0.59
1:U:22:ALA:HA	1:U:25:GLY:CA	2.30	0.59
1:J:19:ARG:O	2:J:201:KIU:OAF	2.20	0.59
1:K:112:ARG:NH1	2:K:201:KIU:OAB	2.25	0.59
1:Q:33:VAL:HG13	1:Q:49:VAL:HB	1.84	0.59
1:H:18:ARG:HH11	1:H:18:ARG:CG	2.14	0.59
1:G:7:VAL:HB	1:G:49:VAL:HB	1.84	0.59
1:X:32:LEU:HD13	1:X:130:ILE:HG12	1.84	0.59
1:E:112:ARG:NH1	2:E:201:KIU:OAD	2.36	0.59
1:L:99:GLU:HB3	1:L:124:VAL:HG13	1.85	0.59
1:Q:33:VAL:O	1:Q:37:GLU:HG2	2.03	0.59
1:U:63:HIS:CD2	1:V:15:ARG:HD2	2.38	0.59
1:W:36:ILE:HG23	1:W:137:LEU:HD11	1.84	0.59
1:O:16:LEU:HD11	1:O:130:ILE:HD11	1.84	0.59
1:W:74:LEU:HD21	1:W:86:LEU:HD21	1.85	0.58
1:M:3:LEU:HB3	1:M:4:ILE:CD1	2.19	0.58
1:T:67:ASP:OD1	1:U:18:ARG:NH2	2.36	0.58
1:N:17:GLY:CA	1:N:18:ARG:CB	2.76	0.58
1:S:74:LEU:HD23	1:S:117:LEU:HD13	1.84	0.58
1:L:19:ARG:HD3	1:L:20:GLU:OE1	2.03	0.58
1:Q:38:ARG:HB3	1:Q:38:ARG:HH11	1.69	0.58
1:O:63:HIS:CG	1:Q:15:ARG:HD3	2.38	0.58
1:A:48:VAL:CG1	1:A:50:ARG:HD2	2.33	0.58
1:E:17:GLY:O	1:E:18:ARG:C	2.42	0.58
1:N:112:ARG:NH1	2:N:201:KIU:OAB	2.34	0.58
1:H:15:ARG:CD	1:J:63:HIS:CD2	2.87	0.58
1:B:48:VAL:HG12	1:B:50:ARG:HD2	1.85	0.58
1:P:21:PRO:O	1:P:22:ALA:HB2	2.04	0.57
1:A:18:ARG:HB3	1:A:19:ARG:CB	2.34	0.57
1:U:29:HIS:O	1:U:33:VAL:HG23	2.03	0.57
1:B:63:HIS:CG	1:C:15:ARG:HD3	2.39	0.57
1:T:15:ARG:HD3	1:V:63:HIS:CG	2.39	0.57
1:A:63:HIS:CD2	1:K:15:ARG:CD	2.88	0.57
1:R:35:LEU:O	1:R:39:GLU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:O	1:A:64:GLN:HG3	2.05	0.57
1:W:36:ILE:HG22	1:W:37:GLU:N	2.17	0.57
1:W:39:GLU:HG2	1:W:134:LEU:HD22	1.86	0.57
1:O:18:ARG:HH21	1:O:28:THR:HB	1.69	0.57
1:A:63:HIS:HE1	1:K:53:ASP:OD2	1.88	0.57
1:J:19:ARG:HA	1:J:21:PRO:HD3	1.86	0.57
1:Q:19:ARG:O	2:Q:201:KIU:OAF	2.23	0.57
1:O:99:GLU:OE2	1:O:101:HIS:NE2	2.38	0.57
1:N:63:HIS:HE1	1:O:53:ASP:OD2	1.87	0.57
1:A:15:ARG:HD2	1:L:63:HIS:CG	2.40	0.56
1:W:15:ARG:HH12	1:W:18:ARG:HD2	1.68	0.56
1:N:19:ARG:HD2	1:Q:92:GLU:OE2	2.05	0.56
1:A:6:ASN:HD21	1:A:70:GLU:HB2	1.70	0.56
1:P:22:ALA:HA	1:P:24:TYR:N	2.21	0.56
1:I:59:LEU:HD12	1:J:53:ASP:HB3	1.87	0.56
1:L:23:VAL:HG23	1:L:24:TYR:CD2	2.41	0.56
1:A:59:LEU:HD22	1:A:89:ALA:HB2	1.87	0.56
1:L:7:VAL:HB	1:L:49:VAL:HG22	1.88	0.56
1:M:50:ARG:HB3	1:M:61:TRP:CZ3	2.40	0.56
1:V:32:LEU:HD13	1:V:130:ILE:CG1	2.35	0.56
1:T:19:ARG:HD3	1:V:92:GLU:OE1	2.06	0.56
1:O:18:ARG:HA	1:O:19:ARG:HE	1.71	0.55
1:P:51:GLN:NE2	1:P:52:SER:N	2.54	0.55
1:W:20:GLU:HG2	1:W:23:VAL:HB	1.89	0.55
1:W:88:ASP:O	1:X:19:ARG:NH1	2.39	0.55
1:S:29:HIS:O	1:S:33:VAL:HG23	2.05	0.55
1:I:57:GLN:HA	1:I:57:GLN:HE21	1.71	0.55
1:H:120:ILE:HD12	1:H:120:ILE:C	2.27	0.55
1:I:32:LEU:HD13	1:I:130:ILE:CG1	2.37	0.55
1:N:99:GLU:HB3	1:N:124:VAL:HG13	1.88	0.55
1:E:48:VAL:HG12	1:E:50:ARG:HD2	1.89	0.55
1:V:139:TYR:O	1:V:143:HIS:N	2.39	0.55
1:C:124:VAL:HG12	1:C:126:VAL:HG23	1.88	0.54
1:P:12:ASN:HB2	2:P:201:KIU:H6	1.89	0.54
1:N:59:LEU:CD2	1:N:89:ALA:HB2	2.36	0.54
1:Q:23:VAL:HG22	1:Q:24:TYR:CD2	2.42	0.54
1:O:58:LEU:O	1:O:62:ILE:HG12	2.07	0.54
1:F:16:LEU:HD21	1:F:130:ILE:HD11	1.89	0.54
1:Q:16:LEU:HD13	1:Q:27:THR:O	2.07	0.54
1:C:112:ARG:HH11	2:C:201:KIU:CAQ	2.20	0.54
1:V:19:ARG:NE	2:V:201:KIU:CAI	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:CYS:HB3	1:F:97:LEU:HD22	1.90	0.54
1:T:12:ASN:HB2	2:T:201:KIU:H6	1.88	0.54
1:P:20:GLU:N	1:P:21:PRO:CA	2.70	0.54
1:M:82:THR:HG21	1:X:84:VAL:HG23	1.88	0.54
1:I:57:GLN:HA	1:I:57:GLN:NE2	2.23	0.54
1:J:104:ASN:HA	1:J:126:VAL:HG13	1.90	0.54
1:M:11:PRO:HA	1:M:53:ASP:OD1	2.07	0.54
1:A:101:HIS:HB2	1:A:126:VAL:HG22	1.89	0.54
1:M:4:ILE:HD12	1:M:4:ILE:N	2.23	0.53
1:W:64:GLN:HA	1:W:64:GLN:NE2	2.23	0.53
1:P:118:SER:HB2	1:P:119:PRO:HD3	1.89	0.53
1:L:22:ALA:O	1:L:23:VAL:HG22	2.08	0.53
1:Q:39:GLU:HG2	1:Q:134:LEU:HB3	1.89	0.53
1:W:15:ARG:CG	1:W:15:ARG:NH1	2.61	0.53
1:G:27:THR:OG1	1:G:130:ILE:CD1	2.56	0.53
1:L:90:CYS:HB2	1:L:120:ILE:HD11	1.90	0.53
1:D:88:ASP:O	1:F:19:ARG:NH1	2.42	0.53
1:Q:131:GLN:O	1:Q:135:LEU:HG	2.08	0.53
1:S:59:LEU:HD22	1:S:89:ALA:HB2	1.90	0.53
1:H:15:ARG:HD3	1:J:63:HIS:CD2	2.44	0.53
1:H:50:ARG:HD3	1:H:61:TRP:CE2	2.43	0.53
1:M:59:LEU:HD23	1:M:86:LEU:HD12	1.91	0.53
1:E:36:ILE:HG23	1:E:137:LEU:HD11	1.89	0.53
1:V:33:VAL:HG22	1:V:49:VAL:CG1	2.39	0.53
1:T:32:LEU:HD13	1:T:130:ILE:HG12	1.90	0.53
1:I:20:GLU:HG2	1:I:23:VAL:CG1	2.38	0.53
1:D:138:ARG:HD2	1:I:138:ARG:HD3	1.89	0.52
1:O:90:CYS:HB3	1:O:97:LEU:HD22	1.91	0.52
1:Q:36:ILE:HG23	1:Q:137:LEU:HD11	1.90	0.52
1:W:138:ARG:HG3	1:W:138:ARG:NH1	2.20	0.52
1:S:14:GLY:H	1:S:51:GLN:NE2	2.06	0.52
1:T:48:VAL:HG12	1:T:50:ARG:HD2	1.90	0.52
1:N:128:LEU:HD21	1:R:98:ILE:CD1	2.39	0.52
1:T:53:ASP:OD2	1:V:63:HIS:HE1	1.91	0.52
1:G:20:GLU:N	1:G:21:PRO:CD	2.71	0.52
1:R:5:VAL:HG22	1:R:71:PRO:HG2	1.92	0.52
1:P:13:LEU:HD23	2:P:201:KIU:H9	1.91	0.52
1:N:23:VAL:HG22	1:N:24:TYR:CE2	2.44	0.52
1:T:117:LEU:O	1:T:120:ILE:HG13	2.10	0.52
1:N:105:VAL:HG22	1:N:126:VAL:HG11	1.91	0.52
1:O:38:ARG:CG	1:O:38:ARG:HH11	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:95:ALA:HB1	1:T:96:PRO:CD	2.40	0.52
1:L:33:VAL:HG22	1:L:49:VAL:HG11	1.91	0.52
1:N:48:VAL:HG12	1:N:50:ARG:HD2	1.92	0.52
1:C:22:ALA:O	1:C:23:VAL:HG23	2.10	0.52
1:W:134:LEU:HA	1:W:137:LEU:HD12	1.92	0.52
1:R:19:ARG:O	1:R:21:PRO:HD3	2.09	0.52
1:K:13:LEU:HD23	2:K:201:KIU:H8	1.92	0.52
1:Q:10:GLY:HA2	1:Q:58:LEU:HD11	1.92	0.52
1:L:112:ARG:HD3	2:L:201:KIU:OAB	2.10	0.52
1:O:36:ILE:HG23	1:O:137:LEU:HD11	1.92	0.52
1:N:76:ALA:HB3	1:N:80:THR:OG1	2.10	0.52
1:D:118:SER:HB2	1:D:119:PRO:HD3	1.92	0.51
1:O:5:VAL:CG1	1:O:140:LEU:HD13	2.40	0.51
1:P:36:ILE:HG23	1:P:137:LEU:HD11	1.93	0.51
1:T:101:HIS:HB2	1:T:126:VAL:HG22	1.93	0.51
1:I:11:PRO:HG2	1:I:79:LEU:HG	1.91	0.51
1:V:19:ARG:HD3	2:V:201:KIU:OAE	2.09	0.51
1:M:59:LEU:HD23	1:M:86:LEU:CD1	2.40	0.51
1:P:20:GLU:N	1:P:20:GLU:CD	2.63	0.51
1:R:80:THR:HG21	1:R:101:HIS:CE1	2.45	0.51
1:M:90:CYS:HB3	1:M:97:LEU:HD22	1.92	0.51
1:F:112:ARG:HG2	2:F:201:KIU:OAC	2.11	0.51
1:R:16:LEU:HD11	1:R:130:ILE:HD11	1.92	0.51
1:Q:3:LEU:N	1:Q:3:LEU:HD12	2.24	0.51
1:J:81:HIS:HE2	2:J:201:KIU:CAP	2.22	0.51
1:W:81:HIS:HE2	2:W:201:KIU:CAQ	2.23	0.51
1:O:18:ARG:HG2	1:O:19:ARG:HH21	1.75	0.51
1:A:102:ILE:HG23	1:A:129:GLY:HA2	1.93	0.51
1:N:32:LEU:HD21	1:N:133:TYR:CE1	2.45	0.51
1:L:36:ILE:HG21	1:L:49:VAL:CG2	2.40	0.51
1:P:59:LEU:HD13	1:R:53:ASP:HB3	1.92	0.51
1:J:19:ARG:HA	1:J:21:PRO:CD	2.41	0.51
1:V:19:ARG:HG2	2:V:201:KIU:OAE	2.07	0.51
1:W:10:GLY:HA2	1:W:58:LEU:HD11	1.91	0.51
1:I:20:GLU:HG2	1:I:23:VAL:HG13	1.92	0.51
1:P:59:LEU:CD1	1:R:53:ASP:HB3	2.40	0.51
1:H:11:PRO:O	1:H:12:ASN:HB2	2.11	0.51
1:G:58:LEU:O	1:G:62:ILE:HG12	2.11	0.51
1:M:102:ILE:HG23	1:M:129:GLY:HA2	1.93	0.51
1:A:48:VAL:HG12	1:A:50:ARG:CD	2.38	0.51
1:E:18:ARG:O	1:E:19:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:81:HIS:NE2	2:U:201:KIU:OAD	2.44	0.51
1:J:59:LEU:HD21	1:J:86:LEU:HA	1.92	0.51
1:R:32:LEU:HD13	1:R:130:ILE:CG1	2.41	0.51
1:R:19:ARG:HG2	1:R:20:GLU:HG3	1.92	0.51
1:F:92:GLU:HG3	1:G:19:ARG:HG2	1.93	0.51
1:A:98:ILE:HD12	1:G:128:LEU:HD21	1.93	0.50
1:U:118:SER:HB2	1:U:119:PRO:HD3	1.92	0.50
1:E:7:VAL:HB	1:E:49:VAL:HG22	1.92	0.50
1:E:27:THR:HG21	1:E:130:ILE:HD12	1.92	0.50
1:U:21:PRO:O	1:U:23:VAL:N	2.38	0.50
1:N:4:ILE:HD13	1:N:70:GLU:HG2	1.93	0.50
1:F:102:ILE:HG23	1:F:129:GLY:HA2	1.92	0.50
1:F:32:LEU:HD11	1:F:36:ILE:HD11	1.93	0.50
1:W:118:SER:HB2	1:W:119:PRO:HD3	1.94	0.50
