



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:57 PM UTC

PDB ID : 3KIP / pdb_00003kip
Title : Crystal structure of type-II 3-dehydroquinase from *C. albicans*
Authors : Trapani, S.; Schoehn, G.; Navaza, J.; Abergel, C.
Deposited on : 2009-11-02
Resolution : 2.95 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

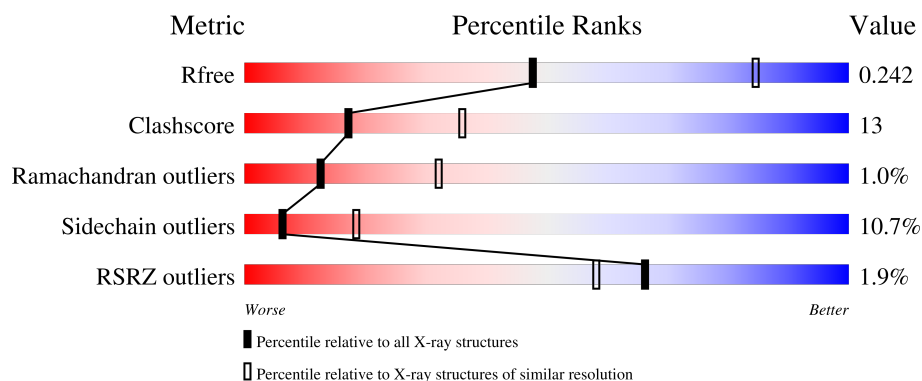
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.



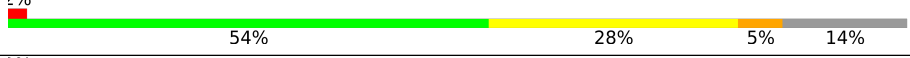
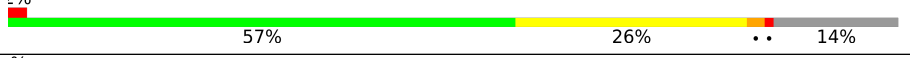
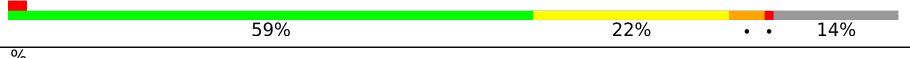
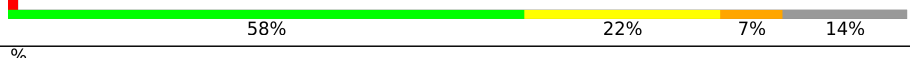
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	167	2% 50% 32% • • 14%
1	B	167	3% 49% 31% 5% • 14%
1	C	167	2% 54% 28% • 14%
1	D	167	2% 58% 23% • • 14%
1	E	167	• 56% 26% • • 13%

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Mol	Chain	Length	Quality of chain
1	F	167	
1	G	167	
1	H	167	
1	I	167	
1	J	167	
1	K	167	
1	L	167	
1	M	167	
1	N	167	
1	O	167	
1	P	167	
1	Q	167	
1	R	167	
1	S	167	
1	T	167	
1	U	167	
1	V	167	
1	W	167	
1	X	167	

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
3	TRS	D	156	-	X	-	-
3	TRS	P	156	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27144 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-dehydroquinase, type II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	B	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	C	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	D	144	Total	C	N	O	S	0	0	0
			1117	711	195	210	1			
1	E	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			
1	F	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			
1	G	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	H	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	I	147	Total	C	N	O	S	0	0	0
			1142	727	198	216	1			
1	J	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	K	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	L	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	M	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	N	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	O	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	P	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	R	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	S	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	T	144	Total	C	N	O	S	0	0	0
			1117	711	195	210	1			
1	U	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	V	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	W	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			
1	X	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			

There are 528 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP Q59Z17
A	-11	HIS	-	expression tag	UNP Q59Z17
A	-10	HIS	-	expression tag	UNP Q59Z17
A	-9	HIS	-	expression tag	UNP Q59Z17
A	-8	HIS	-	expression tag	UNP Q59Z17
A	-7	HIS	-	expression tag	UNP Q59Z17
A	-6	HIS	-	expression tag	UNP Q59Z17
A	-5	GLY	-	expression tag	UNP Q59Z17
A	-4	HIS	-	expression tag	UNP Q59Z17
A	-3	HIS	-	expression tag	UNP Q59Z17
A	-2	HIS	-	expression tag	UNP Q59Z17
A	-1	GLN	-	expression tag	UNP Q59Z17
A	0	LEU	-	expression tag	UNP Q59Z17
A	146	GLN	-	expression tag	UNP Q59Z17
A	147	LEU	-	expression tag	UNP Q59Z17
A	148	ASP	-	expression tag	UNP Q59Z17
A	149	GLY	-	expression tag	UNP Q59Z17
A	150	ASP	-	expression tag	UNP Q59Z17
A	151	LEU	-	expression tag	UNP Q59Z17
A	152	GLU	-	expression tag	UNP Q59Z17
A	153	ALA	-	expression tag	UNP Q59Z17
A	154	ALA	-	expression tag	UNP Q59Z17
B	-12	ALA	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP Q59Z17
B	-10	HIS	-	expression tag	UNP Q59Z17
B	-9	HIS	-	expression tag	UNP Q59Z17
B	-8	HIS	-	expression tag	UNP Q59Z17
B	-7	HIS	-	expression tag	UNP Q59Z17
B	-6	HIS	-	expression tag	UNP Q59Z17
B	-5	GLY	-	expression tag	UNP Q59Z17
B	-4	HIS	-	expression tag	UNP Q59Z17
B	-3	HIS	-	expression tag	UNP Q59Z17
B	-2	HIS	-	expression tag	UNP Q59Z17
B	-1	GLN	-	expression tag	UNP Q59Z17
B	0	LEU	-	expression tag	UNP Q59Z17
B	146	GLN	-	expression tag	UNP Q59Z17
B	147	LEU	-	expression tag	UNP Q59Z17
B	148	ASP	-	expression tag	UNP Q59Z17
B	149	GLY	-	expression tag	UNP Q59Z17
B	150	ASP	-	expression tag	UNP Q59Z17
B	151	LEU	-	expression tag	UNP Q59Z17
B	152	GLU	-	expression tag	UNP Q59Z17
B	153	ALA	-	expression tag	UNP Q59Z17
B	154	ALA	-	expression tag	UNP Q59Z17
C	-12	ALA	-	expression tag	UNP Q59Z17
C	-11	HIS	-	expression tag	UNP Q59Z17
C	-10	HIS	-	expression tag	UNP Q59Z17
C	-9	HIS	-	expression tag	UNP Q59Z17
C	-8	HIS	-	expression tag	UNP Q59Z17
C	-7	HIS	-	expression tag	UNP Q59Z17
C	-6	HIS	-	expression tag	UNP Q59Z17
C	-5	GLY	-	expression tag	UNP Q59Z17
C	-4	HIS	-	expression tag	UNP Q59Z17
C	-3	HIS	-	expression tag	UNP Q59Z17
C	-2	HIS	-	expression tag	UNP Q59Z17
C	-1	GLN	-	expression tag	UNP Q59Z17
C	0	LEU	-	expression tag	UNP Q59Z17
C	146	GLN	-	expression tag	UNP Q59Z17
C	147	LEU	-	expression tag	UNP Q59Z17
C	148	ASP	-	expression tag	UNP Q59Z17
C	149	GLY	-	expression tag	UNP Q59Z17
C	150	ASP	-	expression tag	UNP Q59Z17
C	151	LEU	-	expression tag	UNP Q59Z17
C	152	GLU	-	expression tag	UNP Q59Z17
C	153	ALA	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
C	154	ALA	-	expression tag	UNP Q59Z17
D	-12	ALA	-	expression tag	UNP Q59Z17
D	-11	HIS	-	expression tag	UNP Q59Z17
D	-10	HIS	-	expression tag	UNP Q59Z17
D	-9	HIS	-	expression tag	UNP Q59Z17
D	-8	HIS	-	expression tag	UNP Q59Z17
D	-7	HIS	-	expression tag	UNP Q59Z17
D	-6	HIS	-	expression tag	UNP Q59Z17
D	-5	GLY	-	expression tag	UNP Q59Z17
D	-4	HIS	-	expression tag	UNP Q59Z17
D	-3	HIS	-	expression tag	UNP Q59Z17
D	-2	HIS	-	expression tag	UNP Q59Z17
D	-1	GLN	-	expression tag	UNP Q59Z17
D	0	LEU	-	expression tag	UNP Q59Z17
D	146	GLN	-	expression tag	UNP Q59Z17
D	147	LEU	-	expression tag	UNP Q59Z17
D	148	ASP	-	expression tag	UNP Q59Z17
D	149	GLY	-	expression tag	UNP Q59Z17
D	150	ASP	-	expression tag	UNP Q59Z17
D	151	LEU	-	expression tag	UNP Q59Z17
D	152	GLU	-	expression tag	UNP Q59Z17
D	153	ALA	-	expression tag	UNP Q59Z17
D	154	ALA	-	expression tag	UNP Q59Z17
E	-12	ALA	-	expression tag	UNP Q59Z17
E	-11	HIS	-	expression tag	UNP Q59Z17
E	-10	HIS	-	expression tag	UNP Q59Z17
E	-9	HIS	-	expression tag	UNP Q59Z17
E	-8	HIS	-	expression tag	UNP Q59Z17
E	-7	HIS	-	expression tag	UNP Q59Z17
E	-6	HIS	-	expression tag	UNP Q59Z17
E	-5	GLY	-	expression tag	UNP Q59Z17
E	-4	HIS	-	expression tag	UNP Q59Z17
E	-3	HIS	-	expression tag	UNP Q59Z17
E	-2	HIS	-	expression tag	UNP Q59Z17
E	-1	GLN	-	expression tag	UNP Q59Z17
E	0	LEU	-	expression tag	UNP Q59Z17
E	146	GLN	-	expression tag	UNP Q59Z17
E	147	LEU	-	expression tag	UNP Q59Z17
E	148	ASP	-	expression tag	UNP Q59Z17
E	149	GLY	-	expression tag	UNP Q59Z17
E	150	ASP	-	expression tag	UNP Q59Z17
E	151	LEU	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
E	152	GLU	-	expression tag	UNP Q59Z17
E	153	ALA	-	expression tag	UNP Q59Z17
E	154	ALA	-	expression tag	UNP Q59Z17
F	-12	ALA	-	expression tag	UNP Q59Z17
F	-11	HIS	-	expression tag	UNP Q59Z17
F	-10	HIS	-	expression tag	UNP Q59Z17
F	-9	HIS	-	expression tag	UNP Q59Z17
F	-8	HIS	-	expression tag	UNP Q59Z17
F	-7	HIS	-	expression tag	UNP Q59Z17
F	-6	HIS	-	expression tag	UNP Q59Z17
F	-5	GLY	-	expression tag	UNP Q59Z17
F	-4	HIS	-	expression tag	UNP Q59Z17
F	-3	HIS	-	expression tag	UNP Q59Z17
F	-2	HIS	-	expression tag	UNP Q59Z17
F	-1	GLN	-	expression tag	UNP Q59Z17
F	0	LEU	-	expression tag	UNP Q59Z17
F	146	GLN	-	expression tag	UNP Q59Z17
F	147	LEU	-	expression tag	UNP Q59Z17
F	148	ASP	-	expression tag	UNP Q59Z17
F	149	GLY	-	expression tag	UNP Q59Z17
F	150	ASP	-	expression tag	UNP Q59Z17
F	151	LEU	-	expression tag	UNP Q59Z17
F	152	GLU	-	expression tag	UNP Q59Z17
F	153	ALA	-	expression tag	UNP Q59Z17
F	154	ALA	-	expression tag	UNP Q59Z17
G	-12	ALA	-	expression tag	UNP Q59Z17
G	-11	HIS	-	expression tag	UNP Q59Z17
G	-10	HIS	-	expression tag	UNP Q59Z17
G	-9	HIS	-	expression tag	UNP Q59Z17
G	-8	HIS	-	expression tag	UNP Q59Z17
G	-7	HIS	-	expression tag	UNP Q59Z17
G	-6	HIS	-	expression tag	UNP Q59Z17
G	-5	GLY	-	expression tag	UNP Q59Z17
G	-4	HIS	-	expression tag	UNP Q59Z17
G	-3	HIS	-	expression tag	UNP Q59Z17
G	-2	HIS	-	expression tag	UNP Q59Z17
G	-1	GLN	-	expression tag	UNP Q59Z17
G	0	LEU	-	expression tag	UNP Q59Z17
G	146	GLN	-	expression tag	UNP Q59Z17
G	147	LEU	-	expression tag	UNP Q59Z17
G	148	ASP	-	expression tag	UNP Q59Z17
G	149	GLY	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
G	150	ASP	-	expression tag	UNP Q59Z17
G	151	LEU	-	expression tag	UNP Q59Z17
G	152	GLU	-	expression tag	UNP Q59Z17
G	153	ALA	-	expression tag	UNP Q59Z17
G	154	ALA	-	expression tag	UNP Q59Z17
H	-12	ALA	-	expression tag	UNP Q59Z17
H	-11	HIS	-	expression tag	UNP Q59Z17
H	-10	HIS	-	expression tag	UNP Q59Z17
H	-9	HIS	-	expression tag	UNP Q59Z17
H	-8	HIS	-	expression tag	UNP Q59Z17
H	-7	HIS	-	expression tag	UNP Q59Z17
H	-6	HIS	-	expression tag	UNP Q59Z17
H	-5	GLY	-	expression tag	UNP Q59Z17
H	-4	HIS	-	expression tag	UNP Q59Z17
H	-3	HIS	-	expression tag	UNP Q59Z17
H	-2	HIS	-	expression tag	UNP Q59Z17
H	-1	GLN	-	expression tag	UNP Q59Z17
H	0	LEU	-	expression tag	UNP Q59Z17
H	146	GLN	-	expression tag	UNP Q59Z17
H	147	LEU	-	expression tag	UNP Q59Z17
H	148	ASP	-	expression tag	UNP Q59Z17
H	149	GLY	-	expression tag	UNP Q59Z17
H	150	ASP	-	expression tag	UNP Q59Z17
H	151	LEU	-	expression tag	UNP Q59Z17
H	152	GLU	-	expression tag	UNP Q59Z17
H	153	ALA	-	expression tag	UNP Q59Z17
H	154	ALA	-	expression tag	UNP Q59Z17
I	-12	ALA	-	expression tag	UNP Q59Z17
I	-11	HIS	-	expression tag	UNP Q59Z17
I	-10	HIS	-	expression tag	UNP Q59Z17
I	-9	HIS	-	expression tag	UNP Q59Z17
I	-8	HIS	-	expression tag	UNP Q59Z17
I	-7	HIS	-	expression tag	UNP Q59Z17
I	-6	HIS	-	expression tag	UNP Q59Z17
I	-5	GLY	-	expression tag	UNP Q59Z17
I	-4	HIS	-	expression tag	UNP Q59Z17
I	-3	HIS	-	expression tag	UNP Q59Z17
I	-2	HIS	-	expression tag	UNP Q59Z17
I	-1	GLN	-	expression tag	UNP Q59Z17
I	0	LEU	-	expression tag	UNP Q59Z17
I	146	GLN	-	expression tag	UNP Q59Z17
I	147	LEU	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
I	148	ASP	-	expression tag	UNP Q59Z17
I	149	GLY	-	expression tag	UNP Q59Z17
I	150	ASP	-	expression tag	UNP Q59Z17
I	151	LEU	-	expression tag	UNP Q59Z17
I	152	GLU	-	expression tag	UNP Q59Z17
I	153	ALA	-	expression tag	UNP Q59Z17
I	154	ALA	-	expression tag	UNP Q59Z17
J	-12	ALA	-	expression tag	UNP Q59Z17
J	-11	HIS	-	expression tag	UNP Q59Z17
J	-10	HIS	-	expression tag	UNP Q59Z17
J	-9	HIS	-	expression tag	UNP Q59Z17
J	-8	HIS	-	expression tag	UNP Q59Z17
J	-7	HIS	-	expression tag	UNP Q59Z17
J	-6	HIS	-	expression tag	UNP Q59Z17
J	-5	GLY	-	expression tag	UNP Q59Z17
J	-4	HIS	-	expression tag	UNP Q59Z17
J	-3	HIS	-	expression tag	UNP Q59Z17
J	-2	HIS	-	expression tag	UNP Q59Z17
J	-1	GLN	-	expression tag	UNP Q59Z17
J	0	LEU	-	expression tag	UNP Q59Z17
J	146	GLN	-	expression tag	UNP Q59Z17
J	147	LEU	-	expression tag	UNP Q59Z17
J	148	ASP	-	expression tag	UNP Q59Z17
J	149	GLY	-	expression tag	UNP Q59Z17
J	150	ASP	-	expression tag	UNP Q59Z17
J	151	LEU	-	expression tag	UNP Q59Z17
J	152	GLU	-	expression tag	UNP Q59Z17
J	153	ALA	-	expression tag	UNP Q59Z17
J	154	ALA	-	expression tag	UNP Q59Z17
K	-12	ALA	-	expression tag	UNP Q59Z17
K	-11	HIS	-	expression tag	UNP Q59Z17
K	-10	HIS	-	expression tag	UNP Q59Z17
K	-9	HIS	-	expression tag	UNP Q59Z17
K	-8	HIS	-	expression tag	UNP Q59Z17
K	-7	HIS	-	expression tag	UNP Q59Z17
K	-6	HIS	-	expression tag	UNP Q59Z17
K	-5	GLY	-	expression tag	UNP Q59Z17
K	-4	HIS	-	expression tag	UNP Q59Z17
K	-3	HIS	-	expression tag	UNP Q59Z17
K	-2	HIS	-	expression tag	UNP Q59Z17
K	-1	GLN	-	expression tag	UNP Q59Z17
K	0	LEU	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
K	146	GLN	-	expression tag	UNP Q59Z17
K	147	LEU	-	expression tag	UNP Q59Z17
K	148	ASP	-	expression tag	UNP Q59Z17
K	149	GLY	-	expression tag	UNP Q59Z17
K	150	ASP	-	expression tag	UNP Q59Z17
K	151	LEU	-	expression tag	UNP Q59Z17
K	152	GLU	-	expression tag	UNP Q59Z17
K	153	ALA	-	expression tag	UNP Q59Z17
K	154	ALA	-	expression tag	UNP Q59Z17
L	-12	ALA	-	expression tag	UNP Q59Z17
L	-11	HIS	-	expression tag	UNP Q59Z17
L	-10	HIS	-	expression tag	UNP Q59Z17
L	-9	HIS	-	expression tag	UNP Q59Z17
L	-8	HIS	-	expression tag	UNP Q59Z17
L	-7	HIS	-	expression tag	UNP Q59Z17
L	-6	HIS	-	expression tag	UNP Q59Z17
L	-5	GLY	-	expression tag	UNP Q59Z17
L	-4	HIS	-	expression tag	UNP Q59Z17
L	-3	HIS	-	expression tag	UNP Q59Z17
L	-2	HIS	-	expression tag	UNP Q59Z17
L	-1	GLN	-	expression tag	UNP Q59Z17
L	0	LEU	-	expression tag	UNP Q59Z17
L	146	GLN	-	expression tag	UNP Q59Z17
L	147	LEU	-	expression tag	UNP Q59Z17
L	148	ASP	-	expression tag	UNP Q59Z17
L	149	GLY	-	expression tag	UNP Q59Z17
L	150	ASP	-	expression tag	UNP Q59Z17
L	151	LEU	-	expression tag	UNP Q59Z17
L	152	GLU	-	expression tag	UNP Q59Z17
L	153	ALA	-	expression tag	UNP Q59Z17
L	154	ALA	-	expression tag	UNP Q59Z17
M	-12	ALA	-	expression tag	UNP Q59Z17
M	-11	HIS	-	expression tag	UNP Q59Z17
M	-10	HIS	-	expression tag	UNP Q59Z17
M	-9	HIS	-	expression tag	UNP Q59Z17
M	-8	HIS	-	expression tag	UNP Q59Z17
M	-7	HIS	-	expression tag	UNP Q59Z17
M	-6	HIS	-	expression tag	UNP Q59Z17
M	-5	GLY	-	expression tag	UNP Q59Z17
M	-4	HIS	-	expression tag	UNP Q59Z17
M	-3	HIS	-	expression tag	UNP Q59Z17
M	-2	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	GLN	-	expression tag	UNP Q59Z17
M	0	LEU	-	expression tag	UNP Q59Z17
M	146	GLN	-	expression tag	UNP Q59Z17
M	147	LEU	-	expression tag	UNP Q59Z17
M	148	ASP	-	expression tag	UNP Q59Z17
M	149	GLY	-	expression tag	UNP Q59Z17
M	150	ASP	-	expression tag	UNP Q59Z17
M	151	LEU	-	expression tag	UNP Q59Z17
M	152	GLU	-	expression tag	UNP Q59Z17
M	153	ALA	-	expression tag	UNP Q59Z17
M	154	ALA	-	expression tag	UNP Q59Z17
N	-12	ALA	-	expression tag	UNP Q59Z17
N	-11	HIS	-	expression tag	UNP Q59Z17
N	-10	HIS	-	expression tag	UNP Q59Z17
N	-9	HIS	-	expression tag	UNP Q59Z17
N	-8	HIS	-	expression tag	UNP Q59Z17
N	-7	HIS	-	expression tag	UNP Q59Z17
N	-6	HIS	-	expression tag	UNP Q59Z17
N	-5	GLY	-	expression tag	UNP Q59Z17
N	-4	HIS	-	expression tag	UNP Q59Z17
N	-3	HIS	-	expression tag	UNP Q59Z17
N	-2	HIS	-	expression tag	UNP Q59Z17
N	-1	GLN	-	expression tag	UNP Q59Z17
N	0	LEU	-	expression tag	UNP Q59Z17
N	146	GLN	-	expression tag	UNP Q59Z17
N	147	LEU	-	expression tag	UNP Q59Z17
N	148	ASP	-	expression tag	UNP Q59Z17
N	149	GLY	-	expression tag	UNP Q59Z17
N	150	ASP	-	expression tag	UNP Q59Z17
N	151	LEU	-	expression tag	UNP Q59Z17
N	152	GLU	-	expression tag	UNP Q59Z17
N	153	ALA	-	expression tag	UNP Q59Z17
N	154	ALA	-	expression tag	UNP Q59Z17
O	-12	ALA	-	expression tag	UNP Q59Z17
O	-11	HIS	-	expression tag	UNP Q59Z17
O	-10	HIS	-	expression tag	UNP Q59Z17
O	-9	HIS	-	expression tag	UNP Q59Z17
O	-8	HIS	-	expression tag	UNP Q59Z17
O	-7	HIS	-	expression tag	UNP Q59Z17
O	-6	HIS	-	expression tag	UNP Q59Z17
O	-5	GLY	-	expression tag	UNP Q59Z17
O	-4	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-3	HIS	-	expression tag	UNP Q59Z17
O	-2	HIS	-	expression tag	UNP Q59Z17
O	-1	GLN	-	expression tag	UNP Q59Z17
O	0	LEU	-	expression tag	UNP Q59Z17
O	146	GLN	-	expression tag	UNP Q59Z17
O	147	LEU	-	expression tag	UNP Q59Z17
O	148	ASP	-	expression tag	UNP Q59Z17
O	149	GLY	-	expression tag	UNP Q59Z17
O	150	ASP	-	expression tag	UNP Q59Z17
O	151	LEU	-	expression tag	UNP Q59Z17
O	152	GLU	-	expression tag	UNP Q59Z17
O	153	ALA	-	expression tag	UNP Q59Z17
O	154	ALA	-	expression tag	UNP Q59Z17
P	-12	ALA	-	expression tag	UNP Q59Z17
P	-11	HIS	-	expression tag	UNP Q59Z17
P	-10	HIS	-	expression tag	UNP Q59Z17
P	-9	HIS	-	expression tag	UNP Q59Z17
P	-8	HIS	-	expression tag	UNP Q59Z17
P	-7	HIS	-	expression tag	UNP Q59Z17
P	-6	HIS	-	expression tag	UNP Q59Z17
P	-5	GLY	-	expression tag	UNP Q59Z17
P	-4	HIS	-	expression tag	UNP Q59Z17
P	-3	HIS	-	expression tag	UNP Q59Z17
P	-2	HIS	-	expression tag	UNP Q59Z17
P	-1	GLN	-	expression tag	UNP Q59Z17
P	0	LEU	-	expression tag	UNP Q59Z17
P	146	GLN	-	expression tag	UNP Q59Z17
P	147	LEU	-	expression tag	UNP Q59Z17
P	148	ASP	-	expression tag	UNP Q59Z17
P	149	GLY	-	expression tag	UNP Q59Z17
P	150	ASP	-	expression tag	UNP Q59Z17
P	151	LEU	-	expression tag	UNP Q59Z17
P	152	GLU	-	expression tag	UNP Q59Z17
P	153	ALA	-	expression tag	UNP Q59Z17
P	154	ALA	-	expression tag	UNP Q59Z17
Q	-12	ALA	-	expression tag	UNP Q59Z17
Q	-11	HIS	-	expression tag	UNP Q59Z17
Q	-10	HIS	-	expression tag	UNP Q59Z17
Q	-9	HIS	-	expression tag	UNP Q59Z17
Q	-8	HIS	-	expression tag	UNP Q59Z17
Q	-7	HIS	-	expression tag	UNP Q59Z17
Q	-6	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-5	GLY	-	expression tag	UNP Q59Z17
Q	-4	HIS	-	expression tag	UNP Q59Z17
Q	-3	HIS	-	expression tag	UNP Q59Z17
Q	-2	HIS	-	expression tag	UNP Q59Z17
Q	-1	GLN	-	expression tag	UNP Q59Z17
Q	0	LEU	-	expression tag	UNP Q59Z17
Q	146	GLN	-	expression tag	UNP Q59Z17
Q	147	LEU	-	expression tag	UNP Q59Z17
Q	148	ASP	-	expression tag	UNP Q59Z17
Q	149	GLY	-	expression tag	UNP Q59Z17
Q	150	ASP	-	expression tag	UNP Q59Z17
Q	151	LEU	-	expression tag	UNP Q59Z17
Q	152	GLU	-	expression tag	UNP Q59Z17
Q	153	ALA	-	expression tag	UNP Q59Z17
Q	154	ALA	-	expression tag	UNP Q59Z17
R	-12	ALA	-	expression tag	UNP Q59Z17
R	-11	HIS	-	expression tag	UNP Q59Z17
R	-10	HIS	-	expression tag	UNP Q59Z17
R	-9	HIS	-	expression tag	UNP Q59Z17
R	-8	HIS	-	expression tag	UNP Q59Z17
R	-7	HIS	-	expression tag	UNP Q59Z17
R	-6	HIS	-	expression tag	UNP Q59Z17
R	-5	GLY	-	expression tag	UNP Q59Z17
R	-4	HIS	-	expression tag	UNP Q59Z17
R	-3	HIS	-	expression tag	UNP Q59Z17
R	-2	HIS	-	expression tag	UNP Q59Z17
R	-1	GLN	-	expression tag	UNP Q59Z17
R	0	LEU	-	expression tag	UNP Q59Z17
R	146	GLN	-	expression tag	UNP Q59Z17
R	147	LEU	-	expression tag	UNP Q59Z17
R	148	ASP	-	expression tag	UNP Q59Z17
R	149	GLY	-	expression tag	UNP Q59Z17
R	150	ASP	-	expression tag	UNP Q59Z17
R	151	LEU	-	expression tag	UNP Q59Z17
R	152	GLU	-	expression tag	UNP Q59Z17
R	153	ALA	-	expression tag	UNP Q59Z17
R	154	ALA	-	expression tag	UNP Q59Z17
S	-12	ALA	-	expression tag	UNP Q59Z17
S	-11	HIS	-	expression tag	UNP Q59Z17
S	-10	HIS	-	expression tag	UNP Q59Z17
S	-9	HIS	-	expression tag	UNP Q59Z17
S	-8	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-7	HIS	-	expression tag	UNP Q59Z17
S	-6	HIS	-	expression tag	UNP Q59Z17
S	-5	GLY	-	expression tag	UNP Q59Z17
S	-4	HIS	-	expression tag	UNP Q59Z17
S	-3	HIS	-	expression tag	UNP Q59Z17
S	-2	HIS	-	expression tag	UNP Q59Z17
S	-1	GLN	-	expression tag	UNP Q59Z17
S	0	LEU	-	expression tag	UNP Q59Z17
S	146	GLN	-	expression tag	UNP Q59Z17
S	147	LEU	-	expression tag	UNP Q59Z17
S	148	ASP	-	expression tag	UNP Q59Z17
S	149	GLY	-	expression tag	UNP Q59Z17
S	150	ASP	-	expression tag	UNP Q59Z17
S	151	LEU	-	expression tag	UNP Q59Z17
S	152	GLU	-	expression tag	UNP Q59Z17
S	153	ALA	-	expression tag	UNP Q59Z17
S	154	ALA	-	expression tag	UNP Q59Z17
T	-12	ALA	-	expression tag	UNP Q59Z17
T	-11	HIS	-	expression tag	UNP Q59Z17
T	-10	HIS	-	expression tag	UNP Q59Z17
T	-9	HIS	-	expression tag	UNP Q59Z17
T	-8	HIS	-	expression tag	UNP Q59Z17
T	-7	HIS	-	expression tag	UNP Q59Z17
T	-6	HIS	-	expression tag	UNP Q59Z17
T	-5	GLY	-	expression tag	UNP Q59Z17
T	-4	HIS	-	expression tag	UNP Q59Z17
T	-3	HIS	-	expression tag	UNP Q59Z17
T	-2	HIS	-	expression tag	UNP Q59Z17
T	-1	GLN	-	expression tag	UNP Q59Z17
T	0	LEU	-	expression tag	UNP Q59Z17
T	146	GLN	-	expression tag	UNP Q59Z17
T	147	LEU	-	expression tag	UNP Q59Z17
T	148	ASP	-	expression tag	UNP Q59Z17
T	149	GLY	-	expression tag	UNP Q59Z17
T	150	ASP	-	expression tag	UNP Q59Z17
T	151	LEU	-	expression tag	UNP Q59Z17
T	152	GLU	-	expression tag	UNP Q59Z17
T	153	ALA	-	expression tag	UNP Q59Z17
T	154	ALA	-	expression tag	UNP Q59Z17
U	-12	ALA	-	expression tag	UNP Q59Z17
U	-11	HIS	-	expression tag	UNP Q59Z17
U	-10	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-9	HIS	-	expression tag	UNP Q59Z17
U	-8	HIS	-	expression tag	UNP Q59Z17
U	-7	HIS	-	expression tag	UNP Q59Z17
U	-6	HIS	-	expression tag	UNP Q59Z17
U	-5	GLY	-	expression tag	UNP Q59Z17
U	-4	HIS	-	expression tag	UNP Q59Z17
U	-3	HIS	-	expression tag	UNP Q59Z17
U	-2	HIS	-	expression tag	UNP Q59Z17
U	-1	GLN	-	expression tag	UNP Q59Z17
U	0	LEU	-	expression tag	UNP Q59Z17
U	146	GLN	-	expression tag	UNP Q59Z17
U	147	LEU	-	expression tag	UNP Q59Z17
U	148	ASP	-	expression tag	UNP Q59Z17
U	149	GLY	-	expression tag	UNP Q59Z17
U	150	ASP	-	expression tag	UNP Q59Z17
U	151	LEU	-	expression tag	UNP Q59Z17
U	152	GLU	-	expression tag	UNP Q59Z17
U	153	ALA	-	expression tag	UNP Q59Z17
U	154	ALA	-	expression tag	UNP Q59Z17
V	-12	ALA	-	expression tag	UNP Q59Z17
V	-11	HIS	-	expression tag	UNP Q59Z17
V	-10	HIS	-	expression tag	UNP Q59Z17
V	-9	HIS	-	expression tag	UNP Q59Z17
V	-8	HIS	-	expression tag	UNP Q59Z17
V	-7	HIS	-	expression tag	UNP Q59Z17
V	-6	HIS	-	expression tag	UNP Q59Z17
V	-5	GLY	-	expression tag	UNP Q59Z17
V	-4	HIS	-	expression tag	UNP Q59Z17
V	-3	HIS	-	expression tag	UNP Q59Z17
V	-2	HIS	-	expression tag	UNP Q59Z17
V	-1	GLN	-	expression tag	UNP Q59Z17
V	0	LEU	-	expression tag	UNP Q59Z17
V	146	GLN	-	expression tag	UNP Q59Z17
V	147	LEU	-	expression tag	UNP Q59Z17
V	148	ASP	-	expression tag	UNP Q59Z17
V	149	GLY	-	expression tag	UNP Q59Z17
V	150	ASP	-	expression tag	UNP Q59Z17
V	151	LEU	-	expression tag	UNP Q59Z17
V	152	GLU	-	expression tag	UNP Q59Z17
V	153	ALA	-	expression tag	UNP Q59Z17
V	154	ALA	-	expression tag	UNP Q59Z17
W	-12	ALA	-	expression tag	UNP Q59Z17

