Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 01:46 AM EDT

PDB ID	:	3KIP
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:

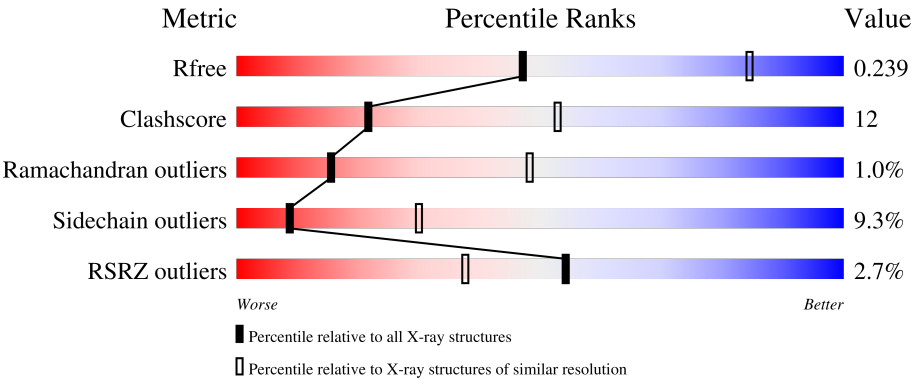
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	59% 22% • • 14%
1	B	167	55% 23% 6% • 14%
1	C	167	% 57% 25% • • 14%
1	D	167	2% 62% 19% • • 14%
1	E	167	63% 19% • • 13%

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Mol	Chain	Length	Quality of chain
1	F	167	61% 23% 13%
1	G	167	2% 59% 24% 14%
1	H	167	% 64% 20% 14%
1	I	167	62% 23% 12%
1	J	167	10% 62% 19% 14%
1	K	167	6% 59% 24% 14%
1	L	167	4% 63% 19% 14%
1	M	167	63% 16% 5% 14%
1	N	167	% 62% 20% 14%
1	O	167	63% 19% 14%
1	P	167	% 65% 17% 14%
1	Q	167	% 65% 15% 7% 14%
1	R	167	% 66% 18% 14%
1	S	167	5% 55% 25% 6% 14%
1	T	167	8% 52% 28% 5% 14%
1	U	167	% 56% 24% 5% 14%
1	V	167	2% 62% 20% 14%
1	W	167	5% 59% 23% 5% 13%
1	X	167	4% 55% 25% 6% 13%

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 (i)

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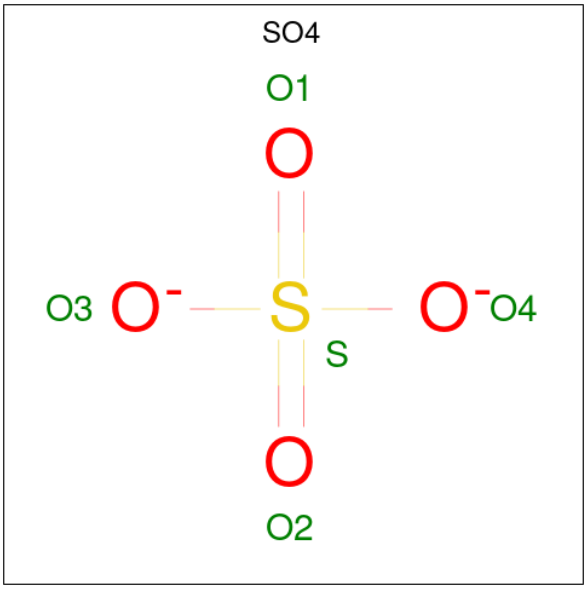
Chain	Residue	Modelled	Actual	Comment	Reference
X	154	ALA	-	expression tag	UNP Q59Z17

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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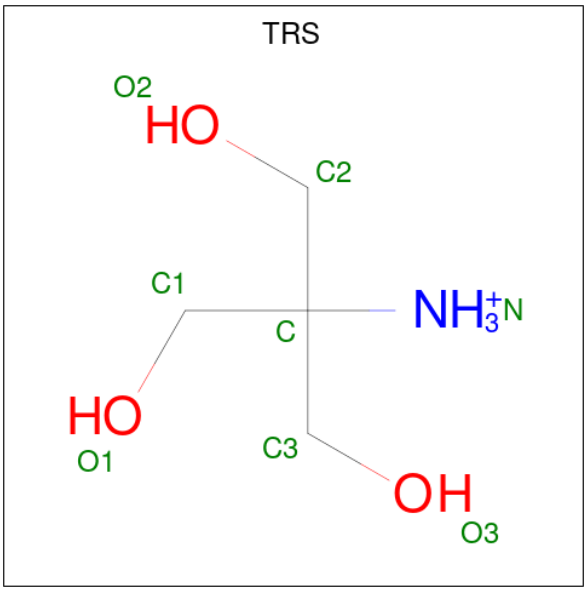
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	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 (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 4 is water.

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

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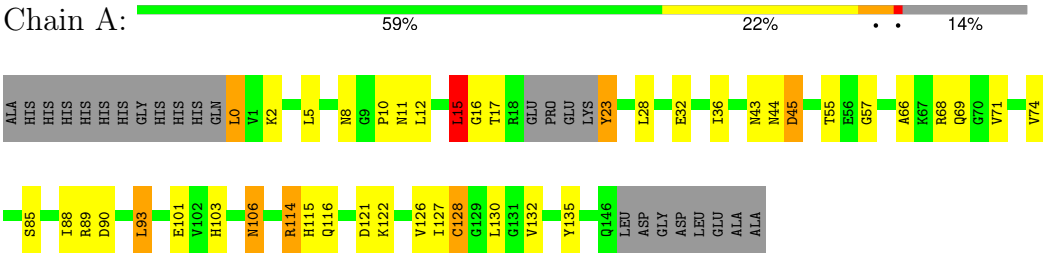
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	17	Total O 17 17	0	0
4	F	10	Total O 10 10	0	0
4	G	9	Total O 9 9	0	0
4	H	4	Total O 4 4	0	0
4	I	11	Total O 11 11	0	0
4	J	4	Total O 4 4	0	0
4	K	5	Total O 5 5	0	0
4	L	4	Total O 4 4	0	0
4	M	4	Total O 4 4	0	0
4	N	11	Total O 11 11	0	0
4	O	2	Total O 2 2	0	0
4	P	8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

3 Residue-property plots (i)

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

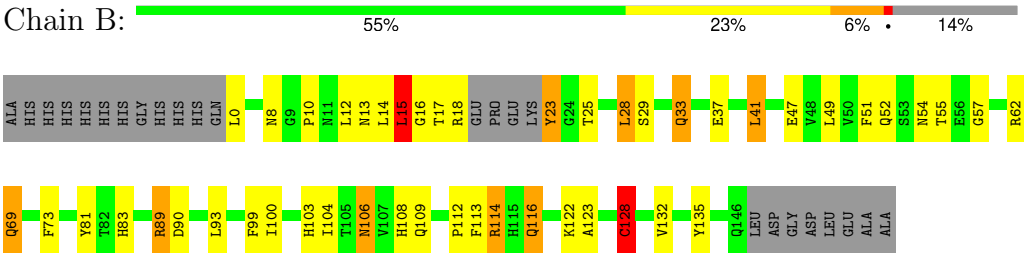
• Molecule 1: 3-dehydroquinase, type II

Chain A:



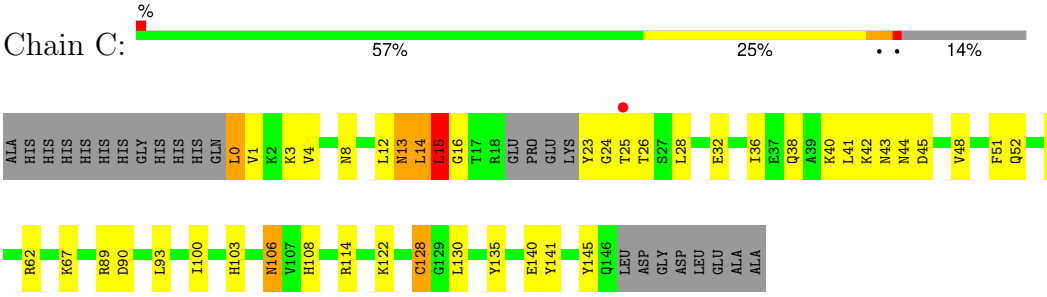
• Molecule 1: 3-dehydroquinase, type II

Chain B:



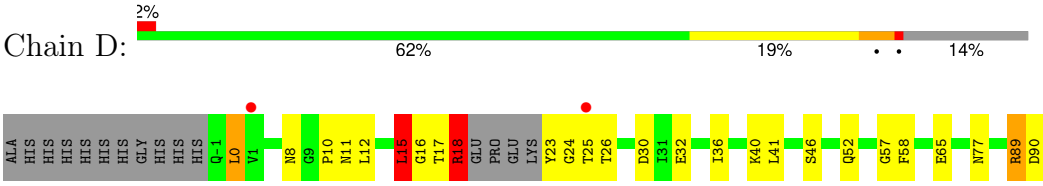
• Molecule 1: 3-dehydroquinase, type II

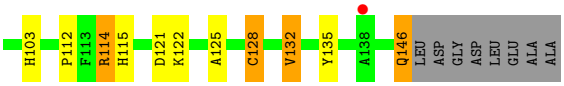
Chain C:



• Molecule 1: 3-dehydroquinase, type II

Chain D:



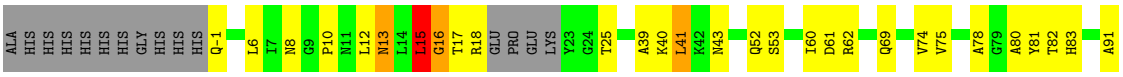


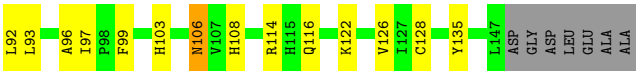
• Molecule 1: 3-dehydroquinase, type II

Chain E:

• Molecule 1: 3-dehydroquinase, type II

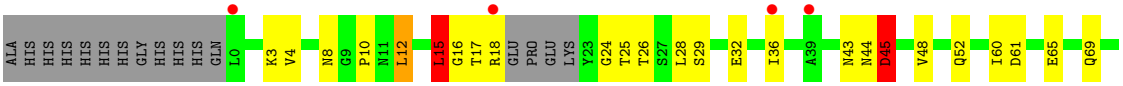
Chain F:





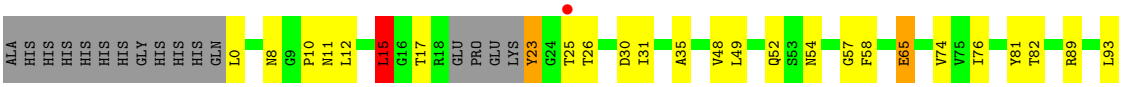
• Molecule 1: 3-dehydroquinase, type II

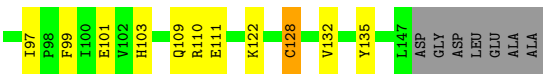
Chain G:



• Molecule 1: 3-dehydroquinase, type II

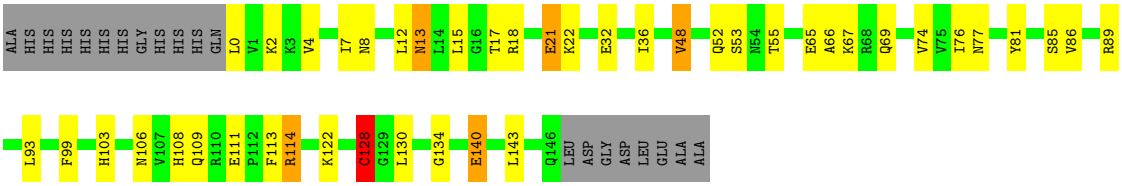
Chain H:





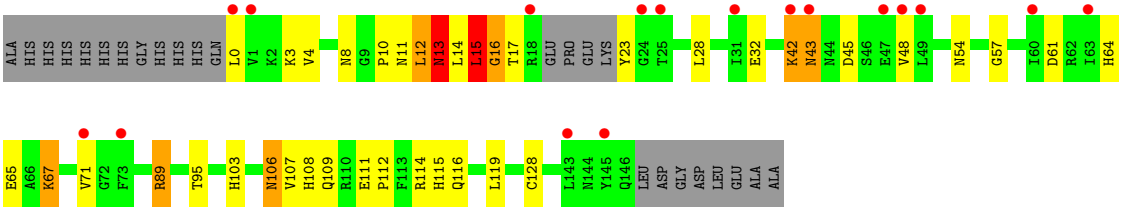
• Molecule 1: 3-dehydroquinase, type II

Chain I:



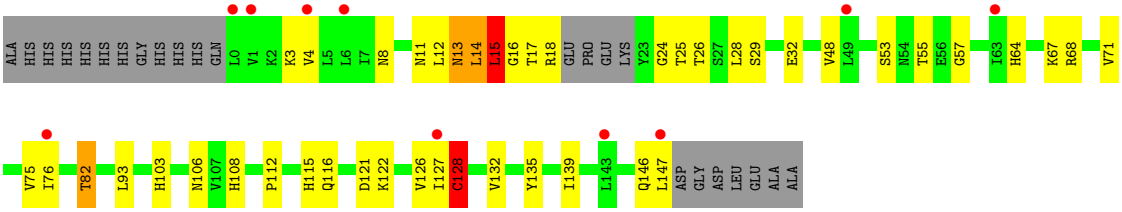
• Molecule 1: 3-dehydroquinase, type II

Chain J:



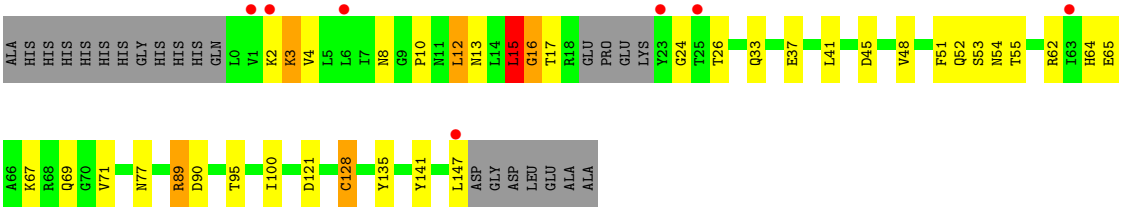
• Molecule 1: 3-dehydroquinase, type II

Chain K:



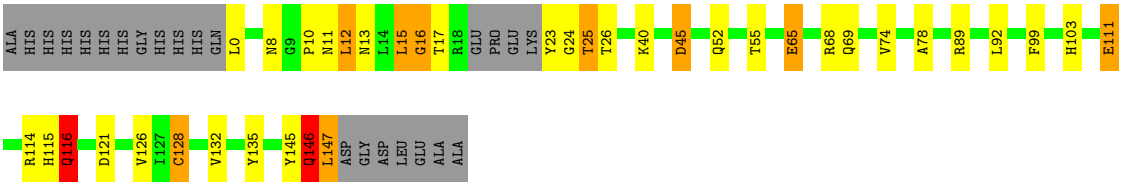
• Molecule 1: 3-dehydroquinase, type II

Chain L:



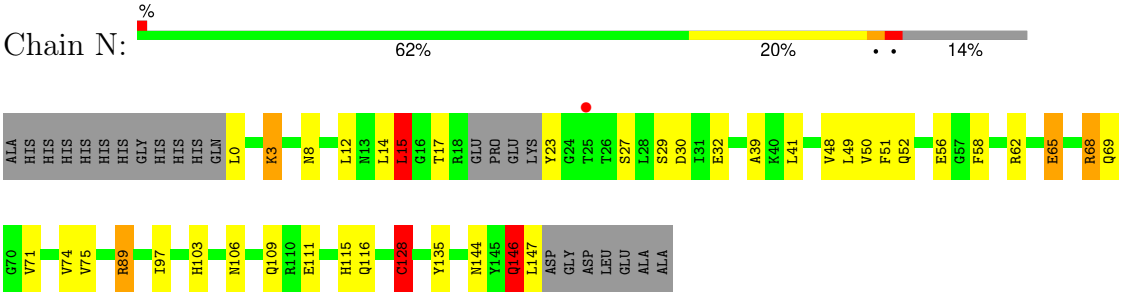
• Molecule 1: 3-dehydroquinase, type II

Chain M:



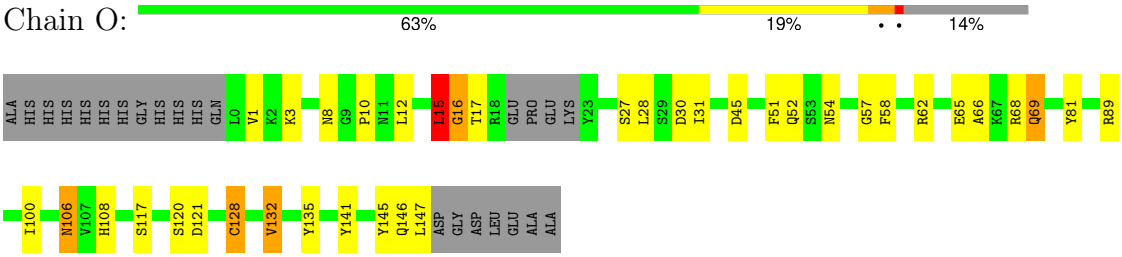
• Molecule 1: 3-dehydroquinase, type II

Chain N:



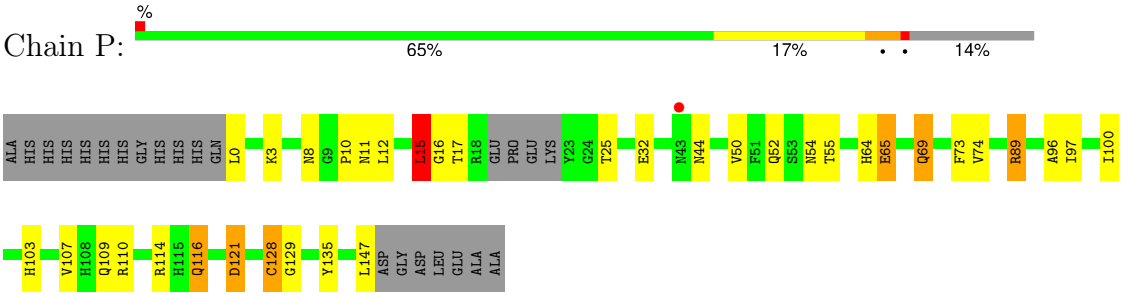
• Molecule 1: 3-dehydroquinase, type II

Chain O:



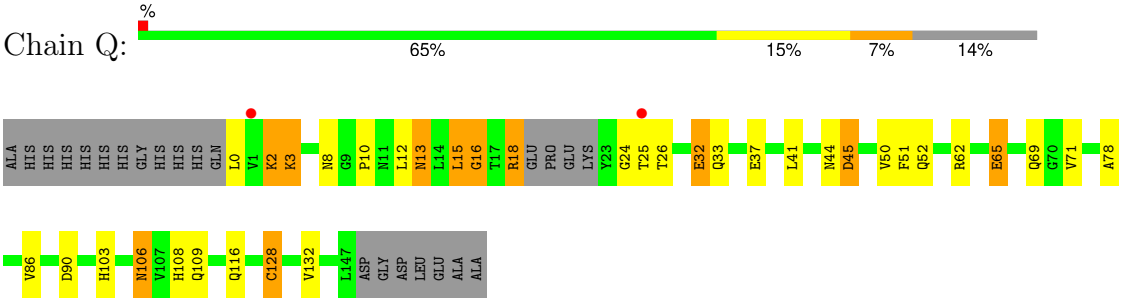
• Molecule 1: 3-dehydroquinase, type II

Chain P:



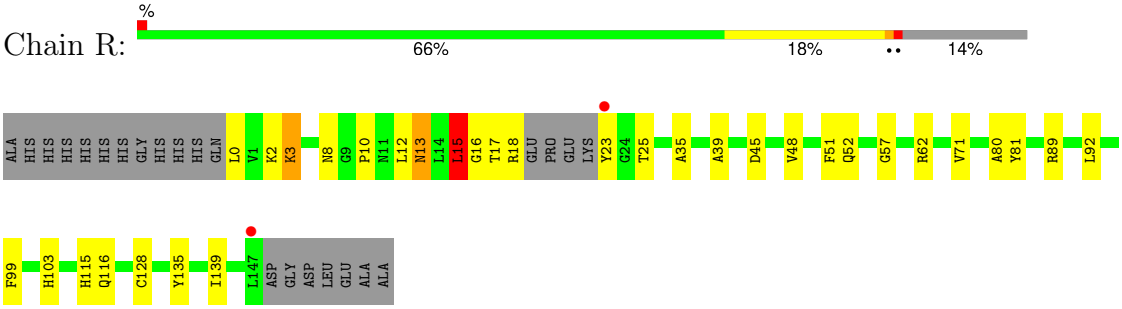
• Molecule 1: 3-dehydroquinase, type II

Chain Q:



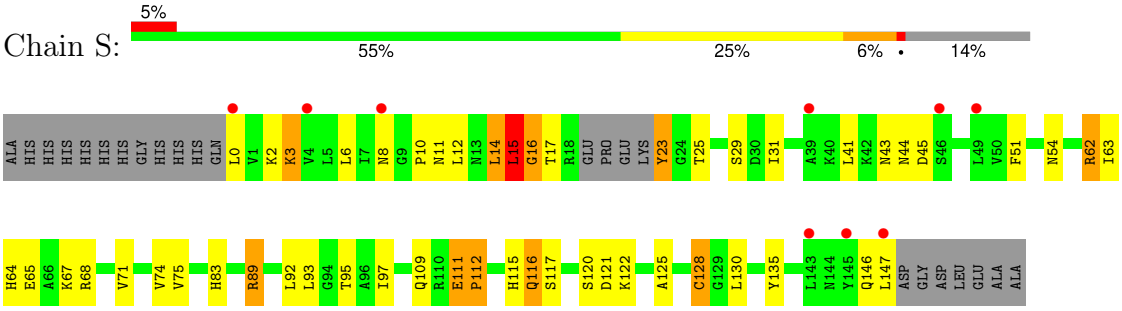
• Molecule 1: 3-dehydroquinase, type II

Chain R:



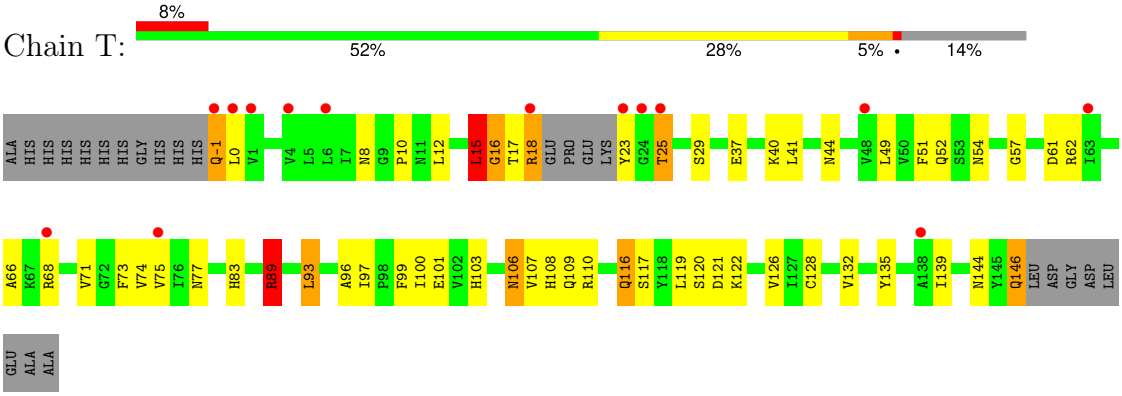
• Molecule 1: 3-dehydroquinase, type II

Chain S:



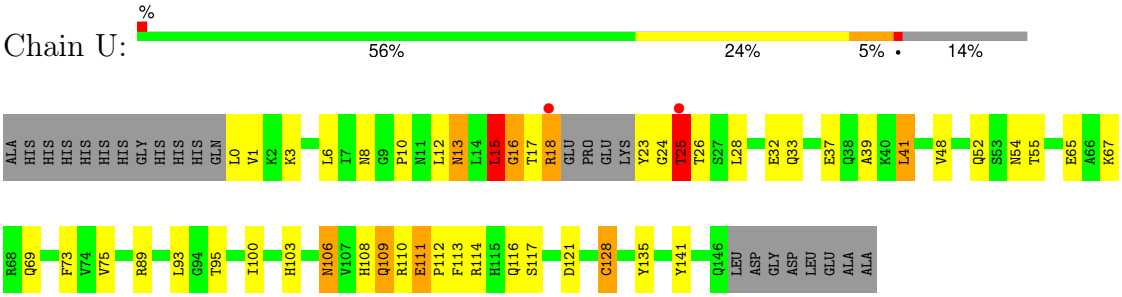
• Molecule 1: 3-dehydroquinase, type II

Chain T:



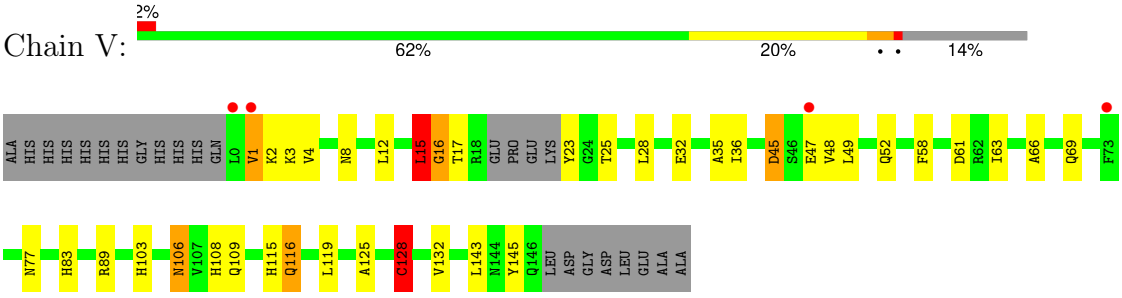
• Molecule 1: 3-dehydroquinase, type II

Chain U:



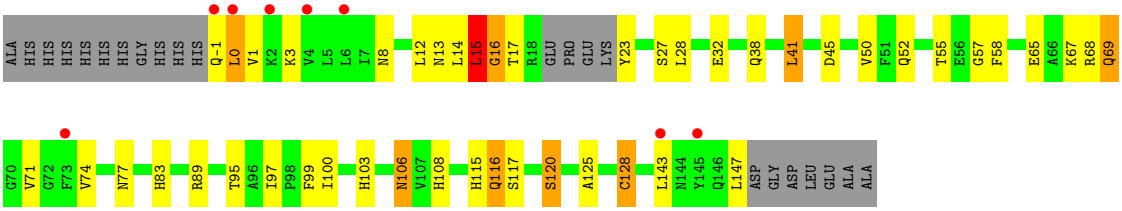
• Molecule 1: 3-dehydroquinase, type II

Chain V:

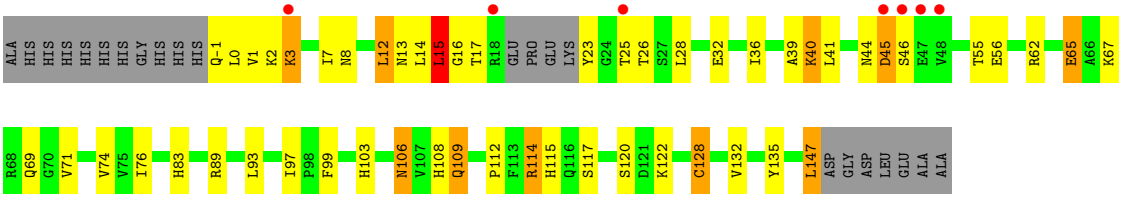


• Molecule 1: 3-dehydroquinase, type II

Chain W:



• Molecule 1: 3-dehydroquinase, type II



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 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
$< I/\sigma(I) >$ [1]	2.71 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.245 0.200 , 0.239	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 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TRS, SO4

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	1.16	0/1126	1.18	9/1527 (0.6%)
1	B	1.25	6/1126 (0.5%)	1.24	11/1527 (0.7%)
1	C	1.18	2/1126 (0.2%)	1.08	5/1527 (0.3%)
1	D	1.15	2/1135 (0.2%)	1.20	13/1539 (0.8%)
1	E	1.24	5/1143 (0.4%)	1.10	3/1550 (0.2%)
1	F	1.27	1/1143 (0.1%)	1.13	6/1550 (0.4%)
1	G	1.19	1/1126 (0.1%)	1.12	6/1527 (0.4%)
1	H	1.19	5/1134 (0.4%)	1.11	5/1538 (0.3%)
1	I	1.25	6/1162 (0.5%)	1.08	3/1577 (0.2%)
1	J	1.07	1/1126 (0.1%)	1.03	5/1527 (0.3%)
1	K	1.06	1/1134 (0.1%)	1.10	6/1538 (0.4%)
1	L	1.07	1/1134 (0.1%)	1.03	4/1538 (0.3%)
1	M	1.18	4/1134 (0.4%)	1.15	5/1538 (0.3%)
1	N	1.19	5/1134 (0.4%)	1.12	4/1538 (0.3%)
1	O	1.08	1/1134 (0.1%)	1.07	3/1538 (0.2%)
1	P	1.10	3/1134 (0.3%)	1.09	5/1538 (0.3%)
1	Q	1.18	1/1134 (0.1%)	1.13	3/1538 (0.2%)
1	R	1.14	0/1134	1.03	4/1538 (0.3%)
1	S	1.15	3/1134 (0.3%)	1.12	3/1538 (0.2%)
1	T	1.12	0/1135	1.10	10/1539 (0.6%)
1	U	1.15	6/1126 (0.5%)	1.10	4/1527 (0.3%)
1	V	1.01	1/1126 (0.1%)	1.04	3/1527 (0.2%)
1	W	1.06	1/1143 (0.1%)	1.06	4/1550 (0.3%)
1	X	1.06	3/1143 (0.3%)	1.13	6/1550 (0.4%)
All	All	1.15	59/27226 (0.2%)	1.11	130/36924 (0.4%)