1:H:95:ALA:HB1	1:H:96:PRO:CD	2.41	0.50
1:V:71:PRO:HB3	1:V:96:PRO:HD2	1.94	0.50
1:T:63:HIS:CG	1:U:15:ARG:HD3	2.47	0.50
1:V:97:LEU:HD23	1:V:121:ALA:HA	1.93	0.50
1:G:92:GLU:O	1:G:92:GLU:HG2	2.10	0.50
1:V:13:LEU:C	1:V:15:ARG:H	2.15	0.50
1:W:138:ARG:CG	1:W:138:ARG:NH1	2.55	0.50
1:O:15:ARG:O	1:O:16:LEU:C	2.50	0.50
1:A:59:LEU:CD2	1:A:89:ALA:HB2	2.41	0.50
1:V:33:VAL:HG22	1:V:49:VAL:HG11	1.93	0.50
1:V:101:HIS:HB2	1:V:126:VAL:HG22	1.93	0.50
1:U:7:VAL:HG21	1:U:36:ILE:HD13	1.94	0.50
1:P:39:GLU:HG2	1:P:134:LEU:HD22	1.92	0.49
1:L:19:ARG:HG2	1:L:20:GLU:HG3	1.94	0.49
1:O:119:PRO:HB3	1:T:106:HIS:O	2.11	0.49
1:M:63:HIS:HE1	1:W:53:ASP:OD2	1.95	0.49
1:H:15:ARG:HD2	1:J:63:HIS:CD2	2.47	0.49
1:T:32:LEU:HD13	1:T:130:ILE:CG1	2.43	0.49
1:R:63:HIS:CG	1:S:15:ARG:HD2	2.47	0.49
1:L:81:HIS:NE2	2:L:201:KIU:OAD	2.45	0.49
1:A:90:CYS:HB3	1:A:97:LEU:HD22	1.95	0.49
1:D:9:ASN:ND2	1:D:29:HIS:NE2	2.59	0.49
1:E:101:HIS:HB2	1:E:126:VAL:HG22	1.93	0.49
1:X:140:LEU:O	1:X:142:GLU:N	2.45	0.49
1:T:3:LEU:HD11	1:T:71:PRO:CD	2.42	0.49
1:I:113:ARG:NH2	3:I:335:HOH:O	2.25	0.49
1:U:77:GLY:HA2	2:U:201:KIU:CAS	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ARG:HB3	1:C:61:TRP:CH2	2.48	0.49
1:N:13:LEU:CG	2:N:201:KIU:H10	2.43	0.49
1:L:36:ILE:HG21	1:L:49:VAL:HG21	1.95	0.49
1:P:80:THR:HG23	1:P:117:LEU:HD12	1.95	0.49
1:D:94:SER:HB2	1:X:68:ALA:HB2	1.92	0.49
1:U:142:GLU:O	1:U:143:HIS:ND1	2.46	0.48
1:G:33:VAL:HG22	1:G:49:VAL:CG2	2.41	0.48
1:R:81:HIS:NE2	2:R:201:KIU:OAD	2.36	0.48
1:D:38:ARG:HH11	1:D:38:ARG:HG2	1.78	0.48
1:B:59:LEU:CD2	1:B:89:ALA:CB	2.89	0.48
1:F:81:HIS:HE2	2:F:201:KIU:CAP	2.26	0.48
1:V:112:ARG:HH11	2:V:201:KIU:CAP	2.27	0.48
1:R:92:GLU:O	1:R:92:GLU:CG	2.61	0.48
1:A:19:ARG:HH21	1:A:19:ARG:CG	2.24	0.48
1:G:27:THR:HG1	1:G:130:ILE:HD13	1.78	0.48
1:E:10:GLY:HA2	1:E:58:LEU:HD11	1.94	0.48
1:W:63:HIS:HE1	1:X:53:ASP:OD2	1.97	0.48
1:M:6:ASN:ND2	1:M:65:ALA:HB2	2.28	0.48
1:T:3:LEU:HD11	1:T:71:PRO:HD3	1.95	0.48
1:I:90:CYS:HB3	1:I:97:LEU:HD22	1.95	0.48
1:R:90:CYS:HB3	1:R:97:LEU:HD22	1.96	0.48
1:R:120:ILE:C	1:R:120:ILE:HD13	2.35	0.48
1:V:4:ILE:HA	1:V:46:LYS:O	2.14	0.48
2:I:201:KIU:H2	2:I:201:KIU:H7	1.60	0.48
1:E:3:LEU:HB3	1:E:45:LEU:HD22	1.96	0.48
1:J:101:HIS:HB2	1:J:126:VAL:HG22	1.96	0.48
1:X:104:ASN:HA	1:X:126:VAL:HG12	1.94	0.48
1:M:63:HIS:CD2	1:W:15:ARG:HD3	2.49	0.47
1:O:11:PRO:HA	1:O:53:ASP:OD1	2.14	0.47
1:A:18:ARG:HB2	1:A:19:ARG:HB2	1.94	0.47
1:H:5:VAL:HG22	1:H:71:PRO:HG2	1.96	0.47
1:Q:18:ARG:O	1:Q:19:ARG:HG2	2.14	0.47
1:J:102:ILE:HG23	1:J:129:GLY:HA2	1.95	0.47
1:K:29:HIS:CE1	1:K:51:GLN:HB2	2.49	0.47
1:J:36:ILE:HG23	1:J:137:LEU:HD11	1.96	0.47
1:M:59:LEU:HD12	1:W:53:ASP:HB3	1.97	0.47
1:K:60:ASP:OD1	1:K:64:GLN:NE2	2.48	0.47
1:P:81:HIS:NE2	2:P:201:KIU:OAB	2.48	0.47
1:X:36:ILE:HG23	1:X:137:LEU:HD11	1.97	0.47
1:N:60:ASP:OD1	1:N:64:GLN:NE2	2.47	0.47
1:W:90:CYS:HB3	1:W:97:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:101:HIS:HB2	1:S:126:VAL:HG22	1.95	0.47
2:I:201:KIU:CAV	2:I:201:KIU:OAF	2.50	0.47
1:B:18:ARG:O	1:B:19:ARG:CB	2.59	0.47
1:V:59:LEU:CD2	1:V:89:ALA:CB	2.93	0.47
1:K:58:LEU:O	1:K:62:ILE:HG12	2.15	0.47
1:G:106:HIS:HA	1:G:113:ARG:HG2	1.96	0.47
1:A:20:GLU:N	1:A:21:PRO:HD3	2.30	0.47
1:B:106:HIS:HA	1:B:113:ARG:HG2	1.96	0.47
1:I:67:ASP:OD1	1:J:15:ARG:NH2	2.35	0.47
1:N:4:ILE:HD12	1:N:4:ILE:H	1.79	0.47
1:G:11:PRO:HG2	1:G:79:LEU:HG	1.97	0.47
1:E:21:PRO:HB3	1:E:25:GLY:O	2.14	0.47
1:O:101:HIS:HB2	1:O:126:VAL:HG22	1.97	0.47
1:C:39:GLU:HG2	1:C:134:LEU:HB3	1.97	0.47
1:F:106:HIS:HA	1:F:113:ARG:HG2	1.97	0.47
1:J:112:ARG:NH1	2:J:201:KIU:OAA	2.47	0.46
1:F:81:HIS:NE2	2:F:201:KIU:OAC	2.46	0.46
1:C:99:GLU:OE1	1:C:118:SER:CB	2.63	0.46
1:E:7:VAL:HG11	1:E:36:ILE:HD13	1.97	0.46
1:G:36:ILE:HG23	1:G:137:LEU:HD11	1.98	0.46
1:V:45:LEU:HD11	1:V:141:ALA:HB2	1.96	0.46
1:U:57:GLN:NE2	1:U:61:TRP:CE2	2.78	0.46
1:L:19:ARG:HG2	1:L:20:GLU:N	2.31	0.46
1:V:5:VAL:HG22	1:V:71:PRO:HG2	1.97	0.46
1:V:36:ILE:HG23	1:V:137:LEU:HD11	1.97	0.46
1:P:13:LEU:CD2	2:P:201:KIU:H9	2.45	0.46
2:U:201:KIU:H7	2:U:201:KIU:H2	1.58	0.46
1:M:66:ALA:HB1	1:M:92:GLU:HG2	1.98	0.46
1:S:74:LEU:HD23	1:S:117:LEU:CD1	2.45	0.46
1:N:80:THR:HG21	1:N:101:HIS:CE1	2.50	0.46
1:J:21:PRO:HB2	1:J:22:ALA:CB	2.37	0.46
1:O:81:HIS:HE2	2:O:201:KIU:CAP	2.27	0.46
1:D:123:GLY:HA3	1:I:128:LEU:HD23	1.98	0.46
1:U:92:GLU:CB	1:V:19:ARG:HH11	2.20	0.46
1:M:3:LEU:HA	1:M:3:LEU:HD12	1.81	0.46
1:M:32:LEU:HD13	1:M:130:ILE:CD1	2.46	0.46
1:K:92:GLU:HB2	1:L:19:ARG:NH1	2.30	0.46
1:N:53:ASP:OD2	1:Q:63:HIS:HE1	1.98	0.46
1:C:20:GLU:HG3	1:C:24:TYR:CD1	2.41	0.46
2:T:201:KIU:H11	2:T:201:KIU:OAE	2.16	0.46
1:N:80:THR:HG21	1:N:101:HIS:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:39:GLU:HG2	1:T:134:LEU:HB3	1.97	0.46
1:C:16:LEU:HD23	1:C:16:LEU:HA	1.62	0.46
1:T:73:ILE:HG12	1:T:136:ALA:HB1	1.98	0.46
1:C:99:GLU:HB3	1:C:124:VAL:HG13	1.97	0.45
1:O:5:VAL:HG13	1:O:140:LEU:HD13	1.98	0.45
2:P:201:KIU:CAV	2:P:201:KIU:OAF	2.55	0.45
1:O:32:LEU:CD1	1:O:130:ILE:HG12	2.41	0.45
1:L:22:ALA:CB	3:L:326:HOH:O	2.60	0.45
1:L:32:LEU:HD13	1:L:130:ILE:CG1	2.42	0.45
1:V:9:ASN:OD1	1:V:75:ASN:HB3	2.17	0.45
1:A:87:ARG:NH1	1:A:116:TYR:O	2.49	0.45
2:C:201:KIU:H7	2:C:201:KIU:H2	1.35	0.45
1:H:92:GLU:HG2	1:I:19:ARG:NH2	2.31	0.45
1:E:111:PHE:CE1	1:E:112:ARG:HG3	2.52	0.45
1:H:36:ILE:HG23	1:H:137:LEU:HD11	1.99	0.45
1:O:29:HIS:O	1:O:33:VAL:HG23	2.17	0.45
1:J:140:LEU:HD23	1:J:140:LEU:HA	1.75	0.45
1:V:59:LEU:HD23	1:V:89:ALA:CB	2.45	0.45
1:H:19:ARG:O	1:H:20:GLU:HB2	2.17	0.45
1:O:9:ASN:O	1:O:51:GLN:HA	2.17	0.45
1:D:92:GLU:O	1:D:92:GLU:HG2	2.17	0.45
1:V:80:THR:HG23	1:V:117:LEU:HD12	1.98	0.45
1:R:131:GLN:O	1:R:135:LEU:HG	2.17	0.45
2:R:201:KIU:H2	2:R:201:KIU:H7	1.44	0.45
1:O:16:LEU:HA	1:O:16:LEU:HD23	1.76	0.45
1:F:101:HIS:HB2	1:F:126:VAL:HG22	1.98	0.45
1:U:63:HIS:CG	1:V:15:ARG:HD2	2.52	0.44
1:B:63:HIS:HE1	1:C:53:ASP:OD2	2.00	0.44
1:V:13:LEU:HD22	2:V:201:KIU:H7	1.99	0.44
1:N:80:THR:HG21	1:N:101:HIS:NE2	2.31	0.44
1:Q:93:LEU:CD1	1:Q:97:LEU:HD13	2.47	0.44
1:B:63:HIS:CD2	1:C:15:ARG:HD3	2.51	0.44
1:L:90:CYS:HB3	1:L:97:LEU:HD22	1.98	0.44
1:F:71:PRO:HB2	1:F:140:LEU:HD13	1.99	0.44
1:E:142:GLU:C	1:E:143:HIS:ND1	2.71	0.44
1:D:36:ILE:HG23	1:D:137:LEU:HD11	1.98	0.44
1:T:18:ARG:O	1:T:19:ARG:HD2	2.17	0.44
1:Q:32:LEU:HD13	1:Q:130:ILE:CG1	2.45	0.44
1:W:63:HIS:CG	1:X:15:ARG:HD2	2.52	0.44
1:U:137:LEU:HD23	1:U:137:LEU:HA	1.54	0.44
1:O:17:GLY:HA2	1:O:18:ARG:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:117:LEU:O	1:M:120:ILE:HG13	2.17	0.44
2:V:201:KIU:H7	2:V:201:KIU:H5	1.62	0.44
1:C:19:ARG:O	1:C:20:GLU:HG2	2.17	0.44
1:U:101:HIS:HB2	1:U:126:VAL:HG22	1.99	0.44
1:C:118:SER:HB3	1:C:124:VAL:HG21	1.98	0.44
1:L:99:GLU:OE1	1:L:118:SER:OG	2.22	0.44
1:K:27:THR:CG2	1:K:31:GLU:HG3	2.45	0.44
1:A:135:LEU:HD22	1:G:135:LEU:HB3	2.00	0.44
1:P:18:ARG:O	1:P:19:ARG:CZ	2.65	0.44
1:N:15:ARG:NH2	1:Q:67:ASP:OD2	2.44	0.44
1:A:21:PRO:CA	1:A:22:ALA:HB3	2.48	0.44
1:W:92:GLU:OE1	1:X:15:ARG:NH2	2.47	0.44
1:O:39:GLU:HG2	1:O:134:LEU:HB3	2.00	0.44
1:H:21:PRO:O	1:H:23:VAL:N	2.48	0.44
1:A:80:THR:CG2	1:A:99:GLU:OE2	2.66	0.44
1:F:96:PRO:HG3	3:F:321:HOH:O	2.18	0.44
1:H:109:GLU:CD	1:H:112:ARG:HE	2.21	0.43
1:V:3:LEU:HD12	1:V:46:LYS:HE2	1.99	0.43
1:K:142:GLU:O	1:K:143:HIS:HB2	2.18	0.43
1:I:139:TYR:C	1:I:139:TYR:CD2	2.91	0.43