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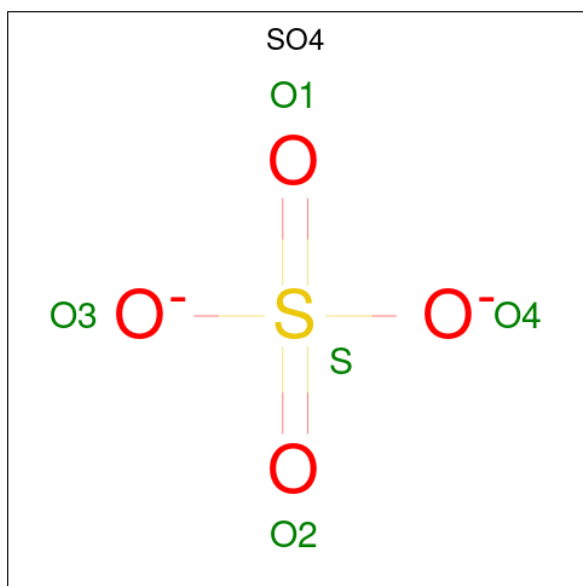
Chain	Residue	Modelled	Actual	Comment	Reference
W	-11	HIS	-	expression tag	UNP Q59Z17
W	-10	HIS	-	expression tag	UNP Q59Z17
W	-9	HIS	-	expression tag	UNP Q59Z17
W	-8	HIS	-	expression tag	UNP Q59Z17
W	-7	HIS	-	expression tag	UNP Q59Z17
W	-6	HIS	-	expression tag	UNP Q59Z17
W	-5	GLY	-	expression tag	UNP Q59Z17
W	-4	HIS	-	expression tag	UNP Q59Z17
W	-3	HIS	-	expression tag	UNP Q59Z17
W	-2	HIS	-	expression tag	UNP Q59Z17
W	-1	GLN	-	expression tag	UNP Q59Z17
W	0	LEU	-	expression tag	UNP Q59Z17
W	146	GLN	-	expression tag	UNP Q59Z17
W	147	LEU	-	expression tag	UNP Q59Z17
W	148	ASP	-	expression tag	UNP Q59Z17
W	149	GLY	-	expression tag	UNP Q59Z17
W	150	ASP	-	expression tag	UNP Q59Z17
W	151	LEU	-	expression tag	UNP Q59Z17
W	152	GLU	-	expression tag	UNP Q59Z17
W	153	ALA	-	expression tag	UNP Q59Z17
W	154	ALA	-	expression tag	UNP Q59Z17
X	-12	ALA	-	expression tag	UNP Q59Z17
X	-11	HIS	-	expression tag	UNP Q59Z17
X	-10	HIS	-	expression tag	UNP Q59Z17
X	-9	HIS	-	expression tag	UNP Q59Z17
X	-8	HIS	-	expression tag	UNP Q59Z17
X	-7	HIS	-	expression tag	UNP Q59Z17
X	-6	HIS	-	expression tag	UNP Q59Z17
X	-5	GLY	-	expression tag	UNP Q59Z17
X	-4	HIS	-	expression tag	UNP Q59Z17
X	-3	HIS	-	expression tag	UNP Q59Z17
X	-2	HIS	-	expression tag	UNP Q59Z17
X	-1	GLN	-	expression tag	UNP Q59Z17
X	0	LEU	-	expression tag	UNP Q59Z17
X	146	GLN	-	expression tag	UNP Q59Z17
X	147	LEU	-	expression tag	UNP Q59Z17
X	148	ASP	-	expression tag	UNP Q59Z17
X	149	GLY	-	expression tag	UNP Q59Z17
X	150	ASP	-	expression tag	UNP Q59Z17
X	151	LEU	-	expression tag	UNP Q59Z17
X	152	GLU	-	expression tag	UNP Q59Z17
X	153	ALA	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
X	154	ALA	-	expression tag	UNP Q59Z17

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



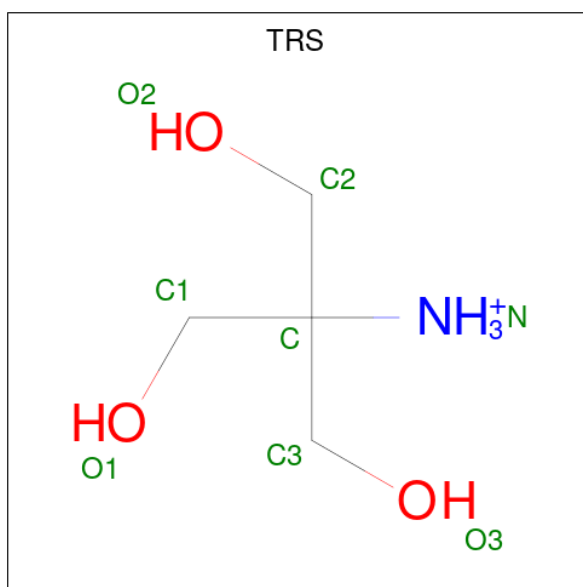
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	U	1	Total	O	S	0	0
			5	4	1		
2	V	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	G	1	Total	C	N	O	0	0
			8	4	1	3		
3	J	1	Total	C	N	O	0	0
			8	4	1	3		
3	N	1	Total	C	N	O	0	0
			8	4	1	3		
3	P	1	Total	C	N	O	0	0
			8	4	1	3		
3	T	1	Total	C	N	O	0	0
			8	4	1	3		
3	W	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	13	Total	O	0	0
			13	13		
4	C	7	Total	O	0	0
			7	7		
4	D	7	Total	O	0	0
			7	7		

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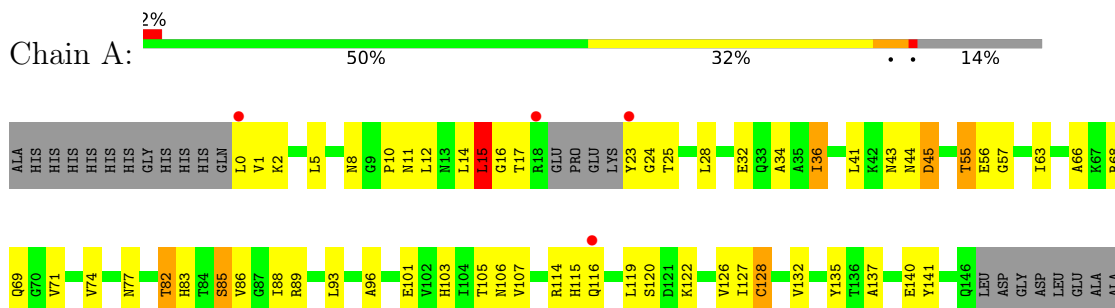
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	17	Total 17	O 17	0	0
4	F	10	Total 10	O 10	0	0
4	G	9	Total 9	O 9	0	0
4	H	4	Total 4	O 4	0	0
4	I	11	Total 11	O 11	0	0
4	J	4	Total 4	O 4	0	0
4	K	5	Total 5	O 5	0	0
4	L	4	Total 4	O 4	0	0
4	M	4	Total 4	O 4	0	0
4	N	11	Total 11	O 11	0	0
4	O	2	Total 2	O 2	0	0
4	P	8	Total 8	O 8	0	0
4	Q	7	Total 7	O 7	0	0
4	R	13	Total 13	O 13	0	0
4	S	4	Total 4	O 4	0	0
4	T	3	Total 3	O 3	0	0
4	U	5	Total 5	O 5	0	0
4	V	5	Total 5	O 5	0	0
4	W	5	Total 5	O 5	0	0
4	X	2	Total 2	O 2	0	0

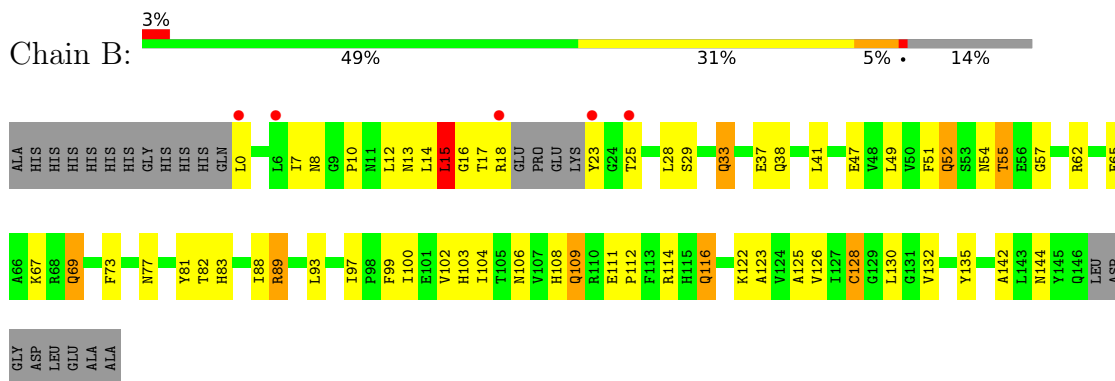
3 Residue-property plots

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 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.