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 (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	128	CYS	CB-SG	-10.19	1.65	1.82
1	Q	65	GLU	CG-CD	8.79	1.65	1.51
1	U	65	GLU	CG-CD	8.76	1.65	1.51
1	E	128	CYS	CB-SG	-8.66	1.67	1.82
1	N	128	CYS	CB-SG	-8.65	1.67	1.82
1	V	128	CYS	CB-SG	-7.87	1.68	1.82
1	W	128	CYS	CB-SG	-7.86	1.68	1.82
1	G	128	CYS	CB-SG	-7.83	1.69	1.82
1	N	65	GLU	CG-CD	7.81	1.63	1.51
1	C	128	CYS	CB-SG	-7.73	1.69	1.82
1	L	128	CYS	CB-SG	-7.48	1.69	1.82
1	I	65	GLU	CG-CD	7.46	1.63	1.51
1	S	65	GLU	CG-CD	7.21	1.62	1.51
1	K	128	CYS	CB-SG	-7.21	1.70	1.82
1	U	65	GLU	CB-CG	6.96	1.65	1.52
1	J	65	GLU	CG-CD	6.91	1.62	1.51
1	I	140	GLU	CD-OE2	6.90	1.33	1.25
1	H	111	GLU	CB-CG	6.79	1.65	1.52
1	I	65	GLU	CB-CG	6.61	1.64	1.52
1	H	128	CYS	CB-SG	-6.50	1.71	1.82
1	P	128	CYS	CB-SG	-6.46	1.71	1.82
1	B	65	GLU	CD-OE2	6.46	1.32	1.25
1	M	128	CYS	CB-SG	-6.38	1.71	1.82
1	S	111	GLU	CB-CG	6.38	1.64	1.52
1	E	118	TYR	CB-CG	-6.27	1.42	1.51
1	U	111	GLU	CG-CD	6.20	1.61	1.51
1	U	25	THR	CA-CB	6.08	1.69	1.53
1	O	128	CYS	CB-SG	-6.06	1.72	1.82
1	B	37	GLU	CG-CD	6.04	1.61	1.51
1	U	128	CYS	CB-SG	-5.96	1.72	1.81
1	B	65	GLU	CG-CD	5.84	1.60	1.51
1	P	65	GLU	CG-CD	5.79	1.60	1.51
1	E	37	GLU	CG-CD	5.74	1.60	1.51
1	M	111	GLU	CB-CG	5.65	1.62	1.52
1	N	23	TYR	CG-CD1	5.61	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	107	VAL	CB-CG1	-5.50	1.41	1.52
1	U	111	GLU	CB-CG	5.47	1.62	1.52
1	B	128	CYS	CB-SG	-5.45	1.73	1.81
1	X	65	GLU	CG-CD	5.45	1.60	1.51
1	M	65	GLU	CG-CD	5.41	1.60	1.51
1	I	128	CYS	CB-SG	-5.34	1.73	1.81
1	N	75	VAL	CB-CG1	-5.29	1.41	1.52
1	H	65	GLU	CD-OE2	5.28	1.31	1.25
1	B	23	TYR	C-O	5.28	1.33	1.23
1	C	51	PHE	CD1-CE1	-5.28	1.28	1.39
1	H	111	GLU	CG-CD	5.25	1.59	1.51
1	D	65	GLU	CG-CD	5.21	1.59	1.51
1	X	25	THR	CA-CB	5.20	1.66	1.53
1	E	71	VAL	CB-CG1	5.18	1.63	1.52
1	H	81	TYR	CE1-CZ	-5.16	1.31	1.38
1	N	23	TYR	CE2-CZ	5.12	1.45	1.38
1	B	113	PHE	CD1-CE1	5.10	1.49	1.39
1	I	48	VAL	CB-CG2	-5.09	1.42	1.52
1	E	111	GLU	CB-CG	5.09	1.61	1.52
1	I	21	GLU	CG-CD	5.08	1.59	1.51
1	D	125	ALA	CA-CB	-5.05	1.41	1.52
1	M	111	GLU	CG-CD	5.02	1.59	1.51
1	X	114	ARG	CZ-NH1	5.01	1.39	1.33
1	F	80	ALA	CA-CB	-5.01	1.42	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	LEU	CA-CB-CG	10.34	139.08	115.30
1	D	114	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	O	15	LEU	CA-CB-CG	9.52	137.19	115.30
1	V	61	ASP	CB-CG-OD1	9.22	126.60	118.30
1	A	15	LEU	CB-CG-CD1	-8.93	95.82	111.00
1	U	110	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	B	15	LEU	CA-CB-CG	8.53	134.91	115.30
1	N	15	LEU	CA-CB-CG	8.23	134.23	115.30
1	U	41	LEU	CA-CB-CG	8.13	134.01	115.30
1	G	16	GLY	N-CA-C	-7.75	93.72	113.10
1	W	15	LEU	CA-CB-CG	7.73	133.08	115.30
1	D	89	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	S	15	LEU	CA-CB-CG	7.29	132.06	115.30
1	X	147	LEU	CA-CB-CG	7.18	131.82	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	16	GLY	N-CA-C	-7.01	95.56	113.10
1	D	15	LEU	CA-CB-CG	6.94	131.26	115.30
1	D	30	ASP	CB-CG-OD1	-6.86	112.12	118.30
1	T	89	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	G	15	LEU	CA-CB-CG	6.74	130.81	115.30
1	I	114	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	D	0	LEU	CA-CB-CG	6.73	130.78	115.30
1	D	16	GLY	N-CA-C	-6.71	96.31	113.10
1	K	15	LEU	CA-CB-CG	6.66	130.63	115.30
1	U	16	GLY	N-CA-C	-6.60	96.60	113.10
1	M	116	GLN	CB-CA-C	-6.59	97.22	110.40
1	M	114	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	122	LYS	CD-CE-NZ	-6.54	96.66	111.70
1	B	89	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	R	0	LEU	CA-CB-CG	6.44	130.12	115.30
1	H	49	LEU	CA-CB-CG	6.43	130.08	115.30
1	N	89	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	E	16	GLY	N-CA-C	-6.39	97.13	113.10
1	P	110	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	E	15	LEU	CA-CB-CG	6.36	129.92	115.30
1	N	41	LEU	CA-CB-CG	6.33	129.86	115.30
1	S	16	GLY	N-CA-C	-6.32	97.31	113.10
1	C	16	GLY	N-CA-C	-6.29	97.38	113.10
1	X	14	LEU	CB-CG-CD1	-6.25	100.38	111.00
1	G	90	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	16	GLY	N-CA-C	-6.21	97.57	113.10
1	B	90	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	M	16	GLY	N-CA-C	-6.20	97.59	113.10
1	P	15	LEU	CA-CB-CG	6.19	129.55	115.30
1	G	15	LEU	CB-CG-CD1	-6.19	100.48	111.00
1	T	110	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	16	GLY	N-CA-C	-6.19	97.63	113.10
1	F	41	LEU	CA-CB-CG	6.16	129.47	115.30
1	E	147	LEU	CA-CB-CG	6.16	129.46	115.30
1	O	16	GLY	N-CA-C	-6.10	97.85	113.10
1	B	68	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	S	14	LEU	CB-CG-CD1	-6.08	100.66	111.00
1	W	16	GLY	N-CA-C	-6.08	97.91	113.10
1	D	114	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	C	89	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	114	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	N	68	ARG	NE-CZ-NH2	-6.02	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	15	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	K	18	ARG	N-CA-C	5.99	127.17	111.00
1	J	89	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	H	30	ASP	CB-CG-OD2	5.91	123.62	118.30
1	K	82	THR	CB-CA-C	-5.91	95.64	111.60
1	L	15	LEU	CA-CB-CG	5.91	128.89	115.30
1	Q	45	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	W	147	LEU	CA-CB-CG	5.90	128.87	115.30
1	L	147	LEU	CA-CB-CG	5.89	128.86	115.30
1	C	89	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	90	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	T	15	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	0	LEU	CA-CB-CG	5.76	128.55	115.30
1	V	16	GLY	N-CA-C	-5.74	98.76	113.10
1	B	114	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	28	LEU	CB-CG-CD1	5.70	120.69	111.00
1	D	90	ASP	CB-CG-OD1	5.69	123.42	118.30
1	U	15	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	P	0	LEU	CA-CB-CG	5.68	128.38	115.30
1	T	18	ARG	N-CA-C	5.65	126.25	111.00
1	X	62	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	H	110	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	L	16	GLY	N-CA-C	-5.60	99.10	113.10
1	X	41	LEU	CA-CB-CG	5.58	128.12	115.30
1	T	93	LEU	CB-CG-CD1	-5.55	101.57	111.00
1	R	16	GLY	N-CA-C	-5.54	99.24	113.10
1	F	18	ARG	N-CA-C	5.53	125.94	111.00
1	F	15	LEU	CB-CA-C	5.53	120.70	110.20
1	O	15	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	C	15	LEU	CA-CB-CG	5.51	127.96	115.30
1	B	18	ARG	N-CA-C	5.48	125.81	111.00
1	G	61	ASP	CB-CG-OD1	5.47	123.23	118.30
1	F	114	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	H	15	LEU	CA-CB-CG	5.43	127.80	115.30
1	Q	90	ASP	CB-CG-OD1	5.43	123.19	118.30
1	T	49	LEU	CA-CB-CG	5.43	127.78	115.30
1	I	0	LEU	CA-CB-CG	5.42	127.78	115.30
1	J	15	LEU	CA-CB-CG	5.41	127.75	115.30
1	C	14	LEU	CA-CB-CG	5.40	127.72	115.30
1	X	15	LEU	CA-CB-CG	5.38	127.67	115.30
1	J	16	GLY	N-CA-C	-5.37	99.69	113.10
1	P	114	ARG	NE-CZ-NH1	-5.37	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	116	GLN	CB-CA-C	-5.35	99.69	110.40
1	V	15	LEU	CA-CB-CG	5.34	127.59	115.30
1	D	89	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	41	LEU	CB-CG-CD1	5.31	120.03	111.00
1	D	18	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	J	61	ASP	CB-CG-OD1	5.29	123.06	118.30
1	R	18	ARG	N-CA-C	5.29	125.29	111.00
1	K	147	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	130	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	K	15	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	A	93	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	A	121	ASP	CB-CG-OD1	5.24	123.01	118.30
1	D	18	ARG	N-CA-C	5.24	125.13	111.00
1	L	12	LEU	CA-CB-CG	-5.23	103.26	115.30
1	T	61	ASP	CB-CG-OD1	5.22	123.00	118.30
1	F	61	ASP	CB-CG-OD1	5.20	122.98	118.30
1	X	12	LEU	CA-CB-CG	-5.20	103.35	115.30
1	I	114	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	T	89	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	M	146	GLN	N-CA-C	5.16	124.92	111.00
1	T	16	GLY	N-CA-C	-5.15	100.22	113.10
1	W	69	GLN	CB-CA-C	-5.14	100.12	110.40
1	B	14	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	P	121	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	F	16	GLY	N-CA-C	-5.09	100.39	113.10
1	H	30	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	K	127	ILE	CB-CA-C	-5.06	101.48	111.60
1	J	12	LEU	CA-CB-CG	-5.03	103.72	115.30
1	G	12	LEU	CA-CB-CG	-5.02	103.74	115.30
1	B	0	LEU	CA-CB-CG	5.01	126.83	115.30
1	D	90	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	M	12	LEU	CA-CB-CG	-5.01	103.78	115.30

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	25	0
1	B	1108	0	1117	32	0
1	C	1108	0	1117	30	0
1	D	1117	0	1125	24	0
1	E	1125	0	1136	25	0
1	F	1125	0	1136	29	0
1	G	1108	0	1117	23	0
1	H	1116	0	1128	22	0
1	I	1142	0	1150	28	0
1	J	1108	0	1117	29	0
1	K	1116	0	1128	24	0
1	L	1116	0	1128	29	0
1	M	1116	0	1128	35	0
1	N	1116	0	1128	30	0
1	O	1116	0	1128	23	0
1	P	1116	0	1128	27	0
1	Q	1116	0	1128	30	0
1	R	1116	0	1128	26	0
1	S	1116	0	1128	33	0
1	T	1117	0	1125	40	0
1	U	1108	0	1117	33	0
1	V	1108	0	1117	28	0
1	W	1125	0	1136	33	0
1	X	1125	0	1136	28	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27144	0	27139	646	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 12.