1:P:3:LEU:O	1:P:45:LEU:HB3	2.17	0.43
1:V:11:PRO:O	2:V:201:KIU:H6	2.18	0.43
1:J:32:LEU:HG	1:J:36:ILE:HD12	2.01	0.43
2:A:201:KIU:H5	2:A:201:KIU:H7	1.51	0.43
1:V:86:LEU:HA	1:V:86:LEU:HD12	1.69	0.43
1:C:77:GLY:HA2	2:C:201:KIU:CAS	2.48	0.43
1:A:112:ARG:NH1	2:A:201:KIU:OAC	2.46	0.43
1:S:30:ASP:N	1:S:30:ASP:OD1	2.51	0.43
1:U:63:HIS:HE1	1:V:53:ASP:OD2	2.01	0.43
1:S:16:LEU:HD21	1:S:102:ILE:HD13	1.99	0.43
1:O:93:LEU:HD12	1:O:97:LEU:HB2	1.99	0.43
1:G:20:GLU:N	1:G:21:PRO:HD2	2.32	0.43
1:D:123:GLY:HA3	1:I:128:LEU:CD2	2.48	0.43
1:P:98:ILE:HD13	1:U:128:LEU:HD21	2.00	0.43
1:X:-5:TYR:CD2	1:X:94:SER:HB2	2.54	0.43
1:H:95:ALA:HB1	1:H:96:PRO:HD2	1.99	0.43
1:T:131:GLN:HG2	1:T:131:GLN:H	1.54	0.43
1:D:16:LEU:HD11	1:D:130:ILE:HD11	2.00	0.43
1:T:19:ARG:HG3	1:V:92:GLU:HG3	2.00	0.43
1:M:50:ARG:HB3	1:M:61:TRP:CH2	2.53	0.43
1:G:11:PRO:HA	1:G:53:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HG	1:A:36:ILE:CD1	2.49	0.43
1:O:27:THR:HG23	1:O:31:GLU:HB3	2.01	0.43
2:W:201:KIU:H7	2:W:201:KIU:H2	1.42	0.43
2:E:201:KIU:H7	2:E:201:KIU:H2	1.48	0.43
1:Q:50:ARG:NH2	1:Q:61:TRP:CD1	2.87	0.43
1:I:4:ILE:HD13	1:I:70:GLU:OE2	2.19	0.43
1:U:8:ILE:HD12	1:U:72:VAL:HG13	2.00	0.43
1:D:130:ILE:HD13	1:D:130:ILE:HA	1.64	0.43
1:D:20:GLU:C	1:D:21:PRO:O	2.56	0.43
1:S:39:GLU:O	1:S:40:ALA:C	2.57	0.43
1:T:19:ARG:HG3	1:V:92:GLU:CD	2.40	0.43
1:D:7:VAL:HG22	1:D:73:ILE:HB	2.00	0.43
1:Q:68:ALA:HB2	3:Q:304:HOH:O	2.18	0.43
1:M:99:GLU:OE2	1:M:101:HIS:NE2	2.49	0.43
1:K:118:SER:O	1:K:119:PRO:C	2.56	0.42
1:X:11:PRO:O	1:X:12:ASN:HB2	2.18	0.42
2:J:201:KIU:CAV	2:J:201:KIU:OAF	2.56	0.42
1:O:23:VAL:CG2	1:O:24:TYR:CE1	2.98	0.42
1:S:7:VAL:O	1:S:49:VAL:HA	2.19	0.42
1:I:18:ARG:O	1:I:19:ARG:CB	2.66	0.42
1:S:59:LEU:CD2	1:S:89:ALA:HB2	2.49	0.42
2:L:201:KIU:H2	2:L:201:KIU:H7	1.60	0.42
1:M:80:THR:HG23	1:M:117:LEU:HD12	2.01	0.42
1:Q:48:VAL:HG12	1:Q:50:ARG:HD2	2.01	0.42
1:R:55:GLU:OE2	1:R:83:SER:OG	2.29	0.42
1:G:9:ASN:O	1:G:51:GLN:HA	2.19	0.42
1:C:19:ARG:C	1:C:20:GLU:HG2	2.40	0.42
1:A:6:ASN:ND2	1:A:70:GLU:HB2	2.33	0.42
1:G:131:GLN:O	1:G:135:LEU:HG	2.20	0.42
1:X:72:VAL:HG12	1:X:73:ILE:N	2.33	0.42
1:H:102:ILE:HD13	1:H:130:ILE:HD12	2.01	0.42
1:F:20:GLU:C	1:F:22:ALA:H	2.23	0.42
1:N:74:LEU:HD12	1:N:75:ASN:N	2.34	0.42
1:P:19:ARG:HA	1:P:20:GLU:HA	1.71	0.42
1:L:81:HIS:NE2	2:L:201:KIU:CAQ	2.83	0.42
1:K:142:GLU:O	1:K:143:HIS:CB	2.67	0.42
1:M:73:ILE:HD13	1:M:136:ALA:HB3	2.02	0.42
1:G:72:VAL:O	1:G:97:LEU:HA	2.20	0.42
1:W:32:LEU:HD13	1:W:130:ILE:HG22	2.01	0.42
1:P:140:LEU:C	1:P:142:GLU:H	2.22	0.42
1:U:13:LEU:O	1:U:16:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:KIU:HB7	2:H:201:KIU:H5	1.44	0.42
1:M:4:ILE:H	1:M:4:ILE:HD12	1.84	0.42
1:B:20:GLU:N	1:B:21:PRO:HD3	2.34	0.42
1:I:92:GLU:O	1:I:92:GLU:HG2	2.19	0.42
1:K:59:LEU:HD22	1:K:89:ALA:HB2	2.01	0.42
1:S:90:CYS:HB3	1:S:97:LEU:HD22	2.02	0.42
1:T:11:PRO:O	1:T:12:ASN:HB2	2.20	0.42
1:P:15:ARG:O	1:P:18:ARG:HB3	2.19	0.42
1:O:16:LEU:CD1	1:O:130:ILE:HD11	2.48	0.42
1:J:118:SER:N	1:J:119:PRO:CD	2.83	0.42
1:U:24:TYR:O	1:U:102:ILE:HG21	2.20	0.42
1:T:19:ARG:HG3	1:V:92:GLU:HG2	2.01	0.41
1:K:11:PRO:HA	1:K:53:ASP:HA	2.02	0.41
1:F:55:GLU:HG3	1:F:79:LEU:HD13	2.02	0.41
1:A:41:ALA:C	1:A:43:LEU:H	2.24	0.41
1:Q:80:THR:CG2	1:Q:99:GLU:OE2	2.68	0.41
1:B:29:HIS:CE1	1:B:51:GLN:HB2	2.55	0.41
1:R:39:GLU:HG2	1:R:134:LEU:HB3	2.02	0.41
1:R:31:GLU:O	1:R:34:ALA:O	2.38	0.41
1:O:19:ARG:O	1:O:20:GLU:CB	2.66	0.41
1:D:15:ARG:CD	1:G:63:HIS:CD2	3.03	0.41
1:D:21:PRO:C	1:D:23:VAL:H	2.23	0.41
1:X:74:LEU:HD23	1:X:117:LEU:HD13	2.01	0.41
1:W:29:HIS:O	1:W:33:VAL:HG23	2.20	0.41
1:T:32:LEU:HA	1:T:32:LEU:HD12	1.92	0.41
1:U:80:THR:HG21	1:U:101:HIS:HE2	1.85	0.41
1:R:62:ILE:HD11	1:R:86:LEU:HD11	2.02	0.41
1:P:19:ARG:HG3	1:S:92:GLU:OE2	2.21	0.41
1:X:19:ARG:HB2	2:X:201:KIU:OAE	2.21	0.41
1:T:20:GLU:N	1:T:21:PRO:HD3	2.35	0.41
1:F:76:ALA:HB3	1:F:80:THR:OG1	2.21	0.41
1:I:27:THR:CG2	1:I:31:GLU:HB2	2.50	0.41
1:T:53:ASP:OD2	1:V:63:HIS:CE1	2.73	0.41
1:T:71:PRO:HB3	1:T:96:PRO:HD2	2.03	0.41
1:D:38:ARG:NH1	1:D:38:ARG:HG2	2.36	0.41
1:X:8:ILE:HD12	1:X:72:VAL:HG13	2.02	0.41
1:L:9:ASN:ND2	1:L:29:HIS:NE2	2.59	0.41
1:W:27:THR:HG23	1:W:31:GLU:HB2	2.02	0.41
1:W:134:LEU:O	1:W:137:LEU:HB2	2.19	0.41
1:D:138:ARG:NE	1:I:138:ARG:HD3	2.36	0.41
1:N:32:LEU:HD13	1:N:130:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:50:ARG:HB3	1:W:61:TRP:CZ3	2.56	0.41
1:B:10:GLY:HA2	1:B:58:LEU:HD11	2.01	0.41
1:N:87:ARG:NH1	1:N:116:TYR:O	2.54	0.41
1:K:81:HIS:CE1	2:K:201:KIU:OAD	2.67	0.41
1:E:3:LEU:HD11	1:E:71:PRO:HD3	2.03	0.41
1:S:29:HIS:CE1	1:S:51:GLN:HB2	2.56	0.41
1:M:13:LEU:HD11	1:M:75:ASN:CG	2.40	0.41
1:M:7:VAL:HB	1:M:49:VAL:HG22	2.03	0.41
1:I:29:HIS:O	1:I:33:VAL:HG23	2.21	0.41
1:I:8:ILE:O	1:I:74:LEU:HD12	2.20	0.41
2:T:201:KIU:CAI	2:T:201:KIU:OAE	2.68	0.41
1:S:42:GLU:HB3	3:S:224:HOH:O	2.21	0.41
1:K:19:ARG:CD	2:K:201:KIU:H11	2.51	0.41
1:N:19:ARG:O	1:N:20:GLU:C	2.58	0.41
1:J:18:ARG:N	1:J:18:ARG:HD3	2.36	0.41
1:F:77:GLY:HA2	2:F:201:KIU:CAS	2.51	0.41
1:A:63:HIS:CD2	1:K:15:ARG:HD3	2.56	0.41
1:Q:134:LEU:O	1:Q:137:LEU:HB2	2.21	0.41
1:J:32:LEU:HD13	1:J:130:ILE:HG12	2.03	0.41
1:G:113:ARG:NH2	3:G:330:HOH:O	2.45	0.41
1:V:137:LEU:HD23	1:V:137:LEU:HA	1.85	0.41
1:E:139:TYR:O	1:E:143:HIS:N	2.43	0.41
1:A:32:LEU:HD13	1:A:130:ILE:HD12	2.03	0.41
1:I:27:THR:HG23	1:I:31:GLU:HB2	2.03	0.41
1:F:117:LEU:HA	1:F:117:LEU:HD23	1.87	0.41
1:G:138:ARG:NH1	3:G:324:HOH:O	2.32	0.41
1:Q:4:ILE:H	1:Q:4:ILE:HD12	1.86	0.41
1:N:82:THR:HG21	1:Q:82:THR:O	2.20	0.41
1:V:13:LEU:HD22	2:V:201:KIU:CAN	2.51	0.41
1:N:13:LEU:HG	2:N:201:KIU:H10	2.03	0.41
1:F:112:ARG:HH11	2:F:201:KIU:CAP	2.31	0.41
1:T:117:LEU:O	1:T:118:SER:C	2.58	0.41
1:P:59:LEU:HD23	1:P:89:ALA:HB2	2.03	0.41
1:E:80:THR:OG1	1:E:101:HIS:HE1	2.04	0.41
1:P:124:VAL:HG12	1:P:126:VAL:HG23	2.02	0.41
1:B:139:TYR:CE1	1:B:143:HIS:CE1	3.09	0.41
1:I:13:LEU:HG	2:I:201:KIU:H6	2.03	0.40
1:V:77:GLY:HA2	2:V:201:KIU:CAS	2.51	0.40
1:B:59:LEU:HD23	1:B:89:ALA:CB	2.51	0.40
1:K:31:GLU:H	1:K:31:GLU:HG2	1.61	0.40
1:I:11:PRO:O	1:I:12:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:11:PRO:O	2:U:201:KIU:H6	2.21	0.40
1:E:139:TYR:HA	1:K:131:GLN:OE1	2.21	0.40
1:I:131:GLN:O	1:I:135:LEU:HG	2.21	0.40
1:S:34:ALA:HA	1:S:37:GLU:HB2	2.03	0.40
1:X:118:SER:N	1:X:119:PRO:CD	2.85	0.40
1:J:58:LEU:O	1:J:62:ILE:HG12	2.21	0.40
1:J:20:GLU:HB3	1:J:22:ALA:HB3	2.02	0.40
1:F:11:PRO:HG2	1:F:79:LEU:HG	2.03	0.40
1:E:102:ILE:HG23	1:E:129:GLY:HA2	2.03	0.40
1:R:102:ILE:O	1:R:127:GLY:HA2	2.21	0.40
1:B:118:SER:HB2	1:B:119:PRO:HD3	2.03	0.40
1:R:10:GLY:HA3	1:R:11:PRO:HD2	1.86	0.40
1:X:13:LEU:HD23	1:X:16:LEU:HD11	2.03	0.40
2:D:201:KIU:H7	2:D:201:KIU:H2	1.72	0.40
1:K:28:THR:HG23	1:K:31:GLU:OE1	2.21	0.40
1:J:59:LEU:HA	1:J:59:LEU:HD23	1.82	0.40
1:J:142:GLU:C	1:J:143:HIS:ND1	2.74	0.40
1:T:58:LEU:HD12	1:T:79:LEU:HD12	2.04	0.40
1:F:120:ILE:C	1:F:120:ILE:HD12	2.42	0.40
1:X:140:LEU:C	1:X:142:GLU:H	2.25	0.40
1:L:27:THR:HG23	1:L:31:GLU:HB2	2.04	0.40
1:V:29:HIS:CE1	1:V:51:GLN:HB2	2.56	0.40
1:N:128:LEU:HD21	1:R:98:ILE:HD11	2.03	0.40
1:G:8:ILE:HD13	1:G:62:ILE:HD13	2.02	0.40
1:A:36:ILE:HG23	1:A:137:LEU:HD11	2.03	0.40
1:M:15:ARG:NH1	1:X:63:HIS:HB3	2.36	0.40
1:V:16:LEU:HB3	1:V:27:THR:O	2.21	0.40
1:R:79:LEU:HD23	1:R:79:LEU:HA	1.91	0.40
1:F:86:LEU:HA	1:F:86:LEU:HD12	1.94	0.40