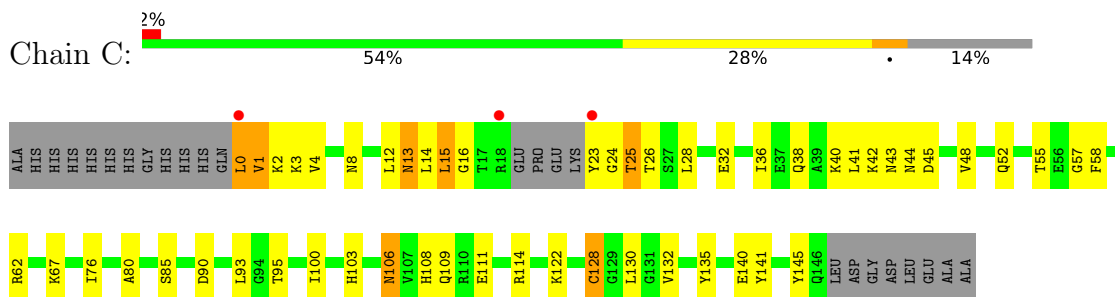
- Molecule 1: 3-dehydroquinase, type II



- Molecule 1: 3-dehydroquinase, type II

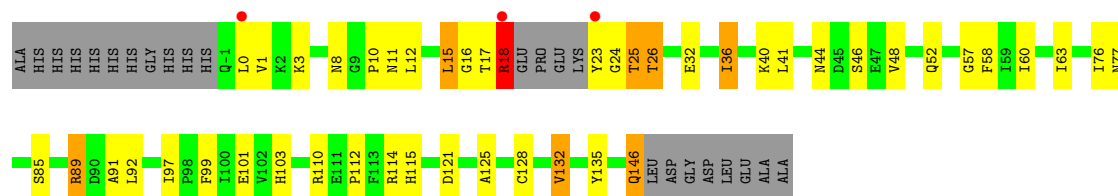


- Molecule 1: 3-dehydroquinase, type II

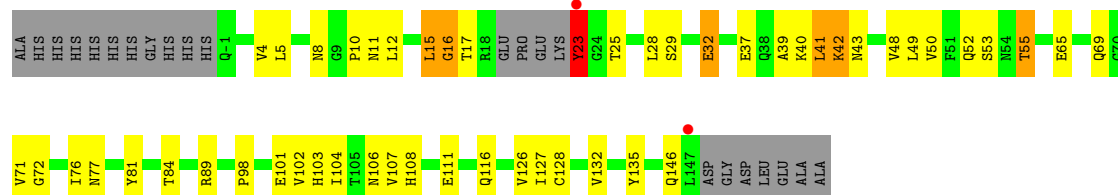


- Molecule 1: 3-dehydroquinase, type II

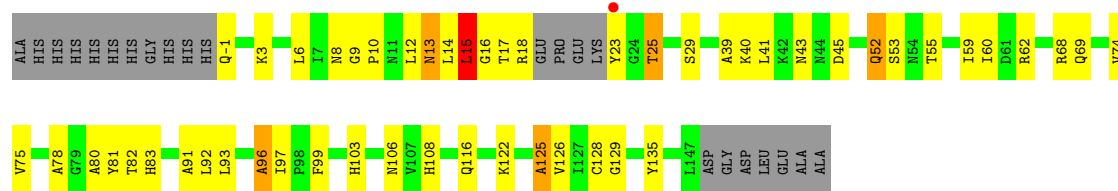




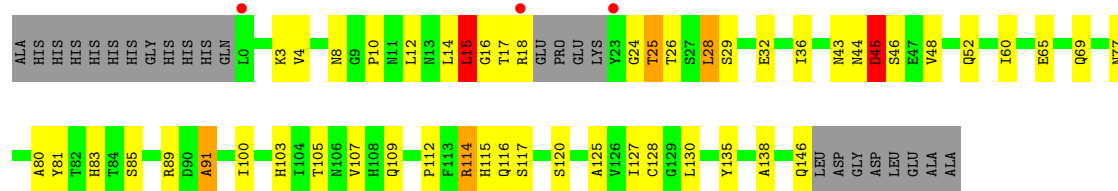
• Molecule 1: 3-dehydroquinase, type II



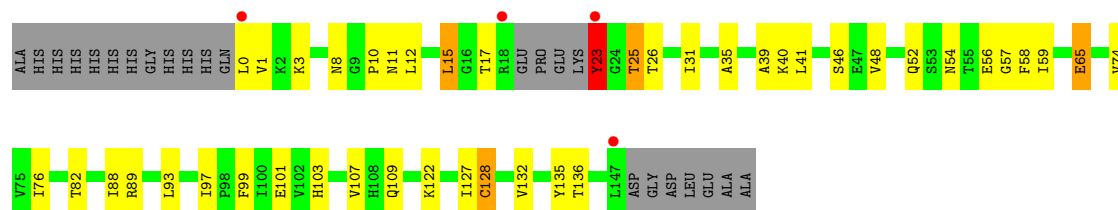
• Molecule 1: 3-dehydroquinase, type II



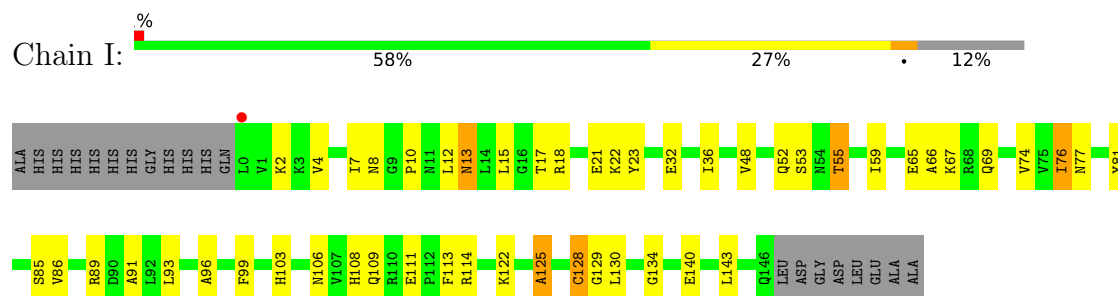
• Molecule 1: 3-dehydroquinase, type II



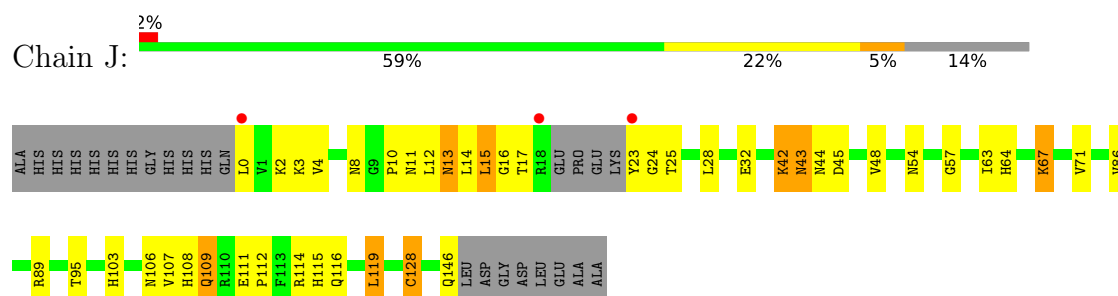
• Molecule 1: 3-dehydroquinase, type II



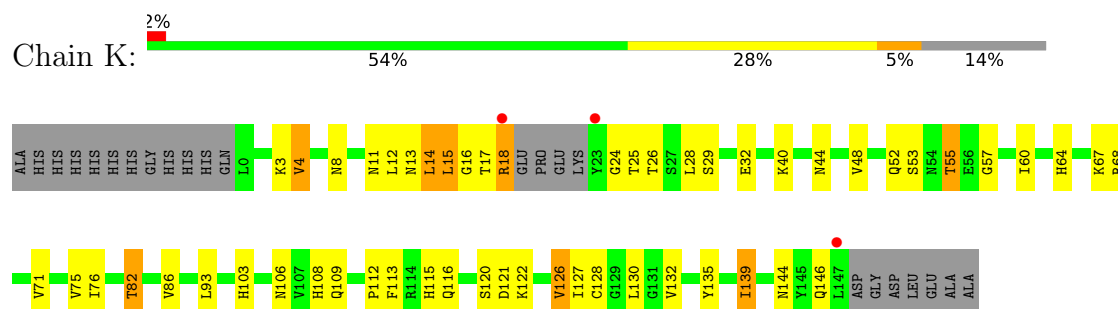
- Molecule 1: 3-dehydroquinase, type II



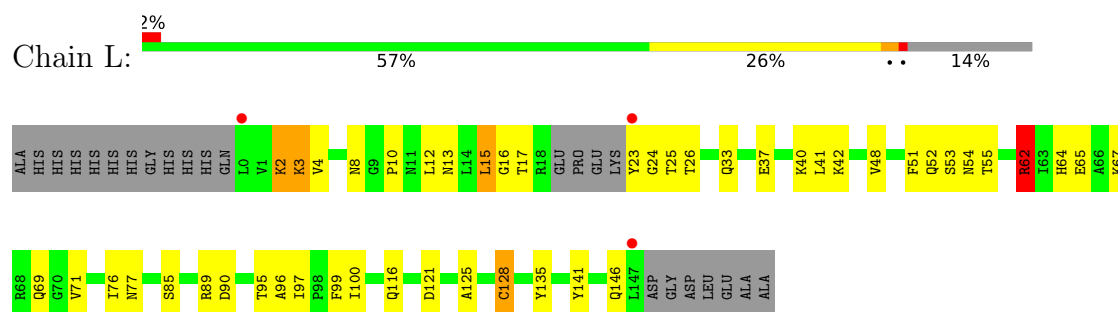
- Molecule 1: 3-dehydroquinase, type II



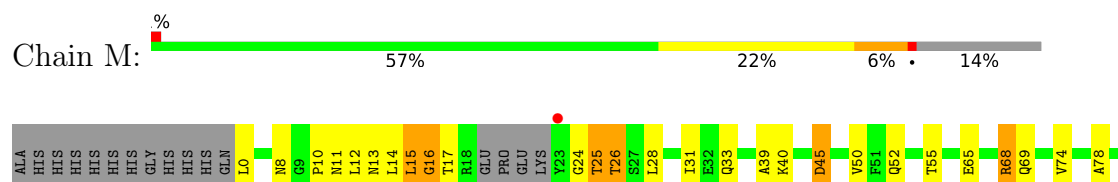
- Molecule 1: 3-dehydroquinase, type II



- Molecule 1: 3-dehydroquinase, type II

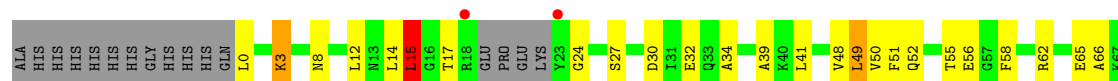


- Molecule 1: 3-dehydroquinase, type II

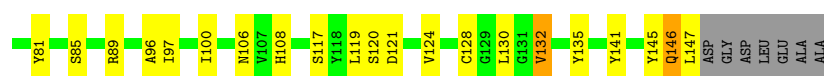
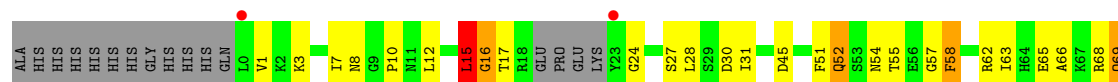




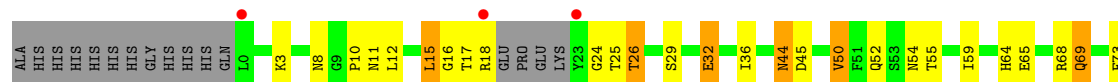
- Molecule 1: 3-dehydroquinase, type II



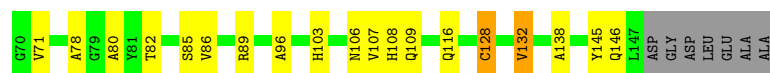
- Molecule 1: 3-dehydroquinase, type II



- Molecule 1: 3-dehydroquinase, type II

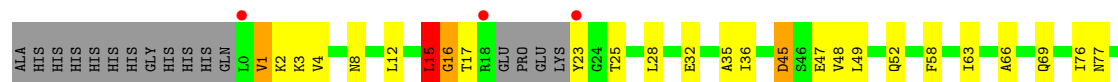


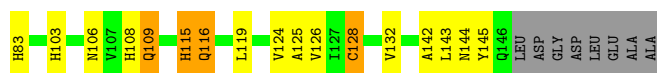
- Molecule 1: 3-dehydroquinase, type II



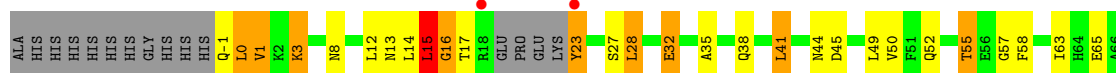
- Molecule 1: 3-dehydroquinase, type II







- Molecule 1: 3-dehydroquinase, type II



- Molecule 1: 3-dehydroquinase, type II



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	159.10Å 308.11Å 97.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.68 – 2.95 70.68 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.68-2.95) 99.9 (70.68-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.245 (Not available) , 0.242	Depositor DCC
R_{free} test set	5090 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27144	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, TRS

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	1.47	6/1126 (0.5%)	1.50	16/1527 (1.0%)
1	B	1.54	8/1126 (0.7%)	1.46	12/1527 (0.8%)
1	C	1.43	3/1126 (0.3%)	1.38	8/1527 (0.5%)
1	D	1.40	5/1135 (0.4%)	1.49	13/1539 (0.8%)
1	E	1.43	4/1143 (0.3%)	1.47	10/1550 (0.6%)
1	F	1.57	10/1143 (0.9%)	1.44	7/1550 (0.5%)
1	G	1.41	5/1126 (0.4%)	1.44	11/1527 (0.7%)
1	H	1.40	6/1134 (0.5%)	1.42	3/1538 (0.2%)
1	I	1.45	4/1162 (0.3%)	1.42	7/1577 (0.4%)
1	J	1.27	3/1126 (0.3%)	1.39	4/1527 (0.3%)
1	K	1.33	6/1134 (0.5%)	1.44	11/1538 (0.7%)
1	L	1.32	3/1134 (0.3%)	1.37	9/1538 (0.6%)
1	M	1.44	7/1134 (0.6%)	1.51	14/1538 (0.9%)
1	N	1.40	4/1134 (0.4%)	1.39	4/1538 (0.3%)
1	O	1.34	3/1134 (0.3%)	1.40	11/1538 (0.7%)
1	P	1.34	4/1134 (0.4%)	1.38	7/1538 (0.5%)
1	Q	1.42	4/1134 (0.4%)	1.47	9/1538 (0.6%)
1	R	1.42	2/1134 (0.2%)	1.40	12/1538 (0.8%)
1	S	1.37	2/1134 (0.2%)	1.45	8/1538 (0.5%)
1	T	1.35	5/1135 (0.4%)	1.40	10/1539 (0.6%)
1	U	1.40	9/1126 (0.8%)	1.39	8/1527 (0.5%)
1	V	1.22	1/1126 (0.1%)	1.32	3/1527 (0.2%)
1	W	1.33	6/1143 (0.5%)	1.40	11/1550 (0.7%)
1	X	1.28	2/1143 (0.2%)	1.42	3/1550 (0.2%)
All	All	1.39	112/27226 (0.4%)	1.42	211/36924 (0.6%)

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	G	0	1
1	M	0	1
1	V	0	1
All	All	0	3

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	25	THR	CA-CB	9.28	1.69	1.53
1	W	63	ILE	CA-CB	-8.42	1.44	1.54
1	F	55	THR	CA-CB	-8.22	1.42	1.53
1	X	25	THR	CA-CB	7.92	1.66	1.53
1	F	96	ALA	CA-CB	-7.47	1.42	1.53
1	R	25	THR	CA-C	7.27	1.62	1.52
1	A	63	ILE	CA-CB	-7.21	1.45	1.54
1	D	25	THR	CA-CB	6.95	1.65	1.53
1	I	96	ALA	CA-CB	-6.90	1.43	1.53
1	L	25	THR	CA-CB	6.84	1.65	1.53
1	F	80	ALA	CA-CB	-6.80	1.42	1.53
1	M	116	GLN	CA-C	-6.66	1.44	1.52
1	Q	80	ALA	CA-CB	-6.66	1.42	1.53
1	C	25	THR	CA-CB	6.64	1.64	1.53
1	L	125	ALA	CA-CB	-6.49	1.42	1.53
1	T	125	ALA	CA-CB	-6.43	1.42	1.53
1	U	25	THR	CA-C	6.36	1.61	1.52
1	F	25	THR	CA-CB	6.32	1.64	1.53
1	B	55	THR	CA-CB	-6.32	1.44	1.53
1	T	25	THR	CA-C	6.30	1.61	1.52
1	F	45	ASP	CA-C	-6.30	1.45	1.53
1	K	60	ILE	CA-CB	6.28	1.61	1.54
1	M	102	VAL	CA-CB	-6.28	1.46	1.54
1	B	125	ALA	N-CA	6.27	1.54	1.45
1	B	7	ILE	CA-CB	-6.27	1.47	1.54
1	G	138	ALA	CA-CB	-6.18	1.43	1.53
1	Q	138	ALA	CA-CB	-6.17	1.43	1.53
1	M	138	ALA	CA-CB	-6.15	1.43	1.53
1	F	68	ARG	C-O	-6.14	1.16	1.24
1	G	125	ALA	CA-CB	-6.13	1.42	1.53
1	U	125	ALA	CA-CB	-6.11	1.42	1.54
1	J	63	ILE	CA-CB	-6.06	1.47	1.54
1	U	24	GLY	N-CA	6.06	1.51	1.44
1	B	142	ALA	CA-C	-6.04	1.45	1.52
1	K	52	GLN	C-O	-6.00	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	23	TYR	CA-C	5.99	1.65	1.52
1	H	136	THR	C-O	5.96	1.31	1.24
1	E	23	TYR	CA-C	5.93	1.65	1.52
1	P	128	CYS	CA-C	-5.93	1.45	1.52
1	E	102	VAL	CA-CB	-5.92	1.47	1.54
1	C	25	THR	CA-C	5.89	1.60	1.52
1	H	25	THR	CA-CB	5.88	1.63	1.53
1	W	15	LEU	CA-C	-5.86	1.45	1.52
1	M	125	ALA	CA-CB	-5.86	1.43	1.53
1	D	125	ALA	CA-CB	-5.85	1.41	1.54
1	I	125	ALA	CA-CB	-5.75	1.43	1.53
1	I	55	THR	CA-CB	-5.72	1.45	1.53
1	F	52	GLN	C-O	-5.71	1.17	1.23
1	M	50	VAL	C-O	-5.70	1.18	1.24
1	U	12	LEU	C-O	-5.67	1.16	1.24
1	A	1	VAL	CA-CB	5.66	1.61	1.53
1	N	55	THR	CA-CB	-5.64	1.45	1.53
1	P	126	VAL	CA-CB	-5.64	1.47	1.54
1	B	52	GLN	C-O	-5.62	1.17	1.23
1	U	80	ALA	CA-CB	-5.56	1.44	1.53
1	U	116	GLN	CA-C	-5.55	1.45	1.52
1	W	35	ALA	CA-CB	-5.54	1.45	1.53
1	K	55	THR	CA-CB	-5.53	1.45	1.53
1	A	24	GLY	N-CA	5.49	1.49	1.44
1	G	100	ILE	CA-CB	-5.49	1.47	1.54
1	J	24	GLY	N-CA	5.46	1.50	1.44
1	G	25	THR	CA-C	5.46	1.60	1.52
1	T	25	THR	CA-CB	5.45	1.62	1.53
1	W	1	VAL	CA-CB	5.45	1.60	1.54
1	S	25	THR	CA-C	5.44	1.60	1.52
1	B	18	ARG	CA-C	5.44	1.64	1.52
1	F	23	TYR	CA-C	5.43	1.64	1.52
1	E	55	THR	CA-CB	-5.42	1.46	1.53
1	X	125	ALA	CA-CB	-5.42	1.43	1.54
1	K	4	VAL	CA-CB	-5.42	1.47	1.54
1	D	25	THR	CA-C	5.41	1.60	1.52
1	H	127	ILE	CA-CB	-5.40	1.47	1.54
1	I	10	PRO	C-O	-5.39	1.17	1.23
1	P	116	GLN	CA-C	-5.39	1.46	1.52
1	R	91	ALA	CA-CB	-5.37	1.45	1.53
1	F	29	SER	N-CA	-5.36	1.39	1.46
1	E	104	ILE	CA-CB	5.36	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	23	TYR	CA-C	5.34	1.64	1.52
1	O	63	ILE	CA-CB	-5.31	1.48	1.54
1	U	50	VAL	C-O	-5.31	1.18	1.24
1	S	137	ALA	CA-CB	-5.30	1.44	1.53
1	C	80	ALA	CA-CB	-5.29	1.44	1.53
1	O	52	GLN	C-O	-5.27	1.17	1.23
1	Q	65	GLU	CG-CD	5.24	1.65	1.52
1	D	18	ARG	CA-C	5.23	1.64	1.52
1	V	15	LEU	CA-C	-5.22	1.46	1.52
1	U	65	GLU	CG-CD	5.22	1.65	1.52
1	H	56	GLU	CA-C	5.19	1.60	1.52
1	W	55	THR	CA-CB	-5.19	1.46	1.53
1	M	31	ILE	CA-CB	-5.18	1.48	1.54
1	B	102	VAL	C-O	-5.17	1.18	1.24
1	O	55	THR	CA-CB	-5.17	1.46	1.53
1	Q	25	THR	CA-CB	5.14	1.62	1.53
1	A	85	SER	C-O	-5.12	1.17	1.23
1	T	116	GLN	CA-C	-5.12	1.46	1.52
1	D	63	ILE	CA-CB	-5.11	1.48	1.54
1	H	23	TYR	CA-C	5.11	1.63	1.52
1	G	15	LEU	CA-C	-5.11	1.46	1.52
1	A	137	ALA	CA-CB	-5.10	1.45	1.53
1	N	24	GLY	N-CA	5.10	1.49	1.44
1	T	80	ALA	CA-CB	-5.08	1.45	1.53
1	N	66	ALA	CA-CB	-5.08	1.45	1.53
1	P	29	SER	N-CA	-5.08	1.40	1.46
1	B	29	SER	N-CA	-5.07	1.39	1.46
1	M	111	GLU	CA-C	5.07	1.58	1.53
1	H	88	ILE	CA-C	5.07	1.59	1.52
1	K	127	ILE	CA-CB	-5.07	1.48	1.54
1	J	25	THR	CA-CB	5.06	1.62	1.53
1	F	125	ALA	CA-CB	-5.05	1.45	1.54
1	K	18	ARG	CA-C	5.03	1.63	1.52
1	N	123	ALA	CA-CB	-5.03	1.44	1.53
1	A	25	THR	CA-CB	5.00	1.61	1.53