All (646) 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:N:146:GLN:HA	1:N:146:GLN:NE2	1.68	1.07
1:J:12:LEU:O	1:J:15:LEU:HD22	1.54	1.07
1:N:146:GLN:HA	1:N:146:GLN:HE21	0.94	1.06
1:T:103:HIS:HB2	1:T:128:CYS:HB2	1.44	0.99
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:0:LEU:H2	1:M:147:LEU:HG	1.48	0.76
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
1:U:13:ASN:H	1:U:13:ASN:ND2	1.85	0.71
1:J:103:HIS:HB2	1:J:128:CYS:HB2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:103:HIS:HB2	1:A:128:CYS:HB2	1.82	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:J:106:ASN:HD22	1:J:106:ASN:C	2.09	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:H:23:TYR:CD2	1:H:23:TYR:C	2.79	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:H:76:ILE:HG23	1:H:76:ILE:O	2.06	0.55
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:I:32:GLU:O	1:I:36:ILE:HG13	2.06	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:106:ASN:HD22	1:Q:106:ASN:C	2.11	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:V:47:GLU:OE2	1:V:49:LEU:HD21	2.07	0.53
1:B:106:ASN:C	1:B:106:ASN:HD22	2.11	0.53
1:O:58:PHE:N	1:O:58:PHE:CD1	2.73	0.53
1:R:15:LEU:HD22	1:R:15:LEU:H	1.72	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
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:P:129:GLY:C	1:V:125:ALA:HB2	2.30	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:C:44:ASN:O	1:C:45:ASP:HB2	2.10	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:S:23:TYR:CD2	1:S:23:TYR:C	2.82	0.52
1:M:10:PRO:O	1:M:11:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:96:ALA:HB2	1:U:18:ARG:HD3	1.93	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:Q:106:ASN:ND2	1:Q:106:ASN:C	2.63	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:M:0:LEU:H1	1:M:147:LEU:HG	1.75	0.49
1:N:49:LEU:N	1:N:49:LEU:HD23	2.28	0.48
1:P:44:ASN:CG	1:P:44:ASN:O	2.50	0.48
1:V:63:ILE:O	1:V:66:ALA:HB3	2.13	0.48
1:V:106:ASN:HD22	1:V:106:ASN:C	2.16	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:J:106:ASN:C	1:J:106:ASN:ND2	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:99:PHE:CE2	1:B:123:ALA:HB2	2.48	0.48
1:E:65:GLU:O	1:E:69:GLN:HG3	2.14	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:C:106:ASN:C	1:C:106:ASN:HD22	2.18	0.47
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:D:23:TYR:CD2	1:D:23:TYR:C	2.87	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:O:106:ASN:C	1:O:106:ASN:HD22	2.17	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:D:146:GLN:NE2	1:D:146:GLN:CA	2.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:51:PHE:CG	1:N:62:ARG:HG2	2.50	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: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: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
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:S:115:HIS:C	1:S:116:GLN:HE21	2.19	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:A:106:ASN:C	1:A:106:ASN:HD22	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:P:15:LEU:HA	1:P:16:GLY:HA2	1.45	0.45
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: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:A:106:ASN:C	1:A:106:ASN:ND2	2.70	0.44
1:O:31:ILE:HG12	1:O:132:VAL:HG22	1.98	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:I:13:ASN:ND2	1:I:13:ASN:N	2.57	0.44
1:X:39:ALA:O	1:X:40:LYS:C	2.56	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: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:P:8:ASN:ND2	1:P:135:TYR:OH	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:J:12:LEU:C	1:J:14:LEU:H	2.21	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
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:B:106:ASN:C	1:B:106:ASN:ND2	2.70	0.43
1:E:32:GLU:HB3	1:E:50:VAL:HG11	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:44:ASN:C	1:A:44:ASN:OD1	2.56	0.43
1:O:89:ARG:HH11	1:O:89:ARG:HD3	1.67	0.43
1:T:106:ASN:C	1:T:106:ASN:HD22	2.21	0.43
1:D:112:PRO:HA	1:D:115:HIS:CD2	2.54	0.43
1:G:43:ASN:O	1:G:43:ASN:CG	2.57	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: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:W:67:LYS:NZ	1:W:95:THR:O	2.38	0.43
1:R:8:ASN:O	1:R:52:GLN:HA	2.19	0.43
1:L:100:ILE:HD11	1:L:141:TYR:CD1	2.54	0.43
1:N:12:LEU:C	1:N:14:LEU:H	2.21	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:G:77:ASN:C	1:G:77:ASN:OD1	2.57	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:Q:13:ASN:H	1:Q:13:ASN:ND2	2.15	0.42
1:R:35:ALA:HB1	1:R:139:ILE:CD1	2.49	0.42
1:A:77:ASN:OD1	1:A:77:ASN:C	2.57	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:HG2	2.20	0.42
1:C:8:ASN:O	1:C:52:GLN:HA	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:M:40:LYS:HE2	1:M:40:LYS:HB3	1.95	0.42
1:W:106:ASN:C	1:W:106:ASN:HD22	2.23	0.42
1:A:23:TYR:O	1:A:23:TYR:CG	2.72	0.42
1:C:106:ASN:ND2	1:C:106:ASN:C	2.72	0.42
1:F:93:LEU:HD21	1:F:122:LYS:HD2	2.02	0.42
1:T:23:TYR:CD2	1:T:23:TYR:C	2.92	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:X:1:VAL:C	1:X:2:LYS:HG2	2.40	0.42
1:B:13:ASN:HA	1:B:28:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:106:ASN:ND2	1:T:106:ASN:C	2.73	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: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:108:HIS:HA	1:W:115:HIS:CD2	2.55	0.41
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: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: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:146:GLN:H	1:O:146:GLN:HG2	1.49	0.41
1:S:11:ASN:O	1:S:14:LEU:HB2	2.20	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:U:1:VAL:HG11	1:U:73:PHE:HB2	2.02	0.41
1:V:106:ASN:ND2	1:V:106:ASN:C	2.74	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: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: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:K:106:ASN:C	1:K:106:ASN:ND2	2.74	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:F:39:ALA:O	1:F:40:LYS:C	2.58	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:F:106:ASN:HD22	1:F:106:ASN:C	2.24	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: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%)	11	39
1	B	139/167 (83%)	131 (94%)	8 (6%)	0	100	100
1	C	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	22	56
1	D	140/167 (84%)	132 (94%)	7 (5%)	1 (1%)	22	56
1	E	141/167 (84%)	127 (90%)	13 (9%)	1 (1%)	22	56
1	F	141/167 (84%)	133 (94%)	7 (5%)	1 (1%)	22	56
1	G	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	22	56
1	H	140/167 (84%)	133 (95%)	6 (4%)	1 (1%)	22	56
1	I	145/167 (87%)	136 (94%)	8 (6%)	1 (1%)	22	56
1	J	139/167 (83%)	127 (91%)	10 (7%)	2 (1%)	11	39
1	K	140/167 (84%)	130 (93%)	9 (6%)	1 (1%)	22	56
1	L	140/167 (84%)	128 (91%)	11 (8%)	1 (1%)	22	56
1	M	140/167 (84%)	127 (91%)	10 (7%)	3 (2%)	7	29
1	N	140/167 (84%)	131 (94%)	8 (6%)	1 (1%)	22	56
1	O	140/167 (84%)	129 (92%)	11 (8%)	0	100	100
1	P	140/167 (84%)	131 (94%)	8 (6%)	1 (1%)	22	56
1	Q	140/167 (84%)	126 (90%)	13 (9%)	1 (1%)	22	56
1	R	140/167 (84%)	133 (95%)	7 (5%)	0	100	100
1	S	140/167 (84%)	124 (89%)	13 (9%)	3 (2%)	7	29
1	T	140/167 (84%)	129 (92%)	7 (5%)	4 (3%)	4	21
1	U	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	22	56
1	V	139/167 (83%)	121 (87%)	16 (12%)	2 (1%)	11	39
1	W	141/167 (84%)	131 (93%)	8 (6%)	2 (1%)	11	39
1	X	141/167 (84%)	127 (90%)	13 (9%)	1 (1%)	22	56
All	All	3362/4008 (84%)	3113 (93%)	217 (6%)	32 (1%)	15	48

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	118/137 (86%)	107 (91%)	11 (9%)	9 30
1	B	118/137 (86%)	106 (90%)	12 (10%)	7 25
1	C	118/137 (86%)	106 (90%)	12 (10%)	7 25
1	D	119/137 (87%)	109 (92%)	10 (8%)	11 35
1	E	120/137 (88%)	110 (92%)	10 (8%)	11 35
1	F	120/137 (88%)	110 (92%)	10 (8%)	11 35
1	G	118/137 (86%)	107 (91%)	11 (9%)	9 30
1	H	119/137 (87%)	114 (96%)	5 (4%)	30 63
1	I	122/137 (89%)	113 (93%)	9 (7%)	13 41
1	J	118/137 (86%)	105 (89%)	13 (11%)	6 22
1	K	119/137 (87%)	105 (88%)	14 (12%)	5 20
1	L	119/137 (87%)	112 (94%)	7 (6%)	19 50
1	M	119/137 (87%)	111 (93%)	8 (7%)	16 45
1	N	119/137 (87%)	109 (92%)	10 (8%)	11 35
1	O	119/137 (87%)	109 (92%)	10 (8%)	11 35
1	P	119/137 (87%)	111 (93%)	8 (7%)	16 45
1	Q	119/137 (87%)	108 (91%)	11 (9%)	9 30
1	R	119/137 (87%)	111 (93%)	8 (7%)	16 45
1	S	119/137 (87%)	103 (87%)	16 (13%)	4 15
1	T	119/137 (87%)	104 (87%)	15 (13%)	4 17
1	U	118/137 (86%)	104 (88%)	14 (12%)	5 20
1	V	118/137 (86%)	107 (91%)	11 (9%)	9 30
1	W	120/137 (88%)	108 (90%)	12 (10%)	7 26
1	X	120/137 (88%)	102 (85%)	18 (15%)	3 12
All	All	2856/3288 (87%)	2591 (91%)	265 (9%)	9 30