There are no symmetry-related clashes.

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	139/153 (91%)	126 (91%)	10 (7%)	3 (2%)	8	9
1	B	139/153 (91%)	129 (93%)	7 (5%)	3 (2%)	8	9
1	C	139/153 (91%)	134 (96%)	4 (3%)	1 (1%)	26	38
1	D	141/153 (92%)	133 (94%)	8 (6%)	0	100	100
1	E	139/153 (91%)	134 (96%)	4 (3%)	1 (1%)	26	38
1	F	139/153 (91%)	131 (94%)	8 (6%)	0	100	100
1	G	139/153 (91%)	133 (96%)	6 (4%)	0	100	100
1	H	139/153 (91%)	129 (93%)	7 (5%)	3 (2%)	8	9
1	I	139/153 (91%)	129 (93%)	9 (6%)	1 (1%)	26	38
1	J	139/153 (91%)	130 (94%)	4 (3%)	5 (4%)	4	3
1	K	139/153 (91%)	131 (94%)	7 (5%)	1 (1%)	26	38
1	L	139/153 (91%)	131 (94%)	5 (4%)	3 (2%)	8	9
1	M	131/153 (86%)	122 (93%)	9 (7%)	0	100	100
1	N	139/153 (91%)	129 (93%)	9 (6%)	1 (1%)	26	38
1	O	139/153 (91%)	131 (94%)	7 (5%)	1 (1%)	26	38
1	P	139/153 (91%)	125 (90%)	8 (6%)	6 (4%)	3	2
1	Q	139/153 (91%)	131 (94%)	6 (4%)	2 (1%)	14	19
1	R	139/153 (91%)	129 (93%)	7 (5%)	3 (2%)	8	9
1	S	139/153 (91%)	126 (91%)	11 (8%)	2 (1%)	14	19
1	T	139/153 (91%)	134 (96%)	5 (4%)	0	100	100
1	U	139/153 (91%)	127 (91%)	11 (8%)	1 (1%)	26	38
1	V	139/153 (91%)	126 (91%)	12 (9%)	1 (1%)	26	38
1	W	139/153 (91%)	126 (91%)	9 (6%)	4 (3%)	6	5
1	X	143/153 (94%)	133 (93%)	9 (6%)	1 (1%)	26	38
All	All	3334/3672 (91%)	3109 (93%)	182 (6%)	43 (1%)	15	21