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	ILE	CA-C-N	-10.01	110.60	120.21
1	D	97	ILE	C-N-CA	-10.01	110.60	120.21
1	S	111	GLU	CA-C-N	9.48	131.69	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	111	GLU	C-N-CA	9.48	131.69	119.84
1	N	34	ALA	N-CA-C	-8.79	100.23	112.45
1	P	44	ASN	N-CA-C	8.56	120.71	110.44
1	H	46	SER	N-CA-C	-7.79	98.99	110.52
1	M	116	GLN	CB-CA-C	-7.74	97.22	109.84
1	L	96	ALA	CA-C-N	-7.69	117.05	122.59
1	L	96	ALA	C-N-CA	-7.69	117.05	122.59
1	K	82	THR	CB-CA-C	-7.64	95.64	110.46
1	R	97	ILE	CA-C-N	-7.62	112.84	120.31
1	R	97	ILE	C-N-CA	-7.62	112.84	120.31
1	P	111	GLU	CA-C-N	7.51	129.23	119.84
1	P	111	GLU	C-N-CA	7.51	129.23	119.84
1	K	55	THR	N-CA-C	7.30	120.58	108.96
1	W	146	GLN	N-CA-C	7.26	120.35	110.55
1	M	128	CYS	N-CA-C	7.25	120.47	109.23
1	A	34	ALA	N-CA-C	-7.08	103.64	111.36
1	O	97	ILE	CA-C-N	-7.00	112.78	119.85
1	O	97	ILE	C-N-CA	-7.00	112.78	119.85
1	J	86	VAL	N-CA-C	-6.95	102.81	113.16
1	O	96	ALA	CA-C-N	-6.86	117.65	122.59
1	O	96	ALA	C-N-CA	-6.86	117.65	122.59
1	A	14	LEU	CA-C-N	-6.78	111.72	121.42
1	A	14	LEU	C-N-CA	-6.78	111.72	121.42
1	G	16	GLY	N-CA-C	-6.75	93.72	113.30
1	W	32	GLU	N-CA-C	-6.67	103.83	112.23
1	N	111	GLU	CA-C-N	6.66	126.91	119.32
1	N	111	GLU	C-N-CA	6.66	126.91	119.32
1	M	146	GLN	N-CA-C	6.63	124.92	110.80
1	F	15	LEU	CB-CA-C	6.61	120.70	109.53
1	G	91	ALA	N-CA-C	-6.53	104.08	111.14
1	L	85	SER	N-CA-C	6.53	120.25	107.98
1	L	146	GLN	N-CA-C	6.53	119.34	108.96
1	F	14	LEU	CA-C-N	-6.52	112.09	121.42
1	F	14	LEU	C-N-CA	-6.52	112.09	121.42
1	A	15	LEU	CA-CB-CG	6.51	139.08	116.30
1	K	86	VAL	N-CA-C	-6.51	102.72	111.44
1	D	76	ILE	N-CA-C	6.48	117.18	108.11
1	D	85	SER	N-CA-C	6.44	120.08	107.98
1	B	144	ASN	N-CA-C	6.43	120.83	112.92
1	D	1	VAL	N-CA-C	6.35	117.24	109.30
1	L	97	ILE	N-CA-C	6.35	114.17	107.76
1	H	128	CYS	N-CA-C	6.27	119.78	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	82	THR	CB-CA-C	-6.27	100.03	110.68
1	Q	96	ALA	CA-C-N	-6.26	118.09	122.59
1	Q	96	ALA	C-N-CA	-6.26	118.09	122.59
1	P	50	VAL	N-CA-C	6.25	118.47	108.85
1	A	82	THR	CB-CA-C	-6.22	99.11	110.63
1	C	95	THR	N-CA-C	-6.22	106.01	113.97
1	D	44	ASN	N-CA-C	6.19	120.10	111.56
1	C	85	SER	N-CA-C	6.18	119.60	107.98
1	K	127	ILE	CB-CA-C	-6.18	101.48	110.63
1	I	23	TYR	N-CA-C	6.17	120.97	113.38
1	K	44	ASN	N-CA-C	6.15	121.28	111.81
1	I	55	THR	N-CA-C	6.14	118.74	108.73
1	M	28	LEU	N-CA-C	-6.12	104.69	111.36
1	Q	16	GLY	N-CA-C	-6.12	95.56	113.30
1	G	46	SER	N-CA-C	-6.11	102.30	110.55
1	E	111	GLU	CA-C-N	6.11	127.48	119.84
1	E	111	GLU	C-N-CA	6.11	127.48	119.84
1	S	125	ALA	N-CA-C	6.10	118.05	108.96
1	U	34	ALA	N-CA-C	-6.10	104.72	111.36
1	T	116	GLN	CB-CA-C	-6.10	99.69	109.75
1	B	97	ILE	CA-C-N	-6.07	113.70	120.14
1	B	97	ILE	C-N-CA	-6.07	113.70	120.14
1	T	46	SER	N-CA-C	-6.03	102.41	110.55
1	U	14	LEU	CA-C-N	-6.03	112.80	121.42
1	U	14	LEU	C-N-CA	-6.03	112.80	121.42
1	E	127	ILE	CB-CA-C	-6.02	103.44	110.91
1	D	26	THR	CB-CA-C	-6.01	100.43	110.29
1	R	14	LEU	CA-C-N	-6.00	112.83	121.42
1	R	14	LEU	C-N-CA	-6.00	112.83	121.42
1	H	1	VAL	N-CA-C	6.00	116.80	109.30
1	C	111	GLU	CA-C-N	5.97	126.13	119.32
1	C	111	GLU	C-N-CA	5.97	126.13	119.32
1	O	15	LEU	CA-CB-CG	5.97	137.19	116.30
1	W	69	GLN	CB-CA-C	-5.94	100.12	110.17
1	R	28	LEU	N-CA-C	-5.94	104.93	111.82
1	F	9	GLY	CA-C-N	-5.94	113.67	119.78
1	F	9	GLY	C-N-CA	-5.94	113.67	119.78
1	Q	85	SER	N-CA-C	5.92	119.04	107.57
1	A	141	TYR	CA-C-N	5.91	128.13	120.44
1	A	141	TYR	C-N-CA	5.91	128.13	120.44
1	X	72	GLY	N-CA-C	5.91	121.98	114.66
1	E	28	LEU	N-CA-C	-5.90	104.85	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ILE	N-CA-C	5.88	116.34	108.11
1	D	16	GLY	N-CA-C	-5.86	96.31	113.30
1	W	127	ILE	CB-CA-C	-5.83	102.48	110.77
1	P	26	THR	CB-CA-C	-5.81	101.07	110.77
1	U	96	ALA	CA-C-N	-5.80	116.99	123.02
1	U	96	ALA	C-N-CA	-5.80	116.99	123.02
1	K	18	ARG	N-CA-C	5.77	127.17	111.00
1	I	76	ILE	N-CA-C	5.77	116.42	108.12
1	W	139	ILE	CB-CA-C	5.76	119.96	112.24
1	U	16	GLY	N-CA-C	-5.76	96.60	113.30
1	R	1	VAL	N-CA-C	5.74	116.48	109.30
1	B	82	THR	CB-CA-C	-5.74	100.93	110.68
1	W	130	LEU	N-CA-C	-5.73	105.87	112.92
1	P	59	ILE	N-CA-C	-5.73	104.93	110.72
1	O	7	ILE	CB-CA-C	-5.71	102.11	110.62
1	R	41	LEU	N-CA-C	5.71	119.35	112.38
1	M	126	VAL	CB-CA-C	5.71	117.89	110.12
1	E	146	GLN	N-CA-C	5.71	117.98	109.59
1	T	55	THR	N-CA-C	5.71	118.04	108.96
1	K	126	VAL	CB-CA-C	5.70	117.88	110.12
1	W	44	ASN	N-CA-C	5.70	119.44	111.30
1	K	139	ILE	CB-CA-C	5.66	120.03	112.22
1	B	111	GLU	CA-C-N	5.64	126.90	119.84
1	B	111	GLU	C-N-CA	5.64	126.90	119.84
1	G	85	SER	N-CA-C	5.64	118.25	107.75
1	G	114	ARG	N-CA-C	-5.63	106.41	113.28
1	Q	146	GLN	N-CA-C	5.62	118.72	110.30
1	C	128	CYS	N-CA-C	5.61	118.35	108.75
1	B	14	LEU	CA-C-N	-5.60	112.91	120.87
1	B	14	LEU	C-N-CA	-5.60	112.91	120.87
1	E	16	GLY	N-CA-C	-5.58	97.13	113.30
1	A	83	HIS	N-CA-C	-5.56	106.49	113.72
1	V	124	VAL	N-CA-C	-5.54	105.33	110.53
1	M	119	LEU	N-CA-C	5.53	120.03	113.12
1	A	86	VAL	N-CA-C	-5.52	104.82	112.50
1	I	96	ALA	CA-C-N	-5.52	117.96	123.04
1	I	96	ALA	C-N-CA	-5.52	117.96	123.04
1	K	130	LEU	N-CA-C	-5.52	106.42	112.72
1	S	16	GLY	N-CA-C	-5.51	97.31	113.30
1	S	46	SER	N-CA-C	-5.51	101.28	109.94
1	C	16	GLY	N-CA-C	-5.49	97.38	113.30
1	M	14	LEU	CA-C-N	-5.49	113.65	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	14	LEU	C-N-CA	-5.49	113.65	121.50
1	A	55	THR	N-CA-C	5.49	117.58	108.20
1	D	101	GLU	CA-C-N	-5.48	116.03	123.10
1	D	101	GLU	C-N-CA	-5.48	116.03	123.10
1	O	85	SER	N-CA-C	5.47	117.92	107.75
1	B	130	LEU	N-CA-C	-5.47	106.49	112.72
1	A	1	VAL	N-CA-C	5.46	116.29	108.93
1	T	18	ARG	N-CA-C	5.45	126.25	111.00
1	M	131	GLY	N-CA-C	-5.44	102.45	112.62
1	M	127	ILE	CB-CA-C	-5.43	102.74	110.83
1	W	127	ILE	N-CA-C	-5.42	99.83	107.75
1	B	16	GLY	N-CA-C	-5.42	97.57	113.30
1	P	126	VAL	CB-CA-C	-5.42	102.42	110.33
1	M	16	GLY	N-CA-C	-5.42	97.59	113.30
1	A	16	GLY	N-CA-C	-5.40	97.63	113.30
1	Q	43	ASN	N-CA-C	5.39	122.28	110.80
1	S	60	ILE	N-CA-C	-5.39	105.13	111.00
1	T	85	SER	N-CA-C	5.38	117.97	108.24
1	I	59	ILE	N-CA-C	-5.34	105.32	110.72
1	W	28	LEU	N-CA-C	-5.34	105.54	111.36
1	F	18	ARG	N-CA-C	5.33	125.94	111.00
1	O	16	GLY	N-CA-C	-5.33	97.85	113.30
1	O	58	PHE	N-CA-C	5.32	117.08	111.28
1	B	15	LEU	CA-CB-CG	5.32	134.91	116.30
1	W	16	GLY	N-CA-C	-5.31	97.91	113.30
1	B	18	ARG	N-CA-C	5.29	125.81	111.00
1	Q	82	THR	CB-CA-C	-5.28	100.87	110.63
1	T	75	VAL	N-CA-C	-5.28	100.15	107.80
1	L	62	ARG	N-CA-C	-5.27	105.61	111.36
1	T	105	THR	N-CA-C	-5.27	102.40	110.14
1	A	96	ALA	CA-C-N	-5.26	117.55	123.02
1	A	96	ALA	C-N-CA	-5.26	117.55	123.02
1	A	105	THR	CA-C-N	-5.26	113.65	122.17
1	A	105	THR	C-N-CA	-5.26	113.65	122.17
1	R	86	VAL	N-CA-C	-5.25	105.92	113.07
1	M	33	GLN	CA-C-N	5.25	127.26	120.44
1	M	33	GLN	C-N-CA	5.25	127.26	120.44
1	F	59	ILE	N-CA-C	-5.24	105.29	111.00
1	K	144	ASN	CB-CA-C	-5.23	101.72	110.56
1	J	128	CYS	N-CA-C	5.19	116.88	108.26
1	G	28	LEU	N-CA-C	-5.18	105.71	111.36
1	U	67	LYS	N-CA-CB	5.16	118.27	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	91	ALA	N-CA-C	-5.15	105.58	111.14
1	E	76	ILE	N-CA-C	5.15	115.53	108.12
1	K	120	SER	N-CA-C	5.13	119.83	111.37
1	T	127	ILE	CB-CA-C	-5.13	103.04	110.63
1	N	15	LEU	CA-CB-CG	5.12	134.23	116.30
1	S	24	GLY	N-CA-C	-5.12	104.80	112.89
1	R	85	SER	N-CA-C	5.12	117.27	107.75
1	G	105	THR	CA-C-N	-5.12	114.37	121.99
1	G	105	THR	C-N-CA	-5.12	114.37	121.99
1	R	18	ARG	N-CA-C	5.10	125.29	111.00
1	X	111	GLU	CA-C-N	5.10	126.21	119.84
1	X	111	GLU	C-N-CA	5.10	126.21	119.84
1	G	120	SER	N-CA-C	5.08	116.50	111.07
1	R	59	ILE	N-CA-C	-5.08	105.59	110.72
1	E	71	VAL	CB-CA-C	-5.07	103.32	111.59
1	C	1	VAL	N-CA-C	5.07	116.12	109.58
1	W	85	SER	N-CA-C	5.06	117.17	107.75
1	Q	145	TYR	CA-C-N	5.06	129.31	121.26
1	Q	145	TYR	C-N-CA	5.06	129.31	121.26
1	U	41	LEU	CA-CB-CG	5.06	134.01	116.30
1	L	99	PHE	N-CA-C	5.06	116.76	109.07
1	D	110	ARG	N-CA-C	5.06	117.16	109.63
1	L	76	ILE	N-CA-C	5.05	115.25	107.77
1	R	63	ILE	N-CA-C	-5.05	105.61	110.72
1	S	127	ILE	CB-CA-C	-5.05	104.06	110.98
1	O	24	GLY	N-CA-C	-5.05	104.91	112.89
1	D	18	ARG	N-CA-C	5.05	125.13	111.00
1	O	124	VAL	N-CA-C	-5.05	105.62	110.72
1	E	42	LYS	N-CA-C	-5.04	106.96	113.01
1	T	9	GLY	CA-C-N	5.04	126.14	119.84
1	T	9	GLY	C-N-CA	5.04	126.14	119.84
1	V	126	VAL	CB-CA-C	-5.04	103.62	110.42
1	J	119	LEU	N-CA-C	5.03	119.41	113.12
1	L	128	CYS	CB-CA-C	5.03	117.37	110.94
1	J	44	ASN	N-CA-C	5.02	117.66	110.68
1	V	16	GLY	N-CA-C	-5.01	98.76	113.30
1	D	60	ILE	N-CA-C	-5.01	105.66	110.72
1	E	72	GLY	N-CA-C	5.01	124.33	115.61
1	G	14	LEU	CA-C-N	-5.01	113.08	121.39
1	G	14	LEU	C-N-CA	-5.01	113.08	121.39