All (265) 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	23	TYR
1	A	82	THR

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Mol	Chain	Res	Type
1	A	89	ARG
1	A	106	ASN
1	A	116	GLN
1	A	128	CYS
1	A	132	VAL
1	B	15	LEU
1	B	25	THR
1	B	29	SER
1	B	33	GLN
1	B	67	LYS
1	B	69	GLN
1	B	89	ARG
1	B	106	ASN
1	B	112	PRO
1	B	116	GLN
1	B	128	CYS
1	B	132	VAL
1	C	0	LEU
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	140	GLU
1	D	0	LEU
1	D	15	LEU
1	D	17	THR
1	D	18	ARG
1	D	40	LYS
1	D	41	LEU
1	D	46	SER
1	D	128	CYS
1	D	132	VAL
1	D	146	GLN
1	E	15	LEU
1	E	17	THR
1	E	23	TYR

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Mol	Chain	Res	Type
1	E	32	GLU
1	E	37	GLU
1	E	53	SER
1	E	89	ARG
1	E	106	ASN
1	E	107	VAL
1	E	128	CYS
1	F	-1	GLN
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	106	ASN
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
1	G	146	GLN
1	H	0	LEU
1	H	15	LEU
1	H	17	THR
1	H	23	TYR
1	H	97	ILE
1	I	13	ASN
1	I	17	THR
1	I	18	ARG
1	I	21	GLU
1	I	53	SER
1	I	67	LYS
1	I	89	ARG
1	I	128	CYS
1	I	140	GLU

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Mol	Chain	Res	Type
1	J	0	LEU
1	J	3	LYS
1	J	13	ASN
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	106	ASN
1	J	107	VAL
1	J	116	GLN
1	K	13	ASN
1	K	14	LEU
1	K	15	LEU
1	K	17	THR
1	K	29	SER
1	K	53	SER
1	K	67	LYS
1	K	68	ARG
1	K	82	THR
1	K	116	GLN
1	K	126	VAL
1	K	128	CYS
1	K	132	VAL
1	K	146	GLN
1	L	3	LYS
1	L	15	LEU
1	L	17	THR
1	L	45	ASP
1	L	53	SER
1	L	89	ARG
1	L	128	CYS
1	M	15	LEU
1	M	17	THR
1	M	23	TYR
1	M	25	THR
1	M	45	ASP
1	M	116	GLN
1	M	126	VAL
1	M	147	LEU

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Mol	Chain	Res	Type
1	N	0	LEU
1	N	3	LYS
1	N	15	LEU
1	N	29	SER
1	N	89	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
1	O	28	LEU
1	O	45	ASP
1	O	69	GLN
1	O	106	ASN
1	O	128	CYS
1	O	132	VAL
1	O	147	LEU
1	P	3	LYS
1	P	15	LEU
1	P	17	THR
1	P	69	GLN
1	P	89	ARG
1	P	109	GLN
1	P	116	GLN
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	106	ASN
1	Q	116	GLN
1	Q	128	CYS
1	R	2	LYS
1	R	3	LYS
1	R	13	ASN

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Mol	Chain	Res	Type
1	R	15	LEU
1	R	17	THR
1	R	25	THR
1	R	89	ARG
1	R	116	GLN
1	S	0	LEU
1	S	3	LYS
1	S	15	LEU
1	S	17	THR
1	S	23	TYR
1	S	29	SER
1	S	41	LEU
1	S	45	ASP
1	S	62	ARG
1	S	68	ARG
1	S	89	ARG
1	S	109	GLN
1	S	112	PRO
1	S	116	GLN
1	S	128	CYS
1	S	147	LEU
1	T	-1	GLN
1	T	0	LEU
1	T	15	LEU
1	T	17	THR
1	T	18	ARG
1	T	25	THR
1	T	29	SER
1	T	40	LYS
1	T	68	ARG
1	T	89	ARG
1	T	106	ASN
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

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Mol	Chain	Res	Type
1	U	25	THR
1	U	41	LEU
1	U	69	GLN
1	U	106	ASN
1	U	109	GLN
1	U	112	PRO
1	U	116	GLN
1	U	117	SER
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	89	ARG
1	V	106	ASN
1	V	116	GLN
1	V	128	CYS
1	W	-1	GLN
1	W	0	LEU
1	W	1	VAL
1	W	15	LEU
1	W	17	THR
1	W	38	GLN
1	W	41	LEU
1	W	45	ASP
1	W	89	ARG
1	W	106	ASN
1	W	116	GLN
1	W	120	SER
1	X	-1	GLN
1	X	0	LEU
1	X	3	LYS
1	X	15	LEU
1	X	17	THR
1	X	26	THR
1	X	40	LYS
1	X	46	SER
1	X	67	LYS
1	X	89	ARG
1	X	106	ASN

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Mol	Chain	Res	Type
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	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) 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	A	144	ASN
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	106	ASN
1	C	109	GLN
1	C	144	ASN
1	D	8	ASN
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
1	F	8	ASN
1	F	13	ASN
1	F	83	HIS
1	F	106	ASN
1	F	109	GLN
1	F	144	ASN
1	G	8	ASN

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Mol	Chain	Res	Type
1	G	83	HIS
1	G	109	GLN
1	H	8	ASN
1	H	115	HIS
1	I	8	ASN
1	I	13	ASN
1	I	106	ASN
1	I	109	GLN
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	146	GLN
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	109	GLN
1	L	115	HIS
1	M	8	ASN
1	M	109	GLN
1	M	115	HIS
1	M	146	GLN
1	N	8	ASN
1	N	106	ASN
1	N	108	HIS
1	N	146	GLN
1	O	8	ASN
1	O	106	ASN
1	O	109	GLN
1	P	8	ASN
1	P	106	ASN
1	P	109	GLN
1	P	115	HIS
1	Q	8	ASN
1	Q	13	ASN
1	Q	106	ASN

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Mol	Chain	Res	Type
1	R	8	ASN
1	R	13	ASN
1	R	109	GLN
1	S	8	ASN
1	S	83	HIS
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
1	U	83	HIS
1	U	106	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	X	8	ASN
1	X	83	HIS
1	X	106	ASN
1	X	108	HIS
1	X	109	GLN
1	X	115	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	TRS	D	156	-	7,7,7	0.66	0	9,9,9	1.79	3 (33%)
2	SO4	U	155	-	4,4,4	0.37	0	6,6,6	1.44	1 (16%)
2	SO4	I	155	-	4,4,4	0.49	0	6,6,6	1.42	1 (16%)
2	SO4	E	155	-	4,4,4	0.32	0	6,6,6	0.97	0
3	TRS	T	156	-	7,7,7	0.55	0	9,9,9	1.08	0
2	SO4	M	155	-	4,4,4	0.59	0	6,6,6	0.95	0
2	SO4	Q	155	-	4,4,4	0.62	0	6,6,6	1.12	1 (16%)
2	SO4	D	155	-	4,4,4	0.56	0	6,6,6	0.71	0
2	SO4	R	155	-	4,4,4	0.28	0	6,6,6	1.19	1 (16%)
2	SO4	G	155	-	4,4,4	0.63	0	6,6,6	1.13	1 (16%)
2	SO4	V	155	-	4,4,4	0.32	0	6,6,6	0.42	0
3	TRS	J	156	-	7,7,7	0.69	0	9,9,9	0.79	0
3	TRS	P	156	-	7,7,7	0.63	0	9,9,9	1.93	5 (55%)
2	SO4	A	156	-	4,4,4	0.58	0	6,6,6	0.77	0
3	TRS	N	156	-	7,7,7	0.39	0	9,9,9	0.63	0
2	SO4	N	155	-	4,4,4	0.27	0	6,6,6	1.02	0
2	SO4	T	155	-	4,4,4	0.40	0	6,6,6	0.88	0
2	SO4	H	155	-	4,4,4	0.54	0	6,6,6	0.83	0
2	SO4	X	155	-	4,4,4	0.50	0	6,6,6	0.79	0
3	TRS	G	156	-	7,7,7	0.81	0	9,9,9	1.44	1 (11%)
2	SO4	O	155	-	4,4,4	0.44	0	6,6,6	0.98	0
2	SO4	W	155	-	4,4,4	0.41	0	6,6,6	0.86	0
2	SO4	P	155	-	4,4,4	0.37	0	6,6,6	0.84	0
2	SO4	A	155	-	4,4,4	0.56	0	6,6,6	1.07	1 (16%)
2	SO4	B	155	-	4,4,4	0.54	0	6,6,6	1.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	S	155	-	4,4,4	0.51	0	6,6,6	1.01	0
3	TRS	W	156	-	7,7,7	0.78	0	9,9,9	1.18	1 (11%)
2	SO4	K	155	-	4,4,4	0.26	0	6,6,6	0.60	0
2	SO4	C	155	-	4,4,4	0.48	0	6,6,6	0.84	0
2	SO4	F	155	-	4,4,4	0.53	0	6,6,6	1.54	1 (16%)
3	TRS	A	157	-	7,7,7	0.75	0	9,9,9	1.33	1 (11%)
2	SO4	J	155	-	4,4,4	0.54	0	6,6,6	0.80	0