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PRO
1	B	19	ARG
1	C	23	VAL
1	H	21	PRO
1	I	19	ARG
1	J	21	PRO

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Mol	Chain	Res	Type
1	J	22	ALA
1	L	23	VAL
1	O	20	GLU
1	P	18	ARG
1	P	21	PRO
1	P	22	ALA
1	P	23	VAL
1	Q	18	ARG
1	R	35	LEU
1	S	21	PRO
1	S	23	VAL
1	U	22	ALA
1	W	20	GLU
1	W	21	PRO
1	W	36	ILE
1	W	37	GLU
1	A	17	GLY
1	A	42	GLU
1	H	18	ARG
1	L	22	ALA
1	N	18	ARG
1	Q	24	TYR
1	R	19	ARG
1	V	4	ILE
1	X	141	ALA
1	P	20	GLU
1	P	141	ALA
1	B	79	LEU
1	E	24	TYR
1	H	20	GLU
1	J	19	ARG
1	J	141	ALA
1	K	42	GLU
1	L	21	PRO
1	R	20	GLU
1	B	110	GLU
1	J	11	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	110/121 (91%)	102 (93%)	8 (7%)	17	27
1	B	110/121 (91%)	102 (93%)	8 (7%)	17	27
1	C	110/121 (91%)	103 (94%)	7 (6%)	22	34
1	D	111/121 (92%)	107 (96%)	4 (4%)	42	63
1	E	110/121 (91%)	102 (93%)	8 (7%)	17	27
1	F	110/121 (91%)	102 (93%)	8 (7%)	17	27
1	G	110/121 (91%)	99 (90%)	11 (10%)	9	14
1	H	110/121 (91%)	103 (94%)	7 (6%)	22	34
1	I	110/121 (91%)	100 (91%)	10 (9%)	12	17
1	J	110/121 (91%)	101 (92%)	9 (8%)	14	21
1	K	109/121 (90%)	102 (94%)	7 (6%)	22	34
1	L	110/121 (91%)	104 (94%)	6 (6%)	27	42
1	M	105/121 (87%)	97 (92%)	8 (8%)	16	25
1	N	110/121 (91%)	104 (94%)	6 (6%)	27	42
1	O	110/121 (91%)	104 (94%)	6 (6%)	27	42
1	P	110/121 (91%)	96 (87%)	14 (13%)	5	6
1	Q	110/121 (91%)	97 (88%)	13 (12%)	6	8
1	R	109/121 (90%)	103 (94%)	6 (6%)	27	42
1	S	110/121 (91%)	100 (91%)	10 (9%)	12	17
1	T	110/121 (91%)	103 (94%)	7 (6%)	22	34
1	U	110/121 (91%)	103 (94%)	7 (6%)	22	34
1	V	110/121 (91%)	100 (91%)	10 (9%)	12	17
1	W	110/121 (91%)	101 (92%)	9 (8%)	14	21
1	X	115/121 (95%)	108 (94%)	7 (6%)	23	36
All	All	2639/2904 (91%)	2443 (93%)	196 (7%)	17	26

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG

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Mol	Chain	Res	Type
1	A	38	ARG
1	A	42	GLU
1	A	46	LYS
1	A	50	ARG
1	A	126	VAL
1	A	130	ILE
1	A	131	GLN
1	B	19	ARG
1	B	35	LEU
1	B	39	GLU
1	B	46	LYS
1	B	50	ARG
1	B	130	ILE
1	B	131	GLN
1	B	142	GLU
1	C	16	LEU
1	C	20	GLU
1	C	30	ASP
1	C	50	ARG
1	C	118	SER
1	C	130	ILE
1	C	131	GLN
1	D	3	LEU
1	D	16	LEU
1	D	20	GLU
1	D	35	LEU
1	E	19	ARG
1	E	20	GLU
1	E	35	LEU
1	E	50	ARG
1	E	122	THR
1	E	130	ILE
1	E	142	GLU
1	E	143	HIS
1	F	3	LEU
1	F	19	ARG
1	F	35	LEU
1	F	50	ARG
1	F	94	SER
1	F	112	ARG
1	F	130	ILE
1	F	138	ARG