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	45	ASP	Peptide
1	M	145	TYR	Peptide
1	V	145	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1108	0	1117	27	0
1	B	1108	0	1117	35	0
1	C	1108	0	1117	30	0
1	D	1117	0	1125	24	0
1	E	1125	0	1136	31	0
1	F	1125	0	1136	32	0
1	G	1108	0	1117	23	0
1	H	1116	0	1128	23	0
1	I	1142	0	1150	30	0
1	J	1108	0	1117	30	0
1	K	1116	0	1128	25	0
1	L	1116	0	1128	30	0
1	M	1116	0	1128	36	0
1	N	1116	0	1128	30	0
1	O	1116	0	1128	25	0
1	P	1116	0	1128	28	0
1	Q	1116	0	1128	32	0
1	R	1116	0	1128	27	0
1	S	1116	0	1128	35	0
1	T	1117	0	1125	42	0
1	U	1108	0	1117	34	0
1	V	1108	0	1117	29	0
1	W	1125	0	1136	38	0
1	X	1125	0	1136	29	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
2	U	5	0	0	0	0
2	V	5	0	0	0	0
2	W	5	0	0	0	0
2	X	5	0	0	0	0
3	A	8	0	12	0	0
3	D	8	0	12	1	0
3	G	8	0	12	0	0
3	J	8	0	12	0	0
3	N	8	0	12	1	0
3	P	8	0	12	1	0
3	T	8	0	12	0	0
3	W	8	0	12	1	0
4	A	8	0	0	0	0
4	B	13	0	0	2	0
4	C	7	0	0	1	0
4	D	7	0	0	1	0
4	E	17	0	0	1	0
4	F	10	0	0	0	0
4	G	9	0	0	0	0
4	H	4	0	0	0	0
4	I	11	0	0	1	0
4	J	4	0	0	0	0
4	K	5	0	0	0	0
4	L	4	0	0	0	0
4	M	4	0	0	0	0
4	N	11	0	0	0	0
4	O	2	0	0	0	0
4	P	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	7	0	0	0	0
4	R	13	0	0	0	0
4	S	4	0	0	1	0
4	T	3	0	0	0	0
4	U	5	0	0	0	0
4	V	5	0	0	1	0
4	W	5	0	0	0	0
4	X	2	0	0	0	0
All	All	27144	0	27139	681	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 (681) 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:J:12:LEU:O	1:J:15:LEU:HD22	1.54	1.07
1:N:146:GLN:HE21	1:N:146:GLN:HA	0.94	1.06
1:T:103:HIS:HB2	1:T:128:CYS:HB2	1.44	0.99
1:N:146:GLN:HA	1:N:146:GLN:NE2	1.68	0.98
1:W:103:HIS:HB2	1:W:128:CYS:HB2	1.46	0.98
1:V:12:LEU:O	1:V:15:LEU:HD22	1.66	0.96
1:M:12:LEU:O	1:M:15:LEU:HD22	1.66	0.96
1:N:146:GLN:HE21	1:N:146:GLN:CA	1.80	0.94
1:U:13:ASN:HD22	1:U:13:ASN:H	1.11	0.92
1:M:0:LEU:N	1:M:147:LEU:HG	1.84	0.91
1:U:15:LEU:HD22	1:U:15:LEU:H	1.36	0.90
1:U:103:HIS:HB2	1:U:128:CYS:HB2	1.54	0.90
1:R:12:LEU:O	1:R:15:LEU:HD22	1.71	0.89
1:W:12:LEU:O	1:W:15:LEU:HD22	1.70	0.89
1:X:12:LEU:O	1:X:15:LEU:CD2	2.21	0.88
1:I:103:HIS:HB2	1:I:128:CYS:HB2	1.54	0.88
1:S:12:LEU:O	1:S:15:LEU:HD22	1.74	0.87
1:K:12:LEU:O	1:K:15:LEU:HD22	1.75	0.87
1:P:12:LEU:O	1:P:15:LEU:HD22	1.76	0.86
1:Q:15:LEU:HD22	1:Q:15:LEU:H	1.38	0.86
1:T:12:LEU:O	1:T:15:LEU:HD22	1.76	0.86
1:F:12:LEU:O	1:F:15:LEU:HD22	1.74	0.86
1:S:23:TYR:O	1:S:23:TYR:CD2	2.30	0.83
1:M:103:HIS:HB2	1:M:128:CYS:HB2	1.61	0.83
1:T:12:LEU:O	1:T:15:LEU:CD2	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:TYR:CD2	1:H:23:TYR:O	2.32	0.82
1:G:24:GLY:O	1:G:26:THR:N	2.12	0.82
1:R:103:HIS:HB2	1:R:128:CYS:HB2	1.62	0.81
1:L:33:GLN:O	1:L:37:GLU:HG2	1.80	0.81
1:B:12:LEU:O	1:B:15:LEU:HD22	1.80	0.80
1:O:12:LEU:O	1:O:15:LEU:HD22	1.80	0.80
1:C:12:LEU:O	1:C:15:LEU:HD22	1.81	0.80
1:N:12:LEU:O	1:N:15:LEU:HD22	1.81	0.80
1:G:103:HIS:HB2	1:G:128:CYS:HB2	1.61	0.79
1:M:8:ASN:HD22	1:M:12:LEU:HD13	1.46	0.79
1:M:12:LEU:O	1:M:15:LEU:CD2	2.30	0.79
1:T:146:GLN:HA	1:T:146:GLN:NE2	1.98	0.79
1:C:24:GLY:O	1:C:26:THR:N	2.14	0.78
1:E:103:HIS:HB2	1:E:128:CYS:HB2	1.64	0.78
1:J:8:ASN:HD22	1:J:12:LEU:HD13	1.47	0.78
1:M:0:LEU:H2	1:M:147:LEU:HG	1.46	0.78
1:H:12:LEU:O	1:H:15:LEU:HD22	1.84	0.78
1:N:39:ALA:HB2	1:N:48:VAL:HG23	1.66	0.78
1:W:8:ASN:HD22	1:W:12:LEU:HD13	1.49	0.77
1:G:12:LEU:O	1:G:15:LEU:HD22	1.84	0.77
1:B:65:GLU:HG3	1:B:69:GLN:NE2	2.01	0.75
1:P:8:ASN:HD22	1:P:12:LEU:HD13	1.51	0.75
1:W:65:GLU:O	1:W:69:GLN:HG3	1.86	0.75
1:E:12:LEU:O	1:E:15:LEU:HD22	1.86	0.75
1:A:44:ASN:O	1:A:45:ASP:HB2	1.86	0.75
1:T:146:GLN:HA	1:T:146:GLN:HE21	1.49	0.74
1:X:12:LEU:O	1:X:15:LEU:HD22	1.85	0.74
1:D:103:HIS:HB2	1:D:128:CYS:HB2	1.68	0.74
1:L:12:LEU:O	1:L:15:LEU:HD22	1.88	0.74
1:M:116:GLN:HA	1:M:116:GLN:OE1	1.87	0.74
1:Q:12:LEU:O	1:Q:15:LEU:HD22	1.88	0.74
1:B:47:GLU:OE2	1:B:49:LEU:HD21	1.87	0.73
1:I:13:ASN:HD22	1:I:13:ASN:H	1.33	0.73
1:R:12:LEU:O	1:R:15:LEU:CD2	2.37	0.73
1:T:-1:GLN:OE1	1:T:-1:GLN:HA	1.89	0.73
1:I:13:ASN:H	1:I:13:ASN:ND2	1.86	0.73
1:J:12:LEU:O	1:J:15:LEU:CD2	2.34	0.72
1:Q:24:GLY:O	1:Q:26:THR:N	2.23	0.72
1:C:15:LEU:HD22	1:C:15:LEU:H	1.53	0.72
1:M:116:GLN:OE1	1:M:116:GLN:CA	2.37	0.72
1:V:12:LEU:O	1:V:15:LEU:CD2	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:HIS:HB2	1:J:128:CYS:HB2	1.70	0.71
1:U:13:ASN:H	1:U:13:ASN:ND2	1.85	0.71
1:J:23:TYR:CD2	1:J:23:TYR:O	2.44	0.71
1:G:65:GLU:O	1:G:69:GLN:HG3	1.90	0.70
1:S:62:ARG:HG3	1:S:62:ARG:HH11	1.57	0.70
1:D:12:LEU:O	1:D:15:LEU:HD22	1.90	0.70
1:A:8:ASN:HD22	1:A:12:LEU:HD13	1.56	0.70
1:B:12:LEU:O	1:B:15:LEU:CD2	2.40	0.69
1:U:12:LEU:O	1:U:15:LEU:HD22	1.91	0.69
1:B:23:TYR:O	1:B:23:TYR:CD1	2.47	0.68
1:K:8:ASN:ND2	1:K:135:TYR:OH	2.26	0.68
1:E:23:TYR:O	1:E:23:TYR:CD2	2.47	0.68
1:N:103:HIS:HB2	1:N:128:CYS:HB2	1.76	0.67
1:J:28:LEU:O	1:J:32:GLU:HG3	1.95	0.67
1:A:12:LEU:O	1:A:15:LEU:HD22	1.95	0.67
1:Q:15:LEU:HD22	1:Q:15:LEU:N	2.10	0.67
1:M:146:GLN:HA	1:M:146:GLN:NE2	2.09	0.66
1:F:8:ASN:O	1:F:52:GLN:HG2	1.95	0.66
1:F:103:HIS:HB2	1:F:128:CYS:HB2	1.77	0.66
1:H:65:GLU:OE1	1:H:65:GLU:HA	1.95	0.66
1:I:8:ASN:HD22	1:I:12:LEU:HD13	1.59	0.66
1:L:12:LEU:O	1:L:15:LEU:CD2	2.42	0.66
1:G:44:ASN:O	1:G:44:ASN:ND2	2.28	0.66
1:N:74:VAL:HG23	1:N:97:ILE:HG21	1.77	0.65
1:S:116:GLN:HE21	1:S:116:GLN:N	1.94	0.65
1:C:8:ASN:ND2	1:C:135:TYR:OH	2.30	0.65
1:V:23:TYR:CG	1:V:23:TYR:O	2.50	0.65
1:R:13:ASN:H	1:R:13:ASN:ND2	1.95	0.64
1:K:12:LEU:O	1:K:15:LEU:CD2	2.44	0.64
1:S:83:HIS:HD2	1:S:116:GLN:O	1.81	0.64
1:F:83:HIS:HD2	1:F:116:GLN:O	1.81	0.64
1:R:10:PRO:HG3	1:R:81:TYR:CE2	2.32	0.64
1:R:23:TYR:CG	1:R:23:TYR:O	2.50	0.64
1:V:103:HIS:HB2	1:V:128:CYS:HB2	1.80	0.64
1:X:93:LEU:HD21	1:X:122:LYS:HD2	1.81	0.63
1:N:39:ALA:CB	1:N:48:VAL:HG23	2.27	0.63
1:Q:13:ASN:H	1:Q:13:ASN:HD22	1.47	0.63
1:E:15:LEU:HD22	1:E:15:LEU:H	1.64	0.63
1:B:83:HIS:HE1	4:B:161:HOH:O	1.82	0.62
1:C:12:LEU:O	1:C:15:LEU:CD2	2.48	0.62
1:V:45:ASP:OD1	1:V:45:ASP:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:15:LEU:H	1:Q:15:LEU:CD2	2.12	0.62
1:Q:8:ASN:HD22	1:Q:12:LEU:HD13	1.64	0.62
1:Q:106:ASN:ND2	1:Q:108:HIS:H	1.96	0.62
1:L:51:PHE:CD1	1:L:62:ARG:HD3	2.35	0.62
1:B:83:HIS:HD2	1:B:116:GLN:O	1.83	0.62
1:O:8:ASN:ND2	1:O:135:TYR:OH	2.32	0.61
1:U:13:ASN:HD22	1:U:13:ASN:N	1.91	0.61
1:V:1:VAL:O	1:V:2:LYS:HD2	1.98	0.61
1:M:45:ASP:OD1	1:M:45:ASP:N	2.34	0.61
1:D:8:ASN:ND2	1:D:135:TYR:OH	2.32	0.61
1:X:103:HIS:HB2	1:X:128:CYS:HB2	1.81	0.61
1:D:24:GLY:O	1:D:26:THR:N	2.30	0.61
1:D:92:LEU:HD13	1:D:99:PHE:CD1	2.36	0.61
1:E:12:LEU:O	1:E:15:LEU:CD2	2.49	0.61
1:H:10:PRO:O	1:H:11:ASN:HB2	2.01	0.61
1:J:106:ASN:HD22	1:J:106:ASN:C	2.09	0.60
1:A:103:HIS:HB2	1:A:128:CYS:HB2	1.82	0.60
1:H:23:TYR:CD2	1:H:23:TYR:C	2.79	0.60
1:N:65:GLU:O	1:N:69:GLN:HG3	2.00	0.60
1:L:8:ASN:HD22	1:L:12:LEU:HD13	1.67	0.60
1:U:23:TYR:CG	1:U:23:TYR:O	2.55	0.60
1:L:62:ARG:HH11	1:L:62:ARG:HG3	1.67	0.60
1:D:146:GLN:HA	1:D:146:GLN:NE2	2.17	0.60
1:P:55:THR:OG1	1:R:57:GLY:HA3	2.01	0.60
1:D:23:TYR:O	1:D:23:TYR:CD2	2.54	0.59
1:R:13:ASN:H	1:R:13:ASN:HD22	1.48	0.59
1:P:116:GLN:OE1	1:P:116:GLN:HA	2.00	0.59
1:Q:15:LEU:N	1:Q:15:LEU:CD2	2.66	0.59
1:D:114:ARG:HD3	4:D:160:HOH:O	2.02	0.59
1:A:8:ASN:ND2	1:A:135:TYR:OH	2.33	0.59
1:A:28:LEU:O	1:A:32:GLU:HG3	2.03	0.59
1:F:15:LEU:HD22	1:F:15:LEU:H	1.67	0.59
1:U:15:LEU:H	1:U:15:LEU:CD2	2.13	0.59
1:U:15:LEU:CD2	1:U:15:LEU:N	2.65	0.59
1:B:33:GLN:HA	1:B:33:GLN:OE1	2.02	0.59
1:W:32:GLU:HB3	1:W:50:VAL:HG11	1.85	0.59
1:A:85:SER:OG	1:A:88:ILE:HG13	2.02	0.59
1:Q:12:LEU:O	1:Q:15:LEU:CD2	2.50	0.59
1:U:24:GLY:O	1:U:26:THR:N	2.35	0.59
1:W:3:LYS:HG2	1:W:71:VAL:HA	1.84	0.59
1:L:3:LYS:HE3	1:L:69:GLN:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:15:LEU:HD22	1:U:15:LEU:N	2.07	0.58
1:M:146:GLN:O	1:M:147:LEU:O	2.22	0.58
1:Q:106:ASN:HD22	1:Q:106:ASN:C	2.11	0.58
1:B:106:ASN:C	1:B:106:ASN:HD22	2.11	0.58
1:C:114:ARG:HD3	4:C:156:HOH:O	2.03	0.58
1:G:4:VAL:HB	1:G:48:VAL:HG22	1.86	0.58
1:L:15:LEU:HD22	1:L:15:LEU:H	1.66	0.58
1:P:73:PHE:CE1	1:P:100:ILE:HG13	2.38	0.58
1:P:12:LEU:O	1:P:15:LEU:CD2	2.50	0.57
1:M:128:CYS:O	1:S:125:ALA:HB1	2.04	0.57
1:T:93:LEU:HD21	1:T:122:LYS:HD2	1.85	0.57
1:H:8:ASN:ND2	1:H:135:TYR:OH	2.37	0.57
1:L:8:ASN:ND2	1:L:135:TYR:OH	2.37	0.57
1:T:-1:GLN:OE1	1:T:-1:GLN:CA	2.52	0.57
1:G:10:PRO:HG3	1:G:81:TYR:CE2	2.39	0.57
1:P:129:GLY:C	1:V:125:ALA:HB2	2.30	0.57
1:B:10:PRO:HG3	1:B:81:TYR:CE2	2.40	0.57
1:W:15:LEU:HD22	1:W:15:LEU:H	1.69	0.57
1:A:10:PRO:O	1:A:11:ASN:HB2	2.04	0.57
1:G:45:ASP:N	1:G:45:ASP:OD1	2.38	0.57
1:T:106:ASN:ND2	1:T:108:HIS:H	2.03	0.57
1:D:8:ASN:O	1:D:52:GLN:HG2	2.06	0.56
1:Q:65:GLU:O	1:Q:69:GLN:HG3	2.04	0.56
1:S:23:TYR:CD2	1:S:23:TYR:C	2.82	0.56
1:N:8:ASN:HD22	1:N:12:LEU:HD13	1.69	0.56
1:S:8:ASN:HB3	1:S:12:LEU:HD13	1.87	0.56
1:U:23:TYR:O	1:U:23:TYR:CD2	2.58	0.56
1:X:15:LEU:CD2	1:X:15:LEU:H	2.18	0.56
1:L:15:LEU:CD2	1:L:15:LEU:H	2.19	0.56
1:V:106:ASN:ND2	1:V:108:HIS:H	2.03	0.56
1:D:12:LEU:O	1:D:15:LEU:CD2	2.54	0.56
1:E:5:LEU:HD12	1:E:49:LEU:O	2.05	0.56
1:N:39:ALA:HB2	1:N:48:VAL:CG2	2.34	0.56
1:U:106:ASN:ND2	1:U:108:HIS:H	2.03	0.56
1:P:103:HIS:HB2	1:P:128:CYS:CB	2.36	0.56
1:P:73:PHE:HE1	1:P:100:ILE:HG13	1.71	0.56
1:Q:106:ASN:ND2	1:Q:106:ASN:C	2.63	0.56
1:T:83:HIS:HD2	1:T:116:GLN:O	1.88	0.55
1:A:69:GLN:HB3	1:N:17:THR:HG22	1.87	0.55
1:H:76:ILE:HG23	1:H:76:ILE:O	2.06	0.55
1:I:32:GLU:O	1:I:36:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:12:LEU:O	1:U:15:LEU:CD2	2.54	0.55
1:O:66:ALA:HA	1:O:69:GLN:HG3	1.89	0.55
1:P:10:PRO:O	1:P:11:ASN:HB2	2.07	0.55
1:Q:103:HIS:HB2	1:Q:128:CYS:HB2	1.89	0.55
1:A:127:ILE:HD11	1:G:130:LEU:HD11	1.89	0.54
1:K:13:ASN:HD22	1:K:13:ASN:H	1.55	0.54
1:R:92:LEU:HD13	1:R:99:PHE:CD1	2.42	0.54
1:E:8:ASN:O	1:E:52:GLN:HG2	2.08	0.54
1:F:103:HIS:HB2	1:F:128:CYS:CB	2.37	0.54
1:V:4:VAL:HB	1:V:48:VAL:HG22	1.87	0.54
1:W:67:LYS:NZ	1:W:95:THR:O	2.38	0.54
1:O:117:SER:HB3	1:O:120:SER:OG	2.07	0.54
1:S:51:PHE:CD1	1:S:62:ARG:HD3	2.42	0.54
1:N:56:GLU:OE1	3:N:156:TRS:H21	2.07	0.54
1:O:106:ASN:ND2	1:O:108:HIS:H	2.06	0.54
1:P:74:VAL:HG23	1:P:97:ILE:HG21	1.90	0.54
1:K:11:ASN:O	1:K:14:LEU:HB2	2.08	0.54
1:A:55:THR:OG1	1:C:57:GLY:HA3	2.08	0.54
1:K:4:VAL:HB	1:K:48:VAL:HG22	1.90	0.54
1:R:8:ASN:ND2	1:R:135:TYR:OH	2.41	0.54
1:H:8:ASN:O	1:H:52:GLN:HG2	2.08	0.53
1:I:4:VAL:HB	1:I:48:VAL:HG22	1.90	0.53
1:O:10:PRO:HA	1:O:54:ASN:OD1	2.07	0.53
1:P:103:HIS:HB2	1:P:128:CYS:HB2	1.89	0.53
1:T:8:ASN:HD22	1:T:12:LEU:HD13	1.73	0.53
1:N:14:LEU:O	1:N:17:THR:OG1	2.23	0.53
1:P:44:ASN:CG	1:P:44:ASN:O	2.50	0.53
1:V:47:GLU:OE2	1:V:49:LEU:HD21	2.07	0.53
1:O:58:PHE:N	1:O:58:PHE:CD1	2.73	0.53
1:J:106:ASN:C	1:J:106:ASN:ND2	2.67	0.53
1:R:15:LEU:HD22	1:R:15:LEU:H	1.72	0.53
1:V:106:ASN:HD22	1:V:106:ASN:C	2.16	0.53
1:I:7:ILE:HB	1:I:76:ILE:HG13	1.91	0.53
1:I:106:ASN:ND2	1:I:108:HIS:H	2.06	0.53
1:U:28:LEU:O	1:U:32:GLU:HG3	2.09	0.53
1:H:10:PRO:HA	1:H:54:ASN:OD1	2.09	0.53
1:M:146:GLN:HA	1:M:146:GLN:HE21	1.73	0.53
1:U:8:ASN:ND2	1:U:135:TYR:OH	2.42	0.53
1:R:115:HIS:N	1:R:115:HIS:CD2	2.76	0.53
1:R:15:LEU:HD23	1:R:15:LEU:O	2.08	0.53
1:J:23:TYR:O	1:J:23:TYR:CG	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:24:GLY:O	1:K:26:THR:N	2.37	0.52
1:I:8:ASN:ND2	1:I:77:ASN:HB3	2.24	0.52
1:U:106:ASN:O	1:U:109:GLN:HB2	2.09	0.52
1:C:1:VAL:HG23	1:C:145:TYR:O	2.09	0.52
1:F:13:ASN:HD22	1:F:13:ASN:H	1.58	0.52
1:F:74:VAL:HG23	1:F:97:ILE:HG21	1.92	0.52
1:G:83:HIS:HD2	1:G:116:GLN:O	1.93	0.52
1:S:93:LEU:HD11	1:S:122:LYS:HG3	1.91	0.52
1:D:23:TYR:CD2	1:D:23:TYR:C	2.87	0.52
1:D:57:GLY:HA3	1:E:55:THR:OG1	2.10	0.52
1:N:115:HIS:N	1:N:115:HIS:CD2	2.77	0.52
1:Q:32:GLU:HG2	1:Q:50:VAL:HG21	1.92	0.52
1:C:44:ASN:O	1:C:45:ASP:HB2	2.10	0.52
1:O:106:ASN:C	1:O:106:ASN:HD22	2.17	0.52
1:W:28:LEU:O	1:W:32:GLU:HG3	2.09	0.52
1:E:98:PRO:HA	4:E:158:HOH:O	2.10	0.52
1:B:106:ASN:ND2	1:B:108:HIS:H	2.08	0.51
1:G:80:ALA:HB1	1:I:86:VAL:HG12	1.92	0.51
1:T:101:GLU:HB3	1:T:126:VAL:HG13	1.91	0.51
1:U:67:LYS:HD3	1:U:95:THR:O	2.10	0.51
1:Q:8:ASN:O	1:Q:52:GLN:HG2	2.11	0.51
1:J:106:ASN:ND2	1:J:108:HIS:H	2.09	0.51
1:K:103:HIS:HB2	1:K:128:CYS:HB2	1.91	0.51
1:M:10:PRO:O	1:M:11:ASN:HB2	2.10	0.51
1:T:96:ALA:HB2	1:U:18:ARG:HD3	1.93	0.51
1:C:106:ASN:C	1:C:106:ASN:HD22	2.18	0.51
1:E:106:ASN:ND2	1:E:108:HIS:H	2.09	0.51
1:J:112:PRO:HA	1:J:115:HIS:CE1	2.46	0.51
1:W:95:THR:OG1	1:W:97:ILE:HD12	2.11	0.51
1:C:103:HIS:HB2	1:C:128:CYS:HB2	1.93	0.51
1:G:8:ASN:O	1:G:52:GLN:HG2	2.11	0.51
1:P:8:ASN:ND2	1:P:12:LEU:HD13	2.23	0.51
1:S:12:LEU:O	1:S:15:LEU:CD2	2.54	0.51
1:W:65:GLU:HA	1:W:68:ARG:NH2	2.26	0.51
1:R:15:LEU:CD2	1:R:15:LEU:N	2.73	0.51
1:S:115:HIS:C	1:S:116:GLN:HE21	2.19	0.51
1:M:8:ASN:O	1:M:52:GLN:HA	2.11	0.50
1:F:12:LEU:O	1:F:15:LEU:CD2	2.54	0.50
1:O:100:ILE:HD11	1:O:141:TYR:CD1	2.46	0.50
1:G:8:ASN:ND2	1:G:135:TYR:OH	2.41	0.50
1:L:8:ASN:ND2	1:L:77:ASN:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:73:PHE:CE1	1:T:100:ILE:HG13	2.46	0.50
1:C:4:VAL:HB	1:C:48:VAL:HG22	1.92	0.50
1:B:65:GLU:OE2	1:N:68:ARG:NH2	2.44	0.50
1:O:1:VAL:HG23	1:O:145:TYR:O	2.12	0.50
1:B:17:THR:HG21	1:M:68:ARG:HB2	1.93	0.50
1:L:3:LYS:HB3	1:L:71:VAL:HA	1.93	0.50
1:T:23:TYR:CD2	1:T:23:TYR:O	2.65	0.50
1:A:68:ARG:HB3	1:N:17:THR:HG21	1.94	0.50
1:N:58:PHE:N	1:N:58:PHE:CD1	2.79	0.50
1:R:23:TYR:O	1:R:23:TYR:CD1	2.65	0.50
1:V:15:LEU:CD2	1:V:15:LEU:H	2.25	0.50
1:T:73:PHE:HE1	1:T:100:ILE:HG13	1.77	0.50
1:A:93:LEU:HD21	1:A:122:LYS:HD2	1.94	0.49
1:E:4:VAL:HB	1:E:48:VAL:HG22	1.94	0.49
1:H:93:LEU:HD21	1:H:122:LYS:HD2	1.93	0.49
1:P:96:ALA:HB2	1:Q:18:ARG:HD3	1.93	0.49
1:A:106:ASN:C	1:A:106:ASN:HD22	2.19	0.49
1:E:10:PRO:HG3	1:E:81:TYR:CE2	2.48	0.49
1:F:15:LEU:H	1:F:15:LEU:CD2	2.25	0.49
1:I:74:VAL:O	1:I:99:PHE:HA	2.12	0.49
1:J:42:LYS:O	1:J:43:ASN:CB	2.60	0.49
1:H:103:HIS:HB2	1:H:128:CYS:HB2	1.94	0.49
1:M:10:PRO:HD2	1:M:78:ALA:O	2.12	0.49
1:C:106:ASN:ND2	1:C:108:HIS:H	2.10	0.49
1:H:57:GLY:HA3	1:I:55:THR:OG1	2.11	0.49
1:J:57:GLY:HA3	1:K:55:THR:OG1	2.13	0.49
1:U:13:ASN:ND2	1:U:13:ASN:N	2.53	0.49
1:W:8:ASN:O	1:W:52:GLN:HG2	2.12	0.49
1:I:93:LEU:HD21	1:I:122:LYS:HD2	1.94	0.49
1:P:116:GLN:OE1	1:P:116:GLN:CA	2.59	0.49
1:B:8:ASN:O	1:B:52:GLN:HG2	2.11	0.49
1:B:41:LEU:O	1:B:41:LEU:HG	2.12	0.49
1:M:8:ASN:O	1:M:52:GLN:HG2	2.13	0.49
1:O:51:PHE:CG	1:O:62:ARG:HG2	2.48	0.49
1:V:8:ASN:HD22	1:V:12:LEU:HD13	1.77	0.49
1:X:23:TYR:O	1:X:23:TYR:CD2	2.66	0.49
1:X:39:ALA:O	1:X:40:LYS:C	2.56	0.49
1:O:117:SER:CB	1:O:120:SER:OG	2.61	0.49
1:R:8:ASN:HD22	1:R:12:LEU:HD13	1.78	0.49
1:S:2:LYS:HE2	1:S:44:ASN:HD22	1.78	0.49
1:G:80:ALA:CB	1:I:86:VAL:HG12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:C	1:A:106:ASN:ND2	2.70	0.48
1:N:49:LEU:N	1:N:49:LEU:HD23	2.28	0.48
1:V:63:ILE:O	1:V:66:ALA:HB3	2.13	0.48
1:J:12:LEU:C	1:J:14:LEU:H	2.21	0.48
1:M:74:VAL:O	1:M:99:PHE:HA	2.13	0.48
1:D:18:ARG:HD3	1:F:96:ALA:HB2	1.94	0.48
1:F:8:ASN:HD22	1:F:12:LEU:HD13	1.78	0.48
1:K:76:ILE:O	1:K:76:ILE:HG23	2.13	0.48
1:M:89:ARG:NH1	1:N:111:GLU:OE2	2.47	0.48
1:W:12:LEU:O	1:W:14:LEU:N	2.46	0.48
1:E:8:ASN:ND2	1:E:135:TYR:OH	2.46	0.48
1:F:62:ARG:NH2	1:F:69:GLN:OE1	2.39	0.48
1:M:24:GLY:O	1:M:26:THR:N	2.46	0.48
1:W:106:ASN:ND2	1:W:108:HIS:H	2.10	0.48
1:N:146:GLN:NE2	1:N:146:GLN:CA	2.50	0.48
1:T:89:ARG:NH1	1:U:111:GLU:OE2	2.47	0.48
1:H:12:LEU:O	1:H:15:LEU:CD2	2.59	0.48
1:M:15:LEU:CD2	1:M:15:LEU:H	2.27	0.48
1:R:15:LEU:CD2	1:R:15:LEU:H	2.26	0.48
1:F:13:ASN:HD22	1:F:13:ASN:N	2.12	0.48
1:N:8:ASN:ND2	1:N:135:TYR:OH	2.44	0.48
1:S:23:TYR:O	1:S:23:TYR:HD2	1.92	0.48
1:L:67:LYS:HD3	1:L:95:THR:O	2.14	0.48
1:W:58:PHE:N	1:W:58:PHE:CD1	2.81	0.48
1:A:44:ASN:C	1:A:44:ASN:OD1	2.56	0.48
1:B:99:PHE:CE2	1:B:123:ALA:HB2	2.48	0.48
1:B:106:ASN:C	1:B:106:ASN:ND2	2.70	0.48
1:E:65:GLU:O	1:E:69:GLN:HG3	2.14	0.48