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	156	TRS	1	0
3	N	156	TRS	1	0
3	W	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, 95^{th} 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%)	-0.02	0 100 100	35, 49, 85, 114	0
1	B	143/167 (85%)	0.05	0 100 100	34, 47, 73, 93	0
1	C	143/167 (85%)	-0.02	1 (0%) 87 76	37, 54, 93, 112	0
1	D	144/167 (86%)	0.17	3 (2%) 63 46	36, 51, 90, 120	0
1	E	145/167 (86%)	0.02	0 100 100	33, 46, 85, 113	0
1	F	145/167 (86%)	0.05	0 100 100	34, 45, 75, 105	0
1	G	143/167 (85%)	0.13	4 (2%) 53 36	37, 52, 96, 113	0
1	H	144/167 (86%)	0.02	1 (0%) 87 76	37, 54, 93, 110	0
1	I	147/167 (88%)	-0.03	0 100 100	36, 45, 78, 102	0
1	J	143/167 (85%)	0.62	17 (11%) 4 2	44, 57, 96, 120	0
1	K	144/167 (86%)	0.35	10 (6%) 16 10	44, 57, 100, 111	0
1	L	144/167 (86%)	0.18	7 (4%) 29 18	46, 59, 104, 118	0
1	M	144/167 (86%)	-0.02	0 100 100	40, 51, 95, 112	0
1	N	144/167 (86%)	0.07	1 (0%) 87 76	39, 49, 81, 96	0
1	O	144/167 (86%)	-0.10	0 100 100	40, 54, 95, 106	0
1	P	144/167 (86%)	0.01	1 (0%) 87 76	39, 53, 97, 113	0
1	Q	144/167 (86%)	0.10	2 (1%) 75 59	37, 50, 92, 112	0
1	R	144/167 (86%)	0.20	2 (1%) 75 59	34, 48, 89, 108	0
1	S	144/167 (86%)	0.34	9 (6%) 20 11	41, 56, 101, 113	0
1	T	144/167 (86%)	0.44	14 (9%) 7 4	43, 60, 109, 127	0
1	U	143/167 (85%)	0.09	2 (1%) 75 59	41, 53, 93, 119	0
1	V	143/167 (85%)	0.18	4 (2%) 53 36	48, 60, 102, 124	0
1	W	145/167 (86%)	0.32	8 (5%) 25 15	49, 60, 110, 121	0
1	X	145/167 (86%)	0.23	7 (4%) 30 19	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%)	0.14	93 (2%) 54 38	33, 54, 97, 127	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	0	LEU	5.2
1	R	147	LEU	5.0
1	W	0	LEU	4.6
1	Q	25	THR	4.6
1	D	25	THR	4.4
1	W	145	TYR	4.2
1	K	6	LEU	4.2
1	X	25	THR	4.1
1	J	18	ARG	4.1
1	V	0	LEU	4.0
1	W	4	VAL	4.0
1	H	25	THR	3.9
1	T	18	ARG	3.8
1	T	25	THR	3.7
1	T	-1	GLN	3.6
1	J	143	LEU	3.5
1	T	1	VAL	3.5
1	S	0	LEU	3.4
1	C	25	THR	3.4
1	J	31	ILE	3.3
1	V	47	GLU	3.3
1	J	25	THR	3.2
1	J	42	LYS	3.1
1	S	4	VAL	3.1
1	J	71	VAL	3.1
1	G	18	ARG	3.0
1	L	25	THR	3.0
1	J	48	VAL	3.0
1	P	43	ASN	3.0
1	G	36	ILE	2.9
1	X	45	ASP	2.9
1	W	143	LEU	2.8
1	T	63	ILE	2.8
1	J	145	TYR	2.8
1	D	138	ALA	2.7
1	J	49	LEU	2.7
1	T	4	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	1	VAL	2.7
1	K	1	VAL	2.7
1	X	3	LYS	2.7
1	T	6	LEU	2.6
1	K	147	LEU	2.6
1	R	23	TYR	2.6
1	W	6	LEU	2.6
1	L	63	ILE	2.6
1	L	6	LEU	2.6
1	T	23	TYR	2.6
1	S	46	SER	2.5
1	S	145	TYR	2.5
1	Q	1	VAL	2.5
1	L	147	LEU	2.5
1	J	73	PHE	2.5
1	K	143	LEU	2.5
1	S	49	LEU	2.5
1	S	143	LEU	2.5
1	V	73	PHE	2.4
1	K	127	ILE	2.4
1	D	1	VAL	2.4
1	X	48	VAL	2.4
1	J	1	VAL	2.3
1	J	63	ILE	2.3
1	X	46	SER	2.2
1	U	18	ARG	2.2
1	T	75	VAL	2.2
1	N	25	THR	2.2
1	J	43	ASN	2.2
1	S	147	LEU	2.2
1	K	0	LEU	2.2
1	J	60	ILE	2.2
1	K	76	ILE	2.1
1	T	138	ALA	2.1
1	J	47	GLU	2.1
1	J	0	LEU	2.1
1	T	68	ARG	2.1
1	K	4	VAL	2.1
1	W	73	PHE	2.1
1	K	49	LEU	2.1
1	K	63	ILE	2.1
1	S	39	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	W	2	LYS	2.1
1	T	24	GLY	2.1
1	U	25	THR	2.1
1	G	39	ALA	2.1
1	L	2	LYS	2.1
1	T	48	VAL	2.1
1	J	24	GLY	2.1
1	G	0	LEU	2.0
1	L	23	TYR	2.0
1	S	8	ASN	2.0
1	X	47	GLU	2.0
1	W	-1	GLN	2.0
1	X	18	ARG	2.0
1	V	1	VAL	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 monosaccharides 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, 95^{th} 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	J	155	5/5	0.77	0.26	116,118,119,119	0
2	SO4	T	155	5/5	0.78	0.22	113,115,116,117	0
2	SO4	A	155	5/5	0.81	0.29	100,102,105,107	0
2	SO4	K	155	5/5	0.82	0.22	116,117,118,118	0
2	SO4	M	155	5/5	0.83	0.25	106,108,111,112	0
2	SO4	H	155	5/5	0.83	0.21	101,103,105,108	0
2	SO4	X	155	5/5	0.83	0.19	107,109,111,113	0
2	SO4	S	155	5/5	0.84	0.32	100,102,105,106	0
2	SO4	O	155	5/5	0.84	0.23	111,114,115,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	Q	155	5/5	0.84	0.25	94,97,99,101	0
2	SO4	P	155	5/5	0.85	0.27	106,107,108,110	0
2	SO4	C	155	5/5	0.86	0.23	111,112,114,117	0
2	SO4	W	155	5/5	0.86	0.26	110,113,114,115	0
2	SO4	E	155	5/5	0.86	0.26	108,110,111,113	0
2	SO4	U	155	5/5	0.89	0.16	101,103,104,105	0
2	SO4	F	155	5/5	0.91	0.24	88,91,96,97	0
2	SO4	G	155	5/5	0.92	0.21	86,90,93,95	0
2	SO4	V	155	5/5	0.92	0.13	110,111,112,112	0
2	SO4	D	155	5/5	0.93	0.19	95,95,97,100	0
2	SO4	R	155	5/5	0.93	0.22	96,98,99,100	0
2	SO4	I	155	5/5	0.94	0.26	67,67,71,72	0
2	SO4	N	155	5/5	0.94	0.22	85,88,88,91	0
2	SO4	B	155	5/5	0.95	0.19	84,84,90,91	0
2	SO4	A	156	5/5	0.95	0.28	88,89,91,91	0
3	TRS	J	156	8/8	0.95	0.23	45,49,50,50	0
3	TRS	W	156	8/8	0.95	0.17	52,55,56,56	0
3	TRS	G	156	8/8	0.96	0.22	41,43,44,44	0
3	TRS	T	156	8/8	0.97	0.23	50,52,52,53	0
3	TRS	A	157	8/8	0.97	0.15	38,44,45,45	0
3	TRS	P	156	8/8	0.98	0.20	35,38,38,41	0
3	TRS	D	156	8/8	0.98	0.23	40,40,41,42	0
3	TRS	N	156	8/8	0.98	0.22	35,38,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.