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Mol	Chain	Res	Type
1	G	16	LEU
1	G	19	ARG
1	G	37	GLU
1	G	42	GLU
1	G	46	LYS
1	G	49	VAL
1	G	50	ARG
1	G	97	LEU
1	G	130	ILE
1	G	131	GLN
1	G	134	LEU
1	H	18	ARG
1	H	19	ARG
1	H	23	VAL
1	H	42	GLU
1	H	126	VAL
1	H	130	ILE
1	H	142	GLU
1	I	3	LEU
1	I	16	LEU
1	I	23	VAL
1	I	38	ARG
1	I	46	LYS
1	I	50	ARG
1	I	51	GLN
1	I	57	GLN
1	I	130	ILE
1	I	138	ARG
1	J	3	LEU
1	J	16	LEU
1	J	18	ARG
1	J	19	ARG
1	J	35	LEU
1	J	42	GLU
1	J	130	ILE
1	J	131	GLN
1	J	143	HIS
1	K	3	LEU
1	K	31	GLU
1	K	35	LEU
1	K	38	ARG
1	K	50	ARG

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Mol	Chain	Res	Type
1	K	110	GLU
1	K	131	GLN
1	L	16	LEU
1	L	19	ARG
1	L	50	ARG
1	L	59	LEU
1	L	126	VAL
1	L	130	ILE
1	M	3	LEU
1	M	38	ARG
1	M	46	LYS
1	M	50	ARG
1	M	64	GLN
1	M	80	THR
1	M	105	VAL
1	M	130	ILE
1	N	4	ILE
1	N	15	ARG
1	N	16	LEU
1	N	20	GLU
1	N	27	THR
1	N	108	ARG
1	O	3	LEU
1	O	16	LEU
1	O	19	ARG
1	O	38	ARG
1	O	54	SER
1	O	130	ILE
1	P	3	LEU
1	P	16	LEU
1	P	19	ARG
1	P	20	GLU
1	P	23	VAL
1	P	30	ASP
1	P	35	LEU
1	P	38	ARG
1	P	45	LEU
1	P	55	GLU
1	P	80	THR
1	P	131	GLN
1	P	138	ARG
1	P	143	HIS

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Mol	Chain	Res	Type
1	Q	3	LEU
1	Q	4	ILE
1	Q	16	LEU
1	Q	18	ARG
1	Q	23	VAL
1	Q	27	THR
1	Q	35	LEU
1	Q	38	ARG
1	Q	42	GLU
1	Q	45	LEU
1	Q	46	LYS
1	Q	55	GLU
1	Q	130	ILE
1	R	16	LEU
1	R	30	ASP
1	R	35	LEU
1	R	50	ARG
1	R	120	ILE
1	R	130	ILE
1	S	20	GLU
1	S	24	TYR
1	S	28	THR
1	S	30	ASP
1	S	35	LEU
1	S	38	ARG
1	S	39	GLU
1	S	49	VAL
1	S	50	ARG
1	S	124	VAL
1	T	11	PRO
1	T	16	LEU
1	T	19	ARG
1	T	46	LYS
1	T	126	VAL
1	T	130	ILE
1	T	131	GLN
1	U	16	LEU
1	U	18	ARG
1	U	50	ARG
1	U	51	GLN
1	U	126	VAL
1	U	130	ILE

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Mol	Chain	Res	Type
1	U	138	ARG
1	V	3	LEU
1	V	4	ILE
1	V	18	ARG
1	V	35	LEU
1	V	50	ARG
1	V	97	LEU
1	V	130	ILE
1	V	138	ARG
1	V	142	GLU
1	V	143	HIS
1	W	3	LEU
1	W	15	ARG
1	W	19	ARG
1	W	30	ASP
1	W	45	LEU
1	W	64	GLN
1	W	130	ILE
1	W	138	ARG
1	W	142	GLU
1	X	3	LEU
1	X	11	PRO
1	X	16	LEU
1	X	37	GLU
1	X	54	SER
1	X	110	GLU
1	X	130	ILE

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

Mol	Chain	Res	Type
1	A	6	ASN
1	A	143	HIS
1	C	63	HIS
1	D	9	ASN
1	D	57	GLN
1	D	143	HIS
1	E	101	HIS
1	F	131	GLN
1	F	143	HIS
1	G	101	HIS
1	H	143	HIS

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Mol	Chain	Res	Type
1	I	51	GLN
1	I	57	GLN
1	I	131	GLN
1	K	63	HIS
1	K	64	GLN
1	M	6	ASN
1	M	57	GLN
1	M	63	HIS
1	M	131	GLN
1	N	63	HIS
1	N	114	HIS
1	N	131	GLN
1	O	131	GLN
1	P	51	GLN
1	P	63	HIS
1	Q	114	HIS
1	S	57	GLN
1	U	51	GLN
1	U	63	HIS
1	U	131	GLN
1	V	131	GLN
1	W	63	HIS
1	W	64	GLN
1	X	6	ASN
1	X	114	HIS
1	X	143	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

22 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	KIU	A	201	-	16,24,24	1.84	2 (12%)	21,33,33	1.20	3 (14%)
2	KIU	B	201	-	16,24,24	5.90	2 (12%)	21,33,33	2.59	10 (47%)
2	KIU	C	201	-	16,24,24	2.71	2 (12%)	21,33,33	1.41	4 (19%)
2	KIU	D	201	-	16,24,24	3.06	2 (12%)	21,33,33	2.65	6 (28%)
2	KIU	E	201	-	16,24,24	3.16	2 (12%)	21,33,33	1.20	3 (14%)
2	KIU	F	201	-	16,24,24	4.02	2 (12%)	21,33,33	2.14	4 (19%)
2	KIU	G	201	-	16,24,24	7.14	3 (18%)	21,33,33	1.85	5 (23%)
2	KIU	H	201	-	16,24,24	6.55	2 (12%)	21,33,33	1.87	9 (42%)
2	KIU	I	201	-	16,24,24	4.93	2 (12%)	21,33,33	1.37	2 (9%)
2	KIU	J	201	-	16,24,24	7.27	3 (18%)	21,33,33	2.52	6 (28%)
2	KIU	K	201	-	16,24,24	1.81	3 (18%)	21,33,33	1.62	7 (33%)
2	KIU	L	201	-	16,24,24	2.10	2 (12%)	21,33,33	2.21	5 (23%)
2	KIU	N	201	-	16,24,24	3.27	2 (12%)	21,33,33	2.10	3 (14%)
2	KIU	O	201	-	16,24,24	2.75	2 (12%)	21,33,33	1.96	7 (33%)
2	KIU	P	201	-	16,24,24	4.98	3 (18%)	21,33,33	4.24	9 (42%)
2	KIU	Q	201	-	16,24,24	5.23	2 (12%)	21,33,33	1.88	5 (23%)
2	KIU	R	201	-	16,24,24	3.24	2 (12%)	21,33,33	1.12	2 (9%)
2	KIU	T	201	-	16,24,24	5.13	3 (18%)	21,33,33	4.24	7 (33%)
2	KIU	U	201	-	16,24,24	4.36	2 (12%)	21,33,33	1.20	2 (9%)
2	KIU	V	201	-	16,24,24	1.56	2 (12%)	21,33,33	1.46	6 (28%)
2	KIU	W	201	-	16,24,24	2.31	2 (12%)	21,33,33	1.78	4 (19%)
2	KIU	X	201	-	16,24,24	3.59	2 (12%)	21,33,33	1.46	3 (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	KIU	A	201	-	-	2/9/17/17	0/2/2/2
2	KIU	B	201	-	-	0/9/17/17	0/2/2/2
2	KIU	C	201	-	-	0/9/17/17	0/2/2/2
2	KIU	D	201	-	-	0/9/17/17	0/2/2/2
2	KIU	E	201	-	-	0/9/17/17	0/2/2/2
2	KIU	F	201	-	-	0/9/17/17	0/2/2/2
2	KIU	G	201	-	-	0/9/17/17	0/2/2/2
2	KIU	H	201	-	-	0/9/17/17	0/2/2/2
2	KIU	I	201	-	-	0/9/17/17	0/2/2/2
2	KIU	J	201	-	-	0/9/17/17	0/2/2/2
2	KIU	K	201	-	-	2/9/17/17	0/2/2/2
2	KIU	L	201	-	-	0/9/17/17	0/2/2/2
2	KIU	N	201	-	-	0/9/17/17	0/2/2/2
2	KIU	O	201	-	-	0/9/17/17	0/2/2/2
2	KIU	P	201	-	-	0/9/17/17	0/2/2/2
2	KIU	Q	201	-	-	0/9/17/17	0/2/2/2
2	KIU	R	201	-	-	0/9/17/17	0/2/2/2
2	KIU	T	201	-	-	0/9/17/17	0/2/2/2
2	KIU	U	201	-	-	0/9/17/17	0/2/2/2
2	KIU	V	201	-	-	0/9/17/17	0/2/2/2
2	KIU	W	201	-	-	0/9/17/17	0/2/2/2
2	KIU	X	201	-	-	0/9/17/17	0/2/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	KIU	CAN-CAR	-5.71	1.37	1.50
2	V	201	KIU	CAN-CAR	-5.42	1.37	1.50
2	O	201	KIU	CAN-CAR	-5.42	1.37	1.50
2	K	201	KIU	CAN-CAR	-5.31	1.38	1.50
2	F	201	KIU	CAN-CAR	-5.25	1.38	1.50
2	X	201	KIU	CAN-CAR	-5.17	1.38	1.50
2	I	201	KIU	CAN-CAR	-5.05	1.38	1.50
2	N	201	KIU	CAN-CAR	-4.93	1.39	1.50
2	W	201	KIU	CAN-CAR	-4.84	1.39	1.50
2	U	201	KIU	CAN-CAR	-4.71	1.39	1.50
2	D	201	KIU	CAN-CAR	-4.59	1.39	1.50
2	R	201	KIU	CAN-CAR	-4.31	1.40	1.50
2	A	201	KIU	CAN-CAR	-4.29	1.40	1.50
2	Q	201	KIU	CAN-CAR	-4.27	1.40	1.50
2	C	201	KIU	CAN-CAR	-4.12	1.40	1.50
2	L	201	KIU	CAN-CAR	-4.00	1.41	1.50
2	H	201	KIU	CAN-CAR	-3.84	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201	KIU	CAN-CAR	-3.61	1.42	1.50
2	G	201	KIU	CAN-CAR	-3.41	1.42	1.50
2	B	201	KIU	CAN-CAR	-3.35	1.42	1.50
2	P	201	KIU	CAN-CAR	-2.55	1.44	1.50
2	K	201	KIU	CAJ-CAS	2.09	1.42	1.38
2	G	201	KIU	OAQ-CAN	2.15	1.50	1.43
2	J	201	KIU	CAL-CAV	2.18	1.43	1.39
2	V	201	KIU	CAK-CAS	2.22	1.43	1.38
2	T	201	KIU	CAL-CAR	2.43	1.43	1.39
2	P	201	KIU	CAL-CAV	2.59	1.44	1.39
2	T	201	KIU	CAL-CAV	3.38	1.45	1.39
2	K	201	KIU	OAE-NAW	4.25	1.31	1.22
2	A	201	KIU	OAE-NAW	5.77	1.34	1.22
2	L	201	KIU	OAE-NAW	6.54	1.35	1.22
2	W	201	KIU	OAE-NAW	7.54	1.37	1.22
2	O	201	KIU	OAE-NAW	9.05	1.40	1.22
2	C	201	KIU	OAE-NAW	9.91	1.42	1.22
2	E	201	KIU	OAE-NAW	11.01	1.44	1.22
2	D	201	KIU	OAE-NAW	11.02	1.44	1.22
2	N	201	KIU	OAE-NAW	11.71	1.46	1.22
2	R	201	KIU	OAE-NAW	12.06	1.46	1.22
2	X	201	KIU	OAE-NAW	13.18	1.48	1.22
2	F	201	KIU	OAE-NAW	14.85	1.52	1.22
2	U	201	KIU	OAE-NAW	16.61	1.55	1.22
2	I	201	KIU	OAE-NAW	18.82	1.60	1.22
2	P	201	KIU	OAE-NAW	19.35	1.61	1.22
2	T	201	KIU	OAE-NAW	19.73	1.61	1.22
2	Q	201	KIU	OAE-NAW	20.34	1.63	1.22
2	B	201	KIU	OAE-NAW	22.87	1.68	1.22
2	H	201	KIU	OAE-NAW	25.72	1.73	1.22
2	G	201	KIU	OAE-NAW	28.13	1.78	1.22
2	J	201	KIU	OAE-NAW	28.58	1.79	1.22