1:G:43:ASN:CG	1:G:43:ASN:O	2.57	0.48
1:V:15:LEU:HD22	1:V:15:LEU:H	1.79	0.48
1:B:8:ASN:ND2	1:B:135:TYR:OH	2.44	0.47
1:C:13:ASN:H	1:C:13:ASN:HD22	1.60	0.47
1:F:15:LEU:CD2	1:F:15:LEU:N	2.77	0.47
1:K:112:PRO:HA	1:K:115:HIS:CD2	2.49	0.47
1:S:8:ASN:ND2	1:S:135:TYR:OH	2.47	0.47
1:T:37:GLU:OE1	1:T:37:GLU:HA	2.14	0.47
1:C:32:GLU:O	1:C:36:ILE:HG13	2.14	0.47
1:J:12:LEU:HD23	1:J:15:LEU:HD13	1.96	0.47
1:C:15:LEU:H	1:C:15:LEU:CD2	2.23	0.47
1:N:12:LEU:C	1:N:14:LEU:H	2.21	0.47
1:T:106:ASN:C	1:T:106:ASN:HD22	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:10:PRO:HA	1:P:54:ASN:OD1	2.15	0.47
1:C:28:LEU:O	1:C:32:GLU:HG3	2.15	0.47
1:M:103:HIS:HB2	1:M:128:CYS:CB	2.38	0.47
1:D:10:PRO:O	1:D:11:ASN:HB2	2.14	0.47
1:J:13:ASN:HD21	1:L:64:HIS:HE1	1.62	0.47
1:J:64:HIS:HE1	1:K:13:ASN:HD21	1.62	0.47
1:J:67:LYS:HG3	1:J:95:THR:HB	1.96	0.47
1:P:8:ASN:O	1:P:52:GLN:HA	2.14	0.47
1:V:115:HIS:N	1:V:115:HIS:CD2	2.82	0.47
1:A:77:ASN:OD1	1:A:77:ASN:C	2.57	0.47
1:D:146:GLN:NE2	1:D:146:GLN:CA	2.77	0.47
1:G:77:ASN:C	1:G:77:ASN:OD1	2.57	0.47
1:S:2:LYS:HE2	1:S:44:ASN:ND2	2.30	0.47
1:S:74:VAL:HG23	1:S:97:ILE:HG21	1.96	0.47
1:X:1:VAL:C	1:X:2:LYS:HG2	2.40	0.47
1:Q:3:LYS:HG2	1:Q:71:VAL:HA	1.97	0.47
1:T:8:ASN:ND2	1:T:77:ASN:HB3	2.29	0.47
1:J:10:PRO:HA	1:J:54:ASN:OD1	2.15	0.47
1:J:11:ASN:O	1:J:14:LEU:HB2	2.15	0.47
1:K:15:LEU:HA	1:K:16:GLY:HA2	1.78	0.47
1:M:8:ASN:ND2	1:M:135:TYR:OH	2.42	0.47
1:M:65:GLU:O	1:M:69:GLN:HG3	2.14	0.47
1:P:32:GLU:HG2	1:P:50:VAL:HG11	1.97	0.47
1:W:15:LEU:O	1:W:27:SER:HA	2.15	0.47
1:W:106:ASN:C	1:W:106:ASN:HD22	2.23	0.47
1:N:51:PHE:CG	1:N:62:ARG:HG2	2.50	0.46
1:T:23:TYR:CD2	1:T:23:TYR:C	2.92	0.46
1:C:106:ASN:C	1:C:106:ASN:ND2	2.72	0.46
1:D:32:GLU:O	1:D:36:ILE:HD12	2.15	0.46
1:S:62:ARG:HG3	1:S:62:ARG:NH1	2.26	0.46
1:X:65:GLU:O	1:X:69:GLN:HG3	2.16	0.46
1:B:23:TYR:O	1:B:23:TYR:CG	2.68	0.46
1:L:24:GLY:O	1:L:26:THR:N	2.44	0.46
1:M:0:LEU:H1	1:M:147:LEU:HG	1.77	0.46
1:T:66:ALA:HB1	1:T:71:VAL:HB	1.98	0.46
1:T:74:VAL:HG23	1:T:97:ILE:HG21	1.98	0.46
1:T:106:ASN:ND2	1:T:106:ASN:C	2.73	0.46
1:V:35:ALA:HB1	1:V:48:VAL:HG11	1.97	0.46
1:W:57:GLY:HA3	1:X:55:THR:OG1	2.16	0.46
1:I:22:LYS:NZ	4:I:158:HOH:O	2.48	0.46
1:K:13:ASN:H	1:K:13:ASN:ND2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:8:ASN:O	1:N:52:GLN:HA	2.16	0.46
1:S:10:PRO:HA	1:S:54:ASN:OD1	2.15	0.46
1:V:58:PHE:CD1	1:V:58:PHE:N	2.83	0.46
1:X:115:HIS:N	1:X:115:HIS:CD2	2.83	0.46
1:A:32:GLU:O	1:A:36:ILE:HG13	2.16	0.46
1:D:23:TYR:O	1:D:23:TYR:CG	2.69	0.46
1:K:93:LEU:HD21	1:K:122:LYS:HD2	1.97	0.46
1:Q:10:PRO:HD2	1:Q:78:ALA:O	2.15	0.46
1:Q:44:ASN:O	1:Q:45:ASP:HB2	2.16	0.46
1:S:15:LEU:HA	1:S:16:GLY:HA2	1.68	0.46
1:I:8:ASN:O	1:I:52:GLN:HA	2.16	0.46
1:U:33:GLN:O	1:U:37:GLU:HG2	2.15	0.46
1:P:8:ASN:O	1:P:52:GLN:HG2	2.16	0.46
1:V:106:ASN:ND2	1:V:106:ASN:C	2.74	0.46
1:B:57:GLY:HA3	1:C:55:THR:OG1	2.16	0.46
1:C:15:LEU:CD2	1:C:15:LEU:N	2.78	0.46
1:C:42:LYS:O	1:C:43:ASN:HB3	2.14	0.46
1:H:26:THR:HG21	1:H:132:VAL:HG11	1.97	0.46
1:J:13:ASN:H	1:J:13:ASN:HD22	1.64	0.46
1:O:8:ASN:O	1:O:52:GLN:HA	2.16	0.46
1:W:83:HIS:HD2	1:W:116:GLN:O	1.99	0.46
1:U:100:ILE:HD11	1:U:141:TYR:CD1	2.51	0.46
1:J:15:LEU:HA	1:J:16:GLY:HA2	1.68	0.45
1:X:13:ASN:HA	1:X:28:LEU:CD2	2.47	0.45
1:Q:15:LEU:O	1:Q:15:LEU:HD23	2.16	0.45
1:R:35:ALA:HB1	1:R:139:ILE:HD13	1.97	0.45
1:S:3:LYS:HB3	1:S:71:VAL:HA	1.98	0.45
1:R:10:PRO:HG3	1:R:81:TYR:CZ	2.51	0.45
1:F:39:ALA:O	1:F:40:LYS:C	2.58	0.45
1:G:115:HIS:CD2	1:G:115:HIS:N	2.85	0.45
1:S:67:LYS:HB2	1:S:95:THR:HB	1.99	0.45
1:U:89:ARG:NH2	1:U:121:ASP:OD1	2.49	0.45
1:F:106:ASN:C	1:F:106:ASN:HD22	2.24	0.45
1:G:103:HIS:HB2	1:G:128:CYS:CB	2.39	0.45
1:P:65:GLU:HG3	1:P:69:GLN:HE22	1.80	0.45
1:W:15:LEU:HA	1:W:16:GLY:HA2	1.55	0.45
1:X:74:VAL:HG23	1:X:97:ILE:HG21	1.98	0.45
1:E:15:LEU:H	1:E:15:LEU:CD2	2.28	0.45
1:K:64:HIS:CE1	1:L:13:ASN:HD21	2.35	0.45
1:K:106:ASN:C	1:K:106:ASN:ND2	2.74	0.45
1:P:15:LEU:HA	1:P:16:GLY:HA2	1.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:51:PHE:CD1	1:T:62:ARG:HD3	2.51	0.45
1:A:101:GLU:HB3	1:A:126:VAL:HG13	1.98	0.45
1:B:103:HIS:HB2	1:B:128:CYS:HB2	1.99	0.45
1:D:89:ARG:NH2	1:D:121:ASP:OD1	2.49	0.45
1:I:2:LYS:HA	1:I:2:LYS:HD2	1.69	0.45
1:I:109:GLN:HE21	1:I:109:GLN:HB2	1.46	0.45
1:U:8:ASN:O	1:U:52:GLN:HA	2.16	0.45
1:A:114:ARG:NH2	1:C:90:ASP:OD1	2.50	0.45
1:B:77:ASN:C	1:B:77:ASN:OD1	2.60	0.45
1:N:3:LYS:HG2	1:N:71:VAL:HA	1.99	0.45
1:Q:33:GLN:O	1:Q:37:GLU:HG2	2.17	0.45
1:T:62:ARG:HG3	1:T:62:ARG:HH11	1.82	0.45
1:T:117:SER:HB3	1:T:120:SER:OG	2.17	0.45
1:X:13:ASN:HA	1:X:28:LEU:HD22	1.97	0.45
1:E:23:TYR:O	1:E:23:TYR:CG	2.70	0.45
1:J:67:LYS:HE3	1:J:95:THR:O	2.17	0.45
1:N:3:LYS:CG	1:N:71:VAL:HA	2.47	0.45
1:O:31:ILE:HG12	1:O:132:VAL:HG22	1.98	0.44
1:V:142:ALA:C	1:V:144:ASN:H	2.25	0.44
1:E:39:ALA:O	1:E:40:LYS:C	2.61	0.44
1:F:10:PRO:HG3	1:F:81:TYR:CE2	2.51	0.44
1:D:58:PHE:N	1:D:58:PHE:CD1	2.83	0.44
1:T:146:GLN:NE2	1:T:146:GLN:CA	2.77	0.44
1:U:106:ASN:C	1:U:106:ASN:HD22	2.24	0.44
1:A:119:LEU:O	1:A:120:SER:C	2.59	0.44
1:I:13:ASN:ND2	1:I:13:ASN:N	2.57	0.44
1:A:115:HIS:CD2	1:A:115:HIS:N	2.84	0.44
1:H:31:ILE:HD13	1:H:135:TYR:CE2	2.53	0.44
1:K:112:PRO:O	1:K:113:PHE:C	2.58	0.44
1:M:55:THR:OG1	1:O:57:GLY:HA3	2.18	0.44
1:O:15:LEU:HA	1:O:16:GLY:HA2	1.78	0.44
1:O:106:ASN:ND2	1:O:106:ASN:C	2.74	0.44
1:P:8:ASN:ND2	1:P:135:TYR:OH	2.44	0.44
1:U:6:LEU:HD12	1:U:75:VAL:O	2.17	0.44
1:B:65:GLU:HG3	1:B:69:GLN:HE22	1.82	0.44
1:E:15:LEU:HA	1:E:16:GLY:HA2	1.78	0.44
1:S:93:LEU:HD21	1:S:122:LYS:HD2	2.00	0.44
1:W:55:THR:HG22	1:W:58:PHE:H	1.82	0.44
3:W:156:TRS:N	1:X:56:GLU:OE1	2.44	0.44
1:C:55:THR:HB	1:C:58:PHE:CD2	2.52	0.44
1:D:121:ASP:O	1:J:109:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:LEU:HD13	1:F:99:PHE:CD1	2.53	0.44
1:T:103:HIS:HB2	1:T:128:CYS:CB	2.31	0.44
1:T:129:GLY:C	1:W:125:ALA:HB2	2.43	0.44
1:V:83:HIS:HD2	1:V:116:GLN:O	2.00	0.44
1:W:103:HIS:HB2	1:W:128:CYS:CB	2.34	0.44
1:B:15:LEU:HD11	1:B:104:ILE:CD1	2.48	0.44
1:C:23:TYR:CD2	1:C:23:TYR:O	2.71	0.44
1:E:8:ASN:ND2	1:E:77:ASN:HB3	2.33	0.44
1:F:15:LEU:HA	1:F:16:GLY:HA2	1.72	0.44
1:R:51:PHE:CD1	1:R:62:ARG:HD3	2.53	0.44
1:X:15:LEU:HA	1:X:16:GLY:HA2	1.74	0.44
1:F:106:ASN:ND2	1:F:108:HIS:H	2.16	0.44
1:G:28:LEU:O	1:G:32:GLU:HG3	2.18	0.44
1:G:60:ILE:HG23	1:G:91:ALA:HB2	2.00	0.44
1:H:65:GLU:OE1	1:H:65:GLU:CA	2.66	0.44
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.89	0.43
1:F:10:PRO:HD2	1:F:78:ALA:O	2.18	0.43
1:F:60:ILE:HG23	1:F:91:ALA:HB2	2.00	0.43
1:I:12:LEU:HD22	1:I:15:LEU:HD11	1.99	0.43
1:S:63:ILE:HD13	1:S:92:LEU:HG	1.99	0.43
1:W:15:LEU:H	1:W:15:LEU:CD2	2.31	0.43
1:C:93:LEU:HD11	1:C:122:LYS:HG3	2.00	0.43
1:L:2:LYS:HD2	1:L:2:LYS:HA	1.50	0.43
1:M:111:GLU:OE2	1:O:89:ARG:NH1	2.51	0.43
3:P:156:TRS:N	1:R:56:GLU:OE1	2.45	0.43
1:Q:51:PHE:CD1	1:Q:62:ARG:HD3	2.53	0.43
1:V:8:ASN:ND2	1:V:77:ASN:HB3	2.33	0.43
1:E:32:GLU:HB3	1:E:50:VAL:HG11	2.00	0.43
1:F:106:ASN:C	1:F:106:ASN:ND2	2.77	0.43
1:G:8:ASN:HD22	1:G:12:LEU:HD13	1.82	0.43
1:W:23:TYR:O	1:W:23:TYR:CD2	2.71	0.43
1:C:100:ILE:HD11	1:C:141:TYR:CD1	2.53	0.43
1:E:29:SER:HA	1:E:32:GLU:HG3	1.98	0.43
1:J:10:PRO:O	1:J:11:ASN:HB2	2.19	0.43
1:K:3:LYS:HG2	1:K:71:VAL:HA	1.99	0.43
1:M:146:GLN:NE2	1:M:146:GLN:CA	2.79	0.43
1:T:8:ASN:O	1:T:52:GLN:HA	2.18	0.43
1:X:15:LEU:CD2	1:X:15:LEU:N	2.80	0.43
1:X:44:ASN:O	1:X:45:ASP:HB2	2.18	0.43
1:O:89:ARG:HH11	1:O:89:ARG:HD3	1.67	0.43
1:D:112:PRO:HA	1:D:115:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LYS:O	1:E:43:ASN:C	2.61	0.43
1:H:39:ALA:O	1:H:40:LYS:C	2.61	0.43
1:I:113:PHE:CE1	1:I:114:ARG:HG2	2.54	0.43
1:N:106:ASN:O	1:N:109:GLN:HB2	2.17	0.43
1:P:65:GLU:HG3	1:P:69:GLN:NE2	2.34	0.43
1:Q:107:VAL:C	1:Q:109:GLN:H	2.25	0.43
1:B:37:GLU:O	1:B:38:GLN:C	2.62	0.43
1:D:26:THR:HG21	1:D:132:VAL:HG21	2.00	0.43
1:I:81:TYR:HB3	1:I:85:SER:HB2	2.01	0.43
1:O:10:PRO:HD3	1:O:81:TYR:CD2	2.54	0.43
1:Q:86:VAL:HG12	1:R:80:ALA:HB1	2.00	0.43
1:V:132:VAL:HG22	4:V:158:HOH:O	2.18	0.43
1:W:100:ILE:HG23	1:W:125:ALA:O	2.19	0.43
1:B:10:PRO:HA	1:B:54:ASN:OD1	2.19	0.43
1:B:106:ASN:O	1:B:109:GLN:HB2	2.18	0.43
1:H:109:GLN:HG3	1:K:121:ASP:O	2.18	0.43
1:L:15:LEU:HA	1:L:16:GLY:HA2	1.66	0.43
1:M:39:ALA:O	1:M:40:LYS:C	2.61	0.43
1:R:8:ASN:O	1:R:52:GLN:HA	2.19	0.43
1:E:106:ASN:ND2	1:E:106:ASN:C	2.76	0.43
1:L:100:ILE:HD11	1:L:141:TYR:CD1	2.54	0.43
1:S:15:LEU:HD22	1:S:15:LEU:H	1.84	0.43
1:W:8:ASN:O	1:W:52:GLN:HA	2.19	0.43
1:J:111:GLU:OE2	1:L:89:ARG:NH1	2.51	0.42
1:L:121:ASP:OD1	1:L:121:ASP:N	2.51	0.42
1:M:115:HIS:CD2	1:M:115:HIS:N	2.87	0.42
1:O:27:SER:O	1:O:30:ASP:HB2	2.19	0.42
1:E:101:GLU:HB3	1:E:126:VAL:HG13	2.00	0.42
1:K:57:GLY:HA3	1:L:55:THR:OG1	2.19	0.42
1:E:23:TYR:CD2	1:E:23:TYR:C	2.97	0.42
1:H:58:PHE:N	1:H:58:PHE:CD1	2.87	0.42
1:I:12:LEU:CD2	1:I:15:LEU:HD11	2.49	0.42
1:K:28:LEU:O	1:K:32:GLU:HG3	2.20	0.42
1:K:108:HIS:HA	1:K:115:HIS:CE1	2.54	0.42
1:T:15:LEU:HA	1:T:16:GLY:HA2	1.72	0.42
1:T:75:VAL:HG21	1:T:139:ILE:HD13	2.00	0.42
1:V:15:LEU:HA	1:V:16:GLY:HA2	1.69	0.42
1:V:28:LEU:O	1:V:32:GLU:HG3	2.19	0.42
1:W:74:VAL:HG23	1:W:97:ILE:HG21	2.00	0.42
1:X:15:LEU:HD22	1:X:15:LEU:H	1.83	0.42
1:X:15:LEU:H	1:X:15:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD21	1:B:122:LYS:HD2	2.00	0.42
1:F:8:ASN:ND2	1:F:135:TYR:OH	2.48	0.42
1:T:8:ASN:ND2	1:T:135:TYR:OH	2.48	0.42
1:A:55:THR:O	1:A:56:GLU:C	2.61	0.42
1:A:66:ALA:HB1	1:A:71:VAL:HG21	2.02	0.42
3:D:156:TRS:H22	1:E:84:THR:HB	2.01	0.42
1:F:15:LEU:HD23	1:F:15:LEU:O	2.20	0.42
1:J:4:VAL:HB	1:J:48:VAL:HG22	2.01	0.42
1:K:75:VAL:HG21	1:K:139:ILE:HG13	2.01	0.42
1:P:64:HIS:CE1	1:Q:13:ASN:HD21	2.38	0.42
1:R:35:ALA:HB1	1:R:139:ILE:CD1	2.49	0.42
1:G:109:GLN:HE21	1:G:109:GLN:HB2	1.60	0.42
1:I:143:LEU:HD23	1:I:143:LEU:HA	1.80	0.42
1:M:89:ARG:NH2	1:M:121:ASP:OD2	2.53	0.42
1:Q:2:LYS:HD2	1:Q:3:LYS:HB2	2.01	0.42
1:S:111:GLU:HA	1:S:112:PRO:HD2	1.78	0.42
1:S:117:SER:HB3	1:S:120:SER:OG	2.20	0.42
1:X:7:ILE:O	1:X:76:ILE:HA	2.20	0.42
1:C:8:ASN:O	1:C:52:GLN:HA	2.20	0.42
1:C:8:ASN:O	1:C:52:GLN:HG2	2.20	0.42
1:D:91:ALA:HB2	1:E:11:ASN:OD1	2.20	0.42
1:E:8:ASN:HD22	1:E:12:LEU:HD13	1.85	0.42
4:S:156:HOH:O	1:U:93:LEU:HD13	2.19	0.42
1:X:83:HIS:CD2	1:X:114:ARG:HA	2.55	0.42
1:E:41:LEU:C	1:E:43:ASN:H	2.27	0.42
1:M:40:LYS:HE2	1:M:40:LYS:HB3	1.95	0.42
1:A:23:TYR:O	1:A:23:TYR:CG	2.72	0.42
1:F:93:LEU:HD21	1:F:122:LYS:HD2	2.02	0.42
1:J:12:LEU:C	1:J:14:LEU:N	2.78	0.42
1:U:39:ALA:HB2	1:U:48:VAL:HG23	2.01	0.42
1:L:15:LEU:CD2	1:L:15:LEU:N	2.81	0.42
1:B:13:ASN:HA	1:B:28:LEU:HD22	2.02	0.41
1:G:107:VAL:HG22	1:G:114:ARG:HB3	2.02	0.41
1:M:15:LEU:HA	1:M:16:GLY:HA2	1.75	0.41
1:W:8:ASN:ND2	1:W:77:ASN:HB3	2.34	0.41
1:X:8:ASN:ND2	1:X:135:TYR:OH	2.49	0.41
1:E:106:ASN:C	1:E:106:ASN:HD22	2.27	0.41
1:F:10:PRO:HG3	1:F:81:TYR:CZ	2.55	0.41
1:W:0:LEU:CD1	1:W:0:LEU:N	2.83	0.41
1:W:23:TYR:CD2	1:W:23:TYR:C	2.98	0.41
1:W:108:HIS:HA	1:W:115:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:26:THR:HG21	1:Q:132:VAL:HG21	2.01	0.41
1:T:8:ASN:O	1:T:52:GLN:HG2	2.20	0.41
1:W:119:LEU:O	1:W:120:SER:C	2.63	0.41
1:P:24:GLY:C	1:P:26:THR:H	2.28	0.41
1:Q:55:THR:O	1:Q:56:GLU:C	2.63	0.41
1:R:3:LYS:HB3	1:R:71:VAL:HA	2.01	0.41
1:W:143:LEU:HA	1:W:143:LEU:HD23	1.85	0.41
1:B:88:ILE:O	1:B:89:ARG:C	2.63	0.41
1:B:114:ARG:HD3	4:B:161:HOH:O	2.19	0.41
1:H:74:VAL:O	1:H:99:PHE:HA	2.20	0.41
1:J:114:ARG:NH2	1:L:90:ASP:OD1	2.53	0.41
1:M:92:LEU:HD13	1:M:99:PHE:CD1	2.56	0.41
1:O:119:LEU:O	1:O:120:SER:C	2.63	0.41
1:O:146:GLN:H	1:O:146:GLN:HG2	1.49	0.41
1:Q:107:VAL:C	1:Q:109:GLN:N	2.79	0.41
1:S:11:ASN:O	1:S:14:LEU:HB2	2.20	0.41
1:S:119:LEU:O	1:S:120:SER:C	2.62	0.41
1:T:57:GLY:HA3	1:U:55:THR:OG1	2.20	0.41
1:U:113:PHE:CE1	1:U:114:ARG:HG2	2.55	0.41
1:X:32:GLU:O	1:X:36:ILE:HD12	2.20	0.41
1:B:73:PHE:CE1	1:B:100:ILE:HG13	2.56	0.41
1:F:13:ASN:N	1:F:13:ASN:ND2	2.69	0.41
1:Q:106:ASN:O	1:Q:109:GLN:HB2	2.21	0.41
1:T:125:ALA:HB2	1:W:129:GLY:C	2.46	0.41
1:U:1:VAL:HG11	1:U:73:PHE:HB2	2.02	0.41
1:C:0:LEU:HD22	1:C:0:LEU:HA	1.91	0.41
1:E:10:PRO:O	1:E:11:ASN:HB2	2.21	0.41
1:L:65:GLU:O	1:L:69:GLN:HB2	2.20	0.41
1:Q:15:LEU:HA	1:Q:16:GLY:HA2	1.67	0.41
1:S:44:ASN:O	1:S:45:ASP:C	2.64	0.41
1:D:8:ASN:ND2	1:D:77:ASN:HB3	2.35	0.41
1:I:130:LEU:HD12	1:I:130:LEU:HA	1.92	0.41
1:L:8:ASN:O	1:L:52:GLN:HA	2.21	0.41
1:L:12:LEU:HD23	1:L:12:LEU:HA	1.94	0.41
1:M:26:THR:HG21	1:M:132:VAL:HG21	2.02	0.41
1:N:32:GLU:HG2	1:N:50:VAL:HB	2.03	0.41
1:U:10:PRO:HA	1:U:54:ASN:OD1	2.21	0.41
1:U:15:LEU:HA	1:U:16:GLY:HA2	1.64	0.41
1:V:119:LEU:HA	1:V:119:LEU:HD23	1.76	0.41
1:H:82:THR:HG21	1:H:101:GLU:OE2	2.21	0.41
1:I:66:ALA:HA	1:I:69:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:40:LYS:C	1:L:42:LYS:H	2.29	0.41
1:N:27:SER:O	1:N:30:ASP:HB2	2.20	0.41
1:S:64:HIS:CE1	1:T:54:ASN:HD21	2.39	0.41
1:T:135:TYR:O	1:T:139:ILE:HG12	2.21	0.41
1:W:74:VAL:O	1:W:99:PHE:HA	2.21	0.41
1:W:117:SER:HB3	1:W:120:SER:OG	2.20	0.41
1:X:106:ASN:ND2	1:X:108:HIS:H	2.19	0.41
1:B:10:PRO:HG3	1:B:81:TYR:CZ	2.56	0.40
1:B:51:PHE:CD1	1:B:62:ARG:HD3	2.56	0.40
1:S:6:LEU:HA	1:S:75:VAL:O	2.21	0.40
1:T:99:PHE:HE2	1:T:119:LEU:HB3	1.86	0.40
1:V:106:ASN:HB3	1:V:109:GLN:NE2	2.36	0.40
1:W:106:ASN:ND2	1:W:106:ASN:C	2.79	0.40
1:X:89:ARG:HH21	1:X:121:ASP:CG	2.29	0.40
1:F:125:ALA:HB2	1:I:129:GLY:C	2.47	0.40
1:L:10:PRO:HA	1:L:54:ASN:OD1	2.21	0.40
1:O:89:ARG:NH2	1:O:121:ASP:OD1	2.54	0.40
1:P:129:GLY:O	1:V:125:ALA:HB2	2.21	0.40
1:R:45:ASP:N	1:R:45:ASP:OD1	2.54	0.40
1:S:130:LEU:HD12	1:S:130:LEU:HA	1.79	0.40
1:T:89:ARG:NH2	1:T:121:ASP:OD1	2.54	0.40
1:X:3:LYS:HG2	1:X:71:VAL:HG22	2.03	0.40
1:X:74:VAL:O	1:X:99:PHE:HA	2.21	0.40
1:F:6:LEU:HD12	1:F:75:VAL:O	2.21	0.40
1:H:35:ALA:HB1	1:H:48:VAL:HG11	2.03	0.40
1:O:65:GLU:HA	1:O:68:ARG:NH2	2.36	0.40
1:S:31:ILE:HD13	1:S:135:TYR:CE2	2.56	0.40
1:T:10:PRO:HA	1:T:54:ASN:HA	2.03	0.40
1:X:106:ASN:HB3	1:X:109:GLN:NE2	2.36	0.40
1:A:5:LEU:HB3	1:A:74:VAL:HG22	2.03	0.40
1:A:57:GLY:HA3	1:B:55:THR:OG1	2.21	0.40
1:F:129:GLY:C	1:I:125:ALA:HB2	2.46	0.40
1:H:89:ARG:NH1	1:I:111:GLU:OE2	2.55	0.40
1:K:13:ASN:HA	1:K:28:LEU:HD22	2.04	0.40
1:L:4:VAL:HB	1:L:48:VAL:HG22	2.02	0.40
1:P:89:ARG:NH2	1:P:121:ASP:OD1	2.54	0.40
1:R:39:ALA:HB2	1:R:48:VAL:HG23	2.03	0.40
1:S:89:ARG:NH2	1:S:121:ASP:OD1	2.54	0.40
1:I:8:ASN:O	1:I:52:GLN:HG2	2.21	0.40
1:J:119:LEU:HD23	1:J:119:LEU:HA	1.92	0.40
1:V:8:ASN:O	1:V:52:GLN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/167 (83%)	131 (94%)	6 (4%)	2 (1%)	9	24
1	B	139/167 (83%)	131 (94%)	8 (6%)	0	100	100
1	C	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	18	40
1	D	140/167 (84%)	132 (94%)	7 (5%)	1 (1%)	18	40
1	E	141/167 (84%)	127 (90%)	13 (9%)	1 (1%)	18	40
1	F	141/167 (84%)	133 (94%)	7 (5%)	1 (1%)	18	40
1	G	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	18	40
1	H	140/167 (84%)	133 (95%)	6 (4%)	1 (1%)	18	40
1	I	145/167 (87%)	136 (94%)	8 (6%)	1 (1%)	18	40
1	J	139/167 (83%)	127 (91%)	10 (7%)	2 (1%)	9	24
1	K	140/167 (84%)	130 (93%)	9 (6%)	1 (1%)	18	40
1	L	140/167 (84%)	128 (91%)	11 (8%)	1 (1%)	18	40
1	M	140/167 (84%)	127 (91%)	10 (7%)	3 (2%)	5	16
1	N	140/167 (84%)	131 (94%)	8 (6%)	1 (1%)	18	40
1	O	140/167 (84%)	129 (92%)	11 (8%)	0	100	100
1	P	140/167 (84%)	131 (94%)	8 (6%)	1 (1%)	18	40
1	Q	140/167 (84%)	126 (90%)	13 (9%)	1 (1%)	18	40
1	R	140/167 (84%)	133 (95%)	7 (5%)	0	100	100
1	S	140/167 (84%)	124 (89%)	13 (9%)	3 (2%)	5	16
1	T	140/167 (84%)	129 (92%)	7 (5%)	4 (3%)	3	10
1	U	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	18	40
1	V	139/167 (83%)	121 (87%)	16 (12%)	2 (1%)	9	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	141/167 (84%)	131 (93%)	8 (6%)	2 (1%)	9	24
1	X	141/167 (84%)	127 (90%)	13 (9%)	1 (1%)	18	40
All	All	3362/4008 (84%)	3113 (93%)	217 (6%)	32 (1%)	12	32

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	25	THR
1	G	25	THR
1	Q	25	THR
1	S	146	GLN
1	U	25	THR
1	V	143	LEU
1	W	13	ASN
1	X	45	ASP
1	D	25	THR
1	E	25	THR
1	F	25	THR
1	K	25	THR
1	L	41	LEU
1	M	146	GLN
1	N	146	GLN
1	P	25	THR
1	S	43	ASN
1	T	25	THR
1	T	44	ASN
1	H	25	THR
1	J	13	ASN
1	J	43	ASN
1	M	25	THR
1	S	25	THR
1	V	25	THR
1	A	45	ASP
1	W	41	LEU
1	A	43	ASN
1	I	134	GLY
1	T	41	LEU
1	T	107	VAL
1	M	13	ASN

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	118/137 (86%)	105 (89%)	13 (11%)	6	17
1	B	118/137 (86%)	105 (89%)	13 (11%)	6	17
1	C	118/137 (86%)	103 (87%)	15 (13%)	4	13
1	D	119/137 (87%)	106 (89%)	13 (11%)	6	18
1	E	120/137 (88%)	109 (91%)	11 (9%)	8	23
1	F	120/137 (88%)	110 (92%)	10 (8%)	10	27
1	G	118/137 (86%)	106 (90%)	12 (10%)	7	20
1	H	119/137 (87%)	109 (92%)	10 (8%)	10	26
1	I	122/137 (89%)	112 (92%)	10 (8%)	10	27
1	J	118/137 (86%)	104 (88%)	14 (12%)	5	15
1	K	119/137 (87%)	104 (87%)	15 (13%)	4	13
1	L	119/137 (87%)	111 (93%)	8 (7%)	15	36
1	M	119/137 (87%)	109 (92%)	10 (8%)	10	26
1	N	119/137 (87%)	107 (90%)	12 (10%)	7	20
1	O	119/137 (87%)	108 (91%)	11 (9%)	8	23
1	P	119/137 (87%)	104 (87%)	15 (13%)	4	13
1	Q	119/137 (87%)	107 (90%)	12 (10%)	7	20
1	R	119/137 (87%)	110 (92%)	9 (8%)	12	31
1	S	119/137 (87%)	101 (85%)	18 (15%)	3	8
1	T	119/137 (87%)	104 (87%)	15 (13%)	4	13
1	U	118/137 (86%)	104 (88%)	14 (12%)	5	15
1	V	118/137 (86%)	106 (90%)	12 (10%)	7	20
1	W	120/137 (88%)	106 (88%)	14 (12%)	5	16
1	X	120/137 (88%)	100 (83%)	20 (17%)	2	6
All	All	2856/3288 (87%)	2550 (89%)	306 (11%)	6	18

All (306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	LEU
1	A	2	LYS
1	A	15	LEU
1	A	17	THR
1	A	36	ILE
1	A	41	LEU
1	A	82	THR
1	A	89	ARG
1	A	107	VAL
1	A	116	GLN
1	A	128	CYS
1	A	132	VAL
1	A	140	GLU
1	B	0	LEU
1	B	15	LEU
1	B	25	THR
1	B	33	GLN
1	B	67	LYS
1	B	69	GLN
1	B	89	ARG
1	B	109	GLN
1	B	112	PRO
1	B	116	GLN
1	B	126	VAL
1	B	128	CYS
1	B	132	VAL
1	C	0	LEU
1	C	2	LYS
1	C	3	LYS
1	C	13	ASN
1	C	14	LEU
1	C	15	LEU
1	C	38	GLN
1	C	40	LYS
1	C	41	LEU
1	C	62	ARG
1	C	67	LYS
1	C	106	ASN
1	C	109	GLN
1	C	132	VAL
1	C	140	GLU
1	D	0	LEU
1	D	3	LYS

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Mol	Chain	Res	Type
1	D	15	LEU
1	D	17	THR
1	D	18	ARG
1	D	36	ILE
1	D	40	LYS
1	D	41	LEU
1	D	46	SER
1	D	48	VAL
1	D	89	ARG
1	D	132	VAL
1	D	146	GLN
1	E	15	LEU
1	E	17	THR
1	E	23	TYR
1	E	32	GLU
1	E	37	GLU
1	E	41	LEU
1	E	53	SER
1	E	89	ARG
1	E	107	VAL
1	E	116	GLN
1	E	132	VAL
1	F	-1	GLN
1	F	3	LYS
1	F	13	ASN
1	F	15	LEU
1	F	17	THR
1	F	41	LEU
1	F	43	ASN
1	F	53	SER
1	F	82	THR
1	F	126	VAL
1	G	3	LYS
1	G	15	LEU
1	G	17	THR
1	G	18	ARG
1	G	29	SER
1	G	36	ILE
1	G	45	ASP
1	G	89	ARG
1	G	112	PRO
1	G	117	SER

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Mol	Chain	Res	Type
1	G	127	ILE
1	G	146	GLN
1	H	0	LEU
1	H	3	LYS
1	H	15	LEU
1	H	17	THR
1	H	23	TYR
1	H	41	LEU
1	H	59	ILE
1	H	65	GLU
1	H	97	ILE
1	H	107	VAL
1	I	13	ASN
1	I	17	THR
1	I	18	ARG
1	I	21	GLU
1	I	53	SER
1	I	65	GLU
1	I	67	LYS
1	I	89	ARG
1	I	128	CYS
1	I	140	GLU
1	J	0	LEU
1	J	2	LYS
1	J	3	LYS
1	J	15	LEU
1	J	17	THR
1	J	42	LYS
1	J	45	ASP
1	J	67	LYS
1	J	71	VAL
1	J	89	ARG
1	J	107	VAL
1	J	109	GLN
1	J	116	GLN
1	J	146	GLN
1	K	14	LEU
1	K	15	LEU
1	K	17	THR
1	K	18	ARG
1	K	29	SER
1	K	40	LYS