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	201	KIU	CAI-CAV-NAW	-11.62	110.11	119.48
2	T	201	KIU	CAI-CAV-NAW	-10.12	111.33	119.48
2	D	201	KIU	CAL-CAV-NAW	-6.70	112.92	118.80
2	J	201	KIU	CAN-OAO-CAS	-6.06	101.44	117.70
2	N	201	KIU	CAI-CAV-NAW	-5.73	114.86	119.48
2	B	201	KIU	CAN-OAO-CAS	-4.56	105.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	201	KIU	CAN-OAO-CAS	-4.49	105.64	117.70
2	P	201	KIU	CAN-CAR-CAH	-4.48	109.91	120.66
2	F	201	KIU	CAL-CAV-NAW	-4.45	114.90	118.80
2	L	201	KIU	CAL-CAV-NAW	-4.39	114.95	118.80
2	J	201	KIU	CAI-CAV-NAW	-4.04	116.22	119.48
2	T	201	KIU	CAN-CAR-CAH	-4.01	111.03	120.66
2	B	201	KIU	CAI-CAV-CAL	-3.96	114.59	120.07
2	G	201	KIU	CAN-OAO-CAS	-3.91	107.19	117.70
2	O	201	KIU	CAN-OAO-CAS	-3.88	107.29	117.70
2	W	201	KIU	CAN-OAO-CAS	-3.77	107.57	117.70
2	C	201	KIU	CAN-OAO-CAS	-3.38	108.63	117.70
2	L	201	KIU	CAN-OAO-CAS	-3.36	108.68	117.70
2	W	201	KIU	CAL-CAV-NAW	-3.30	115.91	118.80
2	H	201	KIU	CAI-CAV-NAW	-3.24	116.87	119.48
2	V	201	KIU	CAN-OAO-CAS	-3.08	109.44	117.70
2	E	201	KIU	CAN-OAO-CAS	-3.05	109.51	117.70
2	A	201	KIU	CAN-OAO-CAS	-2.90	109.91	117.70
2	P	201	KIU	CAI-CAG-CAH	-2.77	116.28	120.24
2	O	201	KIU	CAN-CAR-CAL	-2.73	113.52	120.30
2	G	201	KIU	CAI-CAV-NAW	-2.72	117.29	119.48
2	H	201	KIU	CAN-OAO-CAS	-2.70	110.44	117.70
2	U	201	KIU	CAN-OAO-CAS	-2.65	110.59	117.70
2	I	201	KIU	CAN-OAO-CAS	-2.62	110.66	117.70
2	R	201	KIU	CAN-OAO-CAS	-2.61	110.68	117.70
2	O	201	KIU	CAL-CAV-NAW	-2.60	116.52	118.80
2	D	201	KIU	CAN-CAR-CAL	-2.42	114.29	120.30
2	F	201	KIU	CAN-CAR-CAL	-2.41	114.32	120.30
2	C	201	KIU	CAU-CAK-CAS	-2.41	117.44	119.76
2	K	201	KIU	CAI-CAG-CAH	-2.36	116.87	120.24
2	D	201	KIU	CAN-OAO-CAS	-2.31	111.49	117.70
2	T	201	KIU	CAK-CAS-CAJ	-2.29	117.05	120.99
2	V	201	KIU	CAT-CAJ-CAS	-2.27	117.58	119.76
2	K	201	KIU	CAI-CAV-NAW	-2.22	117.69	119.48
2	H	201	KIU	CAI-CAG-CAH	-2.19	117.11	120.24
2	K	201	KIU	CAN-OAO-CAS	-2.14	111.95	117.70
2	H	201	KIU	CAN-CAR-CAH	-2.09	115.66	120.66
2	B	201	KIU	CAK-CAS-CAJ	-2.08	117.41	120.99
2	L	201	KIU	CAU-CAM-CAT	-2.06	117.36	121.31
2	V	201	KIU	CAI-CAG-CAH	-2.03	117.34	120.24
2	H	201	KIU	CAG-CAH-CAR	2.00	123.83	120.65
2	O	201	KIU	OAE-NAW-CAV	2.01	122.49	118.89
2	V	201	KIU	CAH-CAR-CAL	2.04	121.57	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	201	KIU	OAE-NAW-CAV	2.07	122.61	118.89
2	J	201	KIU	CAU-CAK-CAS	2.08	121.75	119.76
2	K	201	KIU	CAH-CAR-CAL	2.08	121.62	118.55
2	D	201	KIU	CAN-CAR-CAH	2.10	125.71	120.66
2	K	201	KIU	CAG-CAI-CAV	2.12	122.50	119.41
2	P	201	KIU	CAK-CAU-CAM	2.12	121.56	118.29
2	E	201	KIU	CAH-CAR-CAL	2.12	121.69	118.55
2	Q	201	KIU	CAV-CAL-CAR	2.12	121.56	119.02
2	H	201	KIU	CAN-CAR-CAL	2.16	125.67	120.30
2	U	201	KIU	CAI-CAV-NAW	2.20	121.25	119.48
2	J	201	KIU	OAQ-CAN-CAR	2.22	115.88	109.21
2	E	201	KIU	CAK-CAU-CAM	2.25	121.76	118.29
2	R	201	KIU	CAK-CAU-CAM	2.34	121.89	118.29
2	P	201	KIU	OAE-NAW-CAV	2.36	123.13	118.89
2	B	201	KIU	OAE-NAW-CAV	2.37	123.14	118.89
2	B	201	KIU	CAM-CAT-CAJ	2.41	122.00	118.29
2	A	201	KIU	CAU-CAK-CAS	2.42	122.08	119.76
2	T	201	KIU	CAG-CAH-CAR	2.45	124.54	120.65
2	G	201	KIU	CAT-CAJ-CAS	2.45	122.11	119.76
2	O	201	KIU	CAH-CAR-CAL	2.46	122.19	118.55
2	V	201	KIU	CAI-CAV-NAW	2.48	121.49	119.48
2	O	201	KIU	CAM-CAT-CAJ	2.50	122.13	118.29
2	W	201	KIU	CAK-CAU-CAM	2.51	122.16	118.29
2	F	201	KIU	CAM-CAT-CAJ	2.52	122.17	118.29
2	X	201	KIU	CAK-CAU-CAM	2.55	122.22	118.29
2	A	201	KIU	CAM-CAT-CAJ	2.58	122.26	118.29
2	H	201	KIU	CAU-CAK-CAS	2.59	122.25	119.76
2	C	201	KIU	CAT-CAJ-CAS	2.68	122.33	119.76
2	Q	201	KIU	CAU-CAK-CAS	2.70	122.35	119.76
2	C	201	KIU	CAK-CAU-CAM	2.79	122.58	118.29
2	H	201	KIU	OAQ-CAN-CAR	2.81	117.64	109.21
2	V	201	KIU	CAM-CAT-CAJ	2.92	122.78	118.29
2	J	201	KIU	OAE-NAW-CAV	2.92	124.14	118.89
2	D	201	KIU	CAK-CAU-CAM	2.98	122.87	118.29
2	L	201	KIU	CAK-CAU-CAM	2.99	122.89	118.29
2	K	201	KIU	CAK-CAU-CAM	3.04	122.96	118.29
2	B	201	KIU	CAU-CAK-CAS	3.04	122.68	119.76
2	K	201	KIU	CAL-CAV-NAW	3.05	121.47	118.80
2	N	201	KIU	CAK-CAU-CAM	3.14	123.12	118.29
2	I	201	KIU	CAK-CAU-CAM	3.14	123.13	118.29
2	P	201	KIU	CAG-CAH-CAR	3.15	125.65	120.65
2	Q	201	KIU	CAM-CAT-CAJ	3.38	123.49	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	KIU	CAK-CAU-CAM	3.60	123.82	118.29
2	Q	201	KIU	CAL-CAV-NAW	3.61	121.96	118.80
2	H	201	KIU	CAL-CAV-NAW	3.68	122.03	118.80
2	G	201	KIU	CAL-CAV-NAW	3.74	122.08	118.80
2	B	201	KIU	OAO-CAN-CAR	3.77	120.52	109.21
2	X	201	KIU	CAI-CAV-NAW	3.94	122.66	119.48
2	B	201	KIU	CAI-CAV-NAW	4.03	122.73	119.48
2	B	201	KIU	CAL-CAV-NAW	4.41	122.67	118.80
2	O	201	KIU	CAI-CAV-NAW	4.50	123.11	119.48
2	B	201	KIU	CAV-CAL-CAR	4.65	124.57	119.02
2	P	201	KIU	CAN-CAR-CAL	4.78	132.18	120.30
2	P	201	KIU	OAO-CAN-CAR	4.78	123.58	109.21
2	W	201	KIU	CAI-CAV-NAW	4.95	123.47	119.48
2	T	201	KIU	CAN-CAR-CAL	5.05	132.84	120.30
2	N	201	KIU	CAL-CAV-NAW	5.30	123.45	118.80
2	T	201	KIU	OAO-CAN-CAR	5.77	126.54	109.21
2	L	201	KIU	CAI-CAV-NAW	6.09	124.40	119.48
2	F	201	KIU	CAI-CAV-NAW	6.61	124.81	119.48
2	J	201	KIU	CAL-CAV-NAW	7.19	125.11	118.80
2	D	201	KIU	CAI-CAV-NAW	8.04	125.97	119.48
2	P	201	KIU	CAL-CAV-NAW	11.48	128.87	118.80
2	T	201	KIU	CAL-CAV-NAW	13.09	130.28	118.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	201	KIU	CAL-CAV-NAW-OAE
2	A	201	KIU	CAI-CAV-NAW-OAE
2	K	201	KIU	CAI-CAV-NAW-OAE
2	A	201	KIU	CAL-CAV-NAW-OAE