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Mol	Chain	Res	Type
1	K	53	SER
1	K	67	LYS
1	K	68	ARG
1	K	82	THR
1	K	109	GLN
1	K	116	GLN
1	K	126	VAL
1	K	132	VAL
1	K	146	GLN
1	L	2	LYS
1	L	3	LYS
1	L	15	LEU
1	L	17	THR
1	L	53	SER
1	L	62	ARG
1	L	116	GLN
1	L	128	CYS
1	M	15	LEU
1	M	17	THR
1	M	25	THR
1	M	26	THR
1	M	45	ASP
1	M	68	ARG
1	M	116	GLN
1	M	126	VAL
1	M	146	GLN
1	M	147	LEU
1	N	0	LEU
1	N	3	LYS
1	N	15	LEU
1	N	41	LEU
1	N	49	LEU
1	N	89	ARG
1	N	110	ARG
1	N	116	GLN
1	N	128	CYS
1	N	144	ASN
1	N	146	GLN
1	N	147	LEU
1	O	3	LYS
1	O	15	LEU
1	O	17	THR

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Mol	Chain	Res	Type
1	O	28	LEU
1	O	45	ASP
1	O	69	GLN
1	O	128	CYS
1	O	130	LEU
1	O	132	VAL
1	O	146	GLN
1	O	147	LEU
1	P	3	LYS
1	P	15	LEU
1	P	17	THR
1	P	18	ARG
1	P	32	GLU
1	P	36	ILE
1	P	45	ASP
1	P	68	ARG
1	P	69	GLN
1	P	107	VAL
1	P	109	GLN
1	P	112	PRO
1	P	116	GLN
1	P	132	VAL
1	P	147	LEU
1	Q	0	LEU
1	Q	2	LYS
1	Q	3	LYS
1	Q	13	ASN
1	Q	15	LEU
1	Q	18	ARG
1	Q	32	GLU
1	Q	41	LEU
1	Q	89	ARG
1	Q	116	GLN
1	Q	128	CYS
1	Q	132	VAL
1	R	2	LYS
1	R	3	LYS
1	R	13	ASN
1	R	15	LEU
1	R	17	THR
1	R	25	THR
1	R	89	ARG

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Mol	Chain	Res	Type
1	R	107	VAL
1	R	116	GLN
1	S	0	LEU
1	S	3	LYS
1	S	15	LEU
1	S	17	THR
1	S	18	ARG
1	S	23	TYR
1	S	29	SER
1	S	41	LEU
1	S	45	ASP
1	S	62	ARG
1	S	89	ARG
1	S	107	VAL
1	S	109	GLN
1	S	112	PRO
1	S	116	GLN
1	S	128	CYS
1	S	132	VAL
1	S	147	LEU
1	T	-1	GLN
1	T	0	LEU
1	T	1	VAL
1	T	15	LEU
1	T	17	THR
1	T	18	ARG
1	T	25	THR
1	T	29	SER
1	T	36	ILE
1	T	68	ARG
1	T	107	VAL
1	T	109	GLN
1	T	132	VAL
1	T	144	ASN
1	T	146	GLN
1	U	0	LEU
1	U	3	LYS
1	U	13	ASN
1	U	15	LEU
1	U	17	THR
1	U	18	ARG
1	U	25	THR

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Mol	Chain	Res	Type
1	U	41	LEU
1	U	69	GLN
1	U	109	GLN
1	U	112	PRO
1	U	116	GLN
1	U	117	SER
1	U	139	ILE
1	V	1	VAL
1	V	3	LYS
1	V	15	LEU
1	V	17	THR
1	V	36	ILE
1	V	45	ASP
1	V	69	GLN
1	V	76	ILE
1	V	109	GLN
1	V	115	HIS
1	V	116	GLN
1	V	128	CYS
1	W	-1	GLN
1	W	0	LEU
1	W	1	VAL
1	W	3	LYS
1	W	15	LEU
1	W	17	THR
1	W	38	GLN
1	W	41	LEU
1	W	45	ASP
1	W	49	LEU
1	W	89	ARG
1	W	112	PRO
1	W	116	GLN
1	W	120	SER
1	X	-1	GLN
1	X	0	LEU
1	X	1	VAL
1	X	2	LYS
1	X	15	LEU
1	X	17	THR
1	X	26	THR
1	X	36	ILE
1	X	40	LYS

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Mol	Chain	Res	Type
1	X	41	LEU
1	X	46	SER
1	X	67	LYS
1	X	109	GLN
1	X	112	PRO
1	X	117	SER
1	X	120	SER
1	X	128	CYS
1	X	132	VAL
1	X	144	ASN
1	X	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	83	HIS
1	A	106	ASN
1	A	109	GLN
1	A	115	HIS
1	B	8	ASN
1	B	83	HIS
1	B	106	ASN
1	B	109	GLN
1	C	8	ASN
1	C	13	ASN
1	C	103	HIS
1	C	106	ASN
1	C	109	GLN
1	C	115	HIS
1	C	116	GLN
1	C	144	ASN
1	D	8	ASN
1	D	33	GLN
1	D	106	ASN
1	D	109	GLN
1	D	115	HIS
1	D	144	ASN
1	D	146	GLN
1	E	8	ASN
1	E	106	ASN
1	E	109	GLN

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Mol	Chain	Res	Type
1	E	115	HIS
1	F	8	ASN
1	F	13	ASN
1	F	83	HIS
1	F	106	ASN
1	F	109	GLN
1	F	115	HIS
1	F	116	GLN
1	G	8	ASN
1	G	44	ASN
1	G	83	HIS
1	G	109	GLN
1	G	144	ASN
1	H	8	ASN
1	H	33	GLN
1	H	115	HIS
1	H	144	ASN
1	I	8	ASN
1	I	13	ASN
1	I	106	ASN
1	I	109	GLN
1	I	144	ASN
1	I	146	GLN
1	J	8	ASN
1	J	13	ASN
1	J	106	ASN
1	J	109	GLN
1	J	115	HIS
1	J	144	ASN
1	K	8	ASN
1	K	13	ASN
1	K	106	ASN
1	K	109	GLN
1	K	115	HIS
1	K	146	GLN
1	L	8	ASN
1	L	103	HIS
1	L	109	GLN
1	L	115	HIS
1	L	144	ASN
1	M	8	ASN
1	M	33	GLN

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Mol	Chain	Res	Type
1	M	43	ASN
1	M	109	GLN
1	M	115	HIS
1	M	146	GLN
1	N	8	ASN
1	N	33	GLN
1	N	106	ASN
1	N	146	GLN
1	O	8	ASN
1	O	106	ASN
1	O	109	GLN
1	P	8	ASN
1	P	33	GLN
1	P	44	ASN
1	P	106	ASN
1	P	109	GLN
1	P	115	HIS
1	P	144	ASN
1	P	146	GLN
1	Q	8	ASN
1	Q	13	ASN
1	Q	33	GLN
1	Q	106	ASN
1	Q	144	ASN
1	R	8	ASN
1	R	13	ASN
1	R	109	GLN
1	R	144	ASN
1	S	8	ASN
1	S	33	GLN
1	S	83	HIS
1	S	109	GLN
1	S	116	GLN
1	T	8	ASN
1	T	33	GLN
1	T	83	HIS
1	T	106	ASN
1	T	109	GLN
1	T	144	ASN
1	T	146	GLN
1	U	8	ASN
1	U	13	ASN

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Mol	Chain	Res	Type
1	U	83	HIS
1	U	106	ASN
1	U	109	GLN
1	U	144	ASN
1	V	8	ASN
1	V	83	HIS
1	V	106	ASN
1	V	109	GLN
1	W	8	ASN
1	W	83	HIS
1	W	106	ASN
1	W	109	GLN
1	X	8	ASN
1	X	33	GLN
1	X	106	ASN
1	X	108	HIS
1	X	109	GLN
1	X	115	HIS
1	X	144	ASN

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 ⓘ

32 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	SO4	U	155	-	4,4,4	0.37	0	6,6,6	1.44	1 (16%)
2	SO4	G	155	-	4,4,4	0.63	0	6,6,6	1.13	1 (16%)
2	SO4	P	155	-	4,4,4	0.37	0	6,6,6	0.84	0
2	SO4	X	155	-	4,4,4	0.50	0	6,6,6	0.79	0
2	SO4	A	156	-	4,4,4	0.58	0	6,6,6	0.77	0
2	SO4	E	155	-	4,4,4	0.32	0	6,6,6	0.97	0
2	SO4	T	155	-	4,4,4	0.40	0	6,6,6	0.88	0
2	SO4	I	155	-	4,4,4	0.49	0	6,6,6	1.42	1 (16%)
2	SO4	R	155	-	4,4,4	0.28	0	6,6,6	1.19	1 (16%)
2	SO4	V	155	-	4,4,4	0.32	0	6,6,6	0.42	0
2	SO4	O	155	-	4,4,4	0.44	0	6,6,6	0.98	0
3	TRS	D	156	-	7,7,7	0.66	0	9,9,9	1.79	3 (33%)
2	SO4	S	155	-	4,4,4	0.51	0	6,6,6	1.01	0
2	SO4	H	155	-	4,4,4	0.54	0	6,6,6	0.83	0
3	TRS	W	156	-	7,7,7	0.78	0	9,9,9	1.18	1 (11%)
2	SO4	W	155	-	4,4,4	0.41	0	6,6,6	0.86	0
2	SO4	B	155	-	4,4,4	0.54	0	6,6,6	1.41	0
2	SO4	M	155	-	4,4,4	0.59	0	6,6,6	0.95	0
3	TRS	N	156	-	7,7,7	0.39	0	9,9,9	0.63	0
2	SO4	F	155	-	4,4,4	0.53	0	6,6,6	1.54	1 (16%)
3	TRS	J	156	-	7,7,7	0.69	0	9,9,9	0.79	0
2	SO4	K	155	-	4,4,4	0.26	0	6,6,6	0.60	0
2	SO4	D	155	-	4,4,4	0.56	0	6,6,6	0.71	0
2	SO4	A	155	-	4,4,4	0.56	0	6,6,6	1.07	1 (16%)
2	SO4	C	155	-	4,4,4	0.48	0	6,6,6	0.84	0
3	TRS	G	156	-	7,7,7	0.81	0	9,9,9	1.44	1 (11%)
3	TRS	T	156	-	7,7,7	0.55	0	9,9,9	1.08	0
3	TRS	P	156	-	7,7,7	0.63	0	9,9,9	1.93	5 (55%)
2	SO4	Q	155	-	4,4,4	0.62	0	6,6,6	1.12	1 (16%)
2	SO4	N	155	-	4,4,4	0.27	0	6,6,6	1.02	0
2	SO4	J	155	-	4,4,4	0.54	0	6,6,6	0.80	0
3	TRS	A	157	-	7,7,7	0.75	0	9,9,9	1.33	1 (11%)

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
3	TRS	W	156	-	-	5/9/9/9	-
3	TRS	T	156	-	-	2/9/9/9	-
3	TRS	G	156	-	-	2/9/9/9	-
3	TRS	P	156	-	-	5/9/9/9	-
3	TRS	N	156	-	-	3/9/9/9	-
3	TRS	D	156	-	-	9/9/9/9	-
3	TRS	A	157	-	-	2/9/9/9	-
3	TRS	J	156	-	-	0/9/9/9	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	156	TRS	C3-C-N	3.18	116.29	108.17
2	F	155	SO4	O3-S-O1	3.06	125.55	109.56
3	A	157	TRS	O1-C1-C	-2.99	102.55	110.88
3	P	156	TRS	C3-C-C2	-2.83	103.13	110.66
3	D	156	TRS	C2-C-N	2.75	115.20	108.17
3	D	156	TRS	C3-C-N	2.72	115.10	108.17
2	I	155	SO4	O4-S-O1	2.64	123.38	109.56
3	D	156	TRS	C3-C-C2	-2.61	103.70	110.66
2	U	155	SO4	O3-S-O1	-2.58	96.04	109.56
3	G	156	TRS	C2-C-C1	-2.49	104.02	110.66
3	W	156	TRS	C2-C-N	-2.33	102.23	108.17
3	P	156	TRS	C2-C-N	2.30	114.05	108.17
2	Q	155	SO4	O3-S-O1	2.29	121.55	109.56
2	A	155	SO4	O3-S-O1	2.21	121.10	109.56
3	P	156	TRS	O2-C2-C	2.19	116.97	110.88
2	G	155	SO4	O4-S-O1	2.12	120.63	109.56
3	P	156	TRS	C3-C-C1	-2.05	105.18	110.66
2	R	155	SO4	O4-S-O3	2.03	119.72	108.54

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	156	TRS	C1-C-C2-O2
3	D	156	TRS	C3-C-C2-O2
3	D	156	TRS	C1-C-C3-O3
3	N	156	TRS	C3-C-C2-O2

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Mol	Chain	Res	Type	Atoms
3	N	156	TRS	N-C-C2-O2
3	W	156	TRS	N-C-C3-O3
3	D	156	TRS	C2-C-C1-O1
3	W	156	TRS	C2-C-C1-O1
3	W	156	TRS	C1-C-C3-O3
3	D	156	TRS	C3-C-C1-O1
3	D	156	TRS	C2-C-C3-O3
3	D	156	TRS	N-C-C3-O3
3	N	156	TRS	C1-C-C2-O2
3	P	156	TRS	N-C-C2-O2
3	W	156	TRS	N-C-C1-O1
3	P	156	TRS	C1-C-C2-O2
3	P	156	TRS	C3-C-C2-O2
3	P	156	TRS	C1-C-C3-O3
3	T	156	TRS	C2-C-C1-O1
3	A	157	TRS	C1-C-C3-O3
3	D	156	TRS	N-C-C1-O1
3	D	156	TRS	N-C-C2-O2
3	P	156	TRS	N-C-C3-O3
3	G	156	TRS	C3-C-C2-O2
3	W	156	TRS	C2-C-C3-O3
3	A	157	TRS	N-C-C3-O3
3	G	156	TRS	N-C-C2-O2
3	T	156	TRS	C1-C-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	156	TRS	1	0
3	W	156	TRS	1	0
3	N	156	TRS	1	0
3	P	156	TRS	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 ⓘ

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	143/167 (85%)	-0.29	4 (2%)	55	47	35, 49, 85, 114	0
1	B	143/167 (85%)	-0.25	5 (3%)	47	40	34, 47, 73, 93	0
1	C	143/167 (85%)	-0.25	3 (2%)	63	55	37, 54, 93, 112	0
1	D	144/167 (86%)	-0.25	3 (2%)	63	55	36, 51, 90, 120	0
1	E	145/167 (86%)	-0.42	2 (1%)	73	67	33, 46, 85, 113	0
1	F	145/167 (86%)	-0.40	1 (0%)	84	80	34, 45, 75, 105	0
1	G	143/167 (85%)	-0.21	3 (2%)	63	55	37, 52, 96, 113	0
1	H	144/167 (86%)	-0.19	4 (2%)	55	47	37, 54, 93, 110	0
1	I	147/167 (88%)	-0.30	1 (0%)	84	80	36, 45, 78, 102	0
1	J	143/167 (85%)	-0.13	3 (2%)	63	55	44, 57, 96, 120	0
1	K	144/167 (86%)	-0.10	3 (2%)	63	55	44, 57, 100, 111	0
1	L	144/167 (86%)	-0.02	3 (2%)	63	55	46, 59, 104, 118	0
1	M	144/167 (86%)	-0.33	2 (1%)	73	67	40, 51, 95, 112	0
1	N	144/167 (86%)	-0.18	2 (1%)	73	67	39, 49, 81, 96	0
1	O	144/167 (86%)	-0.36	2 (1%)	73	67	40, 54, 95, 106	0
1	P	144/167 (86%)	-0.40	3 (2%)	63	55	39, 53, 97, 113	0
1	Q	144/167 (86%)	-0.41	2 (1%)	73	67	37, 50, 92, 112	0
1	R	144/167 (86%)	-0.30	2 (1%)	73	67	34, 48, 89, 108	0
1	S	144/167 (86%)	-0.22	3 (2%)	63	55	41, 56, 101, 113	0
1	T	144/167 (86%)	-0.07	2 (1%)	73	67	43, 60, 109, 127	0
1	U	143/167 (85%)	-0.24	2 (1%)	73	67	41, 53, 93, 119	0
1	V	143/167 (85%)	-0.25	3 (2%)	63	55	48, 60, 102, 124	0
1	W	145/167 (86%)	-0.04	3 (2%)	63	55	49, 60, 110, 121	0
1	X	145/167 (86%)	-0.19	3 (2%)	63	55	47, 59, 108, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3456/4008 (86%)	-0.24	64 (1%) 66 58	33, 54, 97, 127	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	23	TYR	4.7
1	V	23	TYR	4.6
1	K	23	TYR	4.3
1	B	23	TYR	4.2
1	D	23	TYR	4.2
1	M	147	LEU	4.2
1	W	23	TYR	3.9
1	N	18	ARG	3.8
1	T	0	LEU	3.8
1	B	18	ARG	3.8
1	A	23	TYR	3.7
1	M	23	TYR	3.7
1	G	23	TYR	3.7
1	F	23	TYR	3.5
1	E	23	TYR	3.4
1	W	147	LEU	3.3
1	R	23	TYR	3.3
1	T	23	TYR	3.3
1	S	147	LEU	3.2
1	X	147	LEU	3.2
1	C	0	LEU	3.1
1	Q	23	TYR	3.1
1	U	23	TYR	3.0
1	H	18	ARG	3.0
1	K	147	LEU	2.9
1	H	23	TYR	2.9
1	A	116	GLN	2.9
1	S	23	TYR	2.9
1	J	18	ARG	2.7
1	D	18	ARG	2.7
1	V	0	LEU	2.7
1	V	18	ARG	2.7
1	H	147	LEU	2.6
1	G	18	ARG	2.6
1	J	23	TYR	2.6
1	L	23	TYR	2.6
1	U	18	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	18	ARG	2.5
1	W	18	ARG	2.5
1	G	0	LEU	2.5
1	A	0	LEU	2.4
1	J	0	LEU	2.4
1	P	0	LEU	2.4
1	L	147	LEU	2.4
1	B	25	THR	2.4
1	H	0	LEU	2.4
1	Q	18	ARG	2.3
1	B	6	LEU	2.3
1	B	0	LEU	2.2
1	I	0	LEU	2.2
1	X	0	LEU	2.2
1	X	23	TYR	2.2
1	E	147	LEU	2.2
1	L	0	LEU	2.2
1	D	0	LEU	2.2
1	O	0	LEU	2.2
1	R	18	ARG	2.1
1	P	18	ARG	2.1
1	S	18	ARG	2.1
1	C	23	TYR	2.0
1	O	23	TYR	2.0
1	A	18	ARG	2.0
1	C	18	ARG	2.0
1	P	23	TYR	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	SO4	X	155	5/5	0.74	0.15	107,109,111,113	0
2	SO4	J	155	5/5	0.78	0.17	116,118,119,119	0
2	SO4	M	155	5/5	0.80	0.19	106,108,111,112	0
2	SO4	P	155	5/5	0.80	0.17	106,107,108,110	0
2	SO4	E	155	5/5	0.80	0.15	108,110,111,113	0
2	SO4	U	155	5/5	0.81	0.17	101,103,104,105	0
2	SO4	C	155	5/5	0.81	0.13	111,112,114,117	0
2	SO4	T	155	5/5	0.82	0.13	113,115,116,117	0
2	SO4	K	155	5/5	0.84	0.17	116,117,118,118	0
2	SO4	D	155	5/5	0.85	0.12	95,95,97,100	0
2	SO4	O	155	5/5	0.85	0.12	111,114,115,116	0
2	SO4	H	155	5/5	0.85	0.17	101,103,105,108	0
2	SO4	Q	155	5/5	0.86	0.16	94,97,99,101	0
2	SO4	G	155	5/5	0.87	0.13	86,90,93,95	0
2	SO4	A	155	5/5	0.87	0.14	100,102,105,107	0
2	SO4	W	155	5/5	0.87	0.14	110,113,114,115	0
2	SO4	R	155	5/5	0.87	0.13	96,98,99,100	0
2	SO4	F	155	5/5	0.88	0.15	88,91,96,97	0
2	SO4	S	155	5/5	0.88	0.20	100,102,105,106	0
2	SO4	B	155	5/5	0.89	0.14	84,84,90,91	0
2	SO4	V	155	5/5	0.89	0.09	110,111,112,112	0
2	SO4	A	156	5/5	0.90	0.15	88,89,91,91	0
2	SO4	I	155	5/5	0.91	0.15	67,67,71,72	0
3	TRS	J	156	8/8	0.93	0.09	45,49,50,50	0
3	TRS	W	156	8/8	0.94	0.10	52,55,56,56	0
3	TRS	G	156	8/8	0.95	0.10	41,43,44,44	0
2	SO4	N	155	5/5	0.95	0.10	85,88,88,91	0
3	TRS	A	157	8/8	0.95	0.08	38,44,45,45	0
3	TRS	N	156	8/8	0.96	0.07	35,38,39,39	0
3	TRS	P	156	8/8	0.97	0.07	35,38,38,41	0
3	TRS	T	156	8/8	0.97	0.07	50,52,52,53	0
3	TRS	D	156	8/8	0.97	0.08	40,40,41,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.