There are no ring outliers.

22 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	KIU	2	0
2	B	201	KIU	2	0
2	C	201	KIU	6	0
2	D	201	KIU	3	0
2	E	201	KIU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	201	KIU	6	0
2	G	201	KIU	2	0
2	H	201	KIU	4	0
2	I	201	KIU	7	0
2	J	201	KIU	6	0
2	K	201	KIU	8	0
2	L	201	KIU	4	0
2	N	201	KIU	5	0
2	O	201	KIU	3	0
2	P	201	KIU	7	0
2	Q	201	KIU	2	0
2	R	201	KIU	4	0
2	T	201	KIU	6	0
2	U	201	KIU	4	0
2	V	201	KIU	16	0
2	W	201	KIU	6	0
2	X	201	KIU	5	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/153 (92%)	-0.28	6 (4%) 39 40	15, 23, 59, 109	0
1	B	141/153 (92%)	-0.59	1 (0%) 89 88	12, 20, 41, 76	0
1	C	141/153 (92%)	-0.57	0 100 100	11, 21, 48, 76	0
1	D	143/153 (93%)	-0.44	0 100 100	12, 19, 40, 59	0
1	E	141/153 (92%)	-0.47	2 (1%) 78 77	15, 24, 59, 78	0
1	F	141/153 (92%)	-0.49	0 100 100	14, 21, 48, 71	0
1	G	141/153 (92%)	-0.45	2 (1%) 78 77	12, 20, 43, 66	1 (0%)
1	H	141/153 (92%)	-0.50	2 (1%) 78 77	13, 21, 48, 84	0
1	I	141/153 (92%)	-0.46	0 100 100	11, 21, 49, 63	0
1	J	141/153 (92%)	-0.51	2 (1%) 78 77	12, 19, 44, 75	0
1	K	141/153 (92%)	-0.36	1 (0%) 89 88	13, 23, 49, 68	0
1	L	141/153 (92%)	-0.42	0 100 100	13, 21, 42, 54	0
1	M	135/153 (88%)	-0.27	4 (2%) 54 53	18, 30, 54, 98	0
1	N	141/153 (92%)	-0.17	0 100 100	21, 31, 66, 85	0
1	O	141/153 (92%)	-0.50	2 (1%) 78 77	15, 23, 43, 77	0
1	P	141/153 (92%)	-0.23	5 (3%) 48 48	18, 31, 65, 103	0
1	Q	141/153 (92%)	-0.02	6 (4%) 39 40	22, 36, 67, 108	0
1	R	141/153 (92%)	-0.21	2 (1%) 78 77	21, 30, 64, 79	0
1	S	141/153 (92%)	-0.14	3 (2%) 67 66	19, 29, 72, 111	1 (0%)
1	T	141/153 (92%)	-0.35	1 (0%) 89 88	13, 22, 51, 83	0
1	U	141/153 (92%)	-0.19	4 (2%) 56 55	16, 28, 57, 92	0
1	V	141/153 (92%)	-0.15	4 (2%) 56 55	17, 25, 59, 76	0
1	W	141/153 (92%)	0.06	5 (3%) 48 48	25, 35, 66, 99	0
1	X	147/153 (96%)	-0.49	0 100 100	17, 26, 49, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3386/3672 (92%)	-0.34	52 (1%) 76 75	11, 26, 58, 111	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	23	VAL	6.6
1	Q	21	PRO	5.2
1	V	22	ALA	5.0
1	A	21	PRO	4.6
1	P	21	PRO	4.3
1	S	21	PRO	3.9
1	Q	24	TYR	3.8
1	M	25	GLY	3.7
1	P	24	TYR	3.5
1	J	21	PRO	3.4
1	W	25	GLY	3.2
1	A	18	ARG	3.2
1	A	19	ARG	3.1
1	W	20	GLU	3.1
1	Q	19	ARG	3.1
1	M	24	TYR	3.1
1	M	17	GLY	3.0
1	P	17	GLY	3.0
1	P	20	GLU	3.0
1	Q	20	GLU	3.0
1	U	19	ARG	2.8
1	W	19	ARG	2.8
1	P	19	ARG	2.8
1	W	21	PRO	2.7
1	A	22	ALA	2.7
1	G	3	LEU	2.7
1	V	44	GLY	2.7
1	J	19	ARG	2.6
1	A	23	VAL	2.6
1	A	25	GLY	2.6
1	W	23	VAL	2.4
1	R	22	ALA	2.4
1	U	18	ARG	2.4
1	B	19	ARG	2.4
1	H	20	GLU	2.4
1	V	26	GLY	2.3
1	K	22	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	19	ARG	2.2
1	U	3	LEU	2.2
1	Q	38	ARG	2.2
1	Q	41	ALA	2.2
1	T	19	ARG	2.2
1	H	23	VAL	2.2
1	S	24	TYR	2.2
1	V	41	ALA	2.1
1	E	18	ARG	2.1
1	R	143	HIS	2.1
1	O	19	ARG	2.1
1	E	3	LEU	2.1
1	O	18	ARG	2.0
1	U	23	VAL	2.0
1	M	26	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	KIU	X	201	23/23	0.93	0.25	3.50	47,57,65,73	0
2	KIU	L	201	23/23	0.95	0.17	2.90	30,34,42,43	0
2	KIU	Q	201	23/23	0.66	0.43	2.85	41,50,57,59	23
2	KIU	C	201	23/23	0.93	0.22	2.07	31,42,50,58	0
2	KIU	V	201	23/23	0.93	0.24	1.88	49,62,66,67	0
2	KIU	W	201	23/23	0.89	0.30	1.75	20,28,37,39	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	KIU	P	201	23/23	0.83	0.31	1.66	48,66,74,80	0
2	KIU	E	201	23/23	0.90	0.22	1.66	42,53,63,66	0
2	KIU	N	201	23/23	0.90	0.21	1.59	52,63,88,96	0
2	KIU	U	201	23/23	0.91	0.25	1.54	40,56,60,70	0
2	KIU	A	201	23/23	0.90	0.26	1.35	45,60,64,67	0
2	KIU	R	201	23/23	0.91	0.21	1.30	51,56,73,77	0
2	KIU	O	201	23/23	0.94	0.22	1.25	36,45,50,52	0
2	KIU	H	201	23/23	0.89	0.21	1.16	34,51,70,79	0
2	KIU	T	201	23/23	0.90	0.19	1.07	44,53,57,58	0
2	KIU	K	201	23/23	0.94	0.15	1.01	32,45,55,58	0
2	KIU	B	201	23/23	0.84	0.19	0.94	35,45,53,55	0
2	KIU	G	201	23/23	0.88	0.17	0.79	26,40,54,57	0
2	KIU	I	201	23/23	0.95	0.16	0.74	19,31,53,66	0
2	KIU	F	201	23/23	0.94	0.14	0.71	32,40,50,56	0
2	KIU	D	201	23/23	0.96	0.15	0.69	25,39,48,56	0
2	KIU	J	201	23/23	0.89	0.17	0.66	34,41,53,55	0

6.5 Other polymers

There are no such residues in this entry.