wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 06:58 am BST

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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

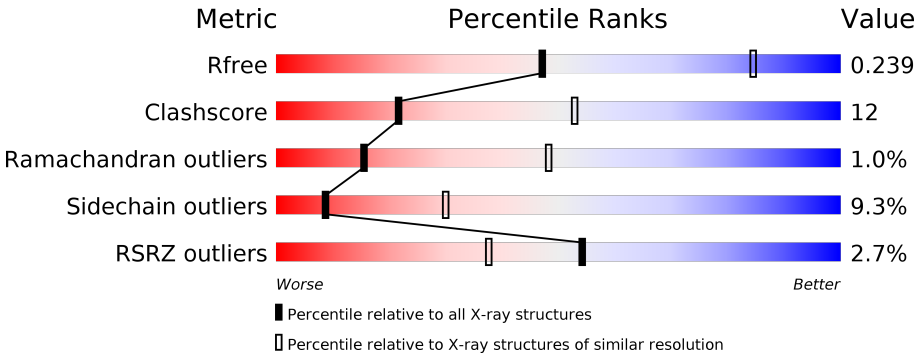
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 on 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%
1	F	167	61% 23% • • 13%

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Mol	Chain	Length	Quality of chain
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	-	-

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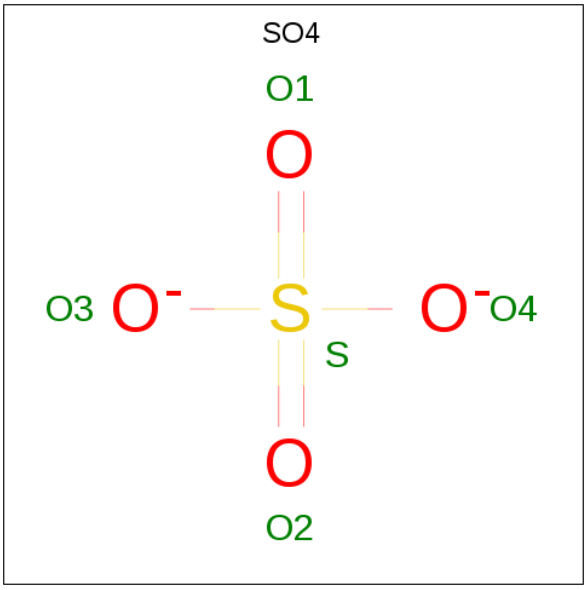
Chain	Residue	Modelled	Actual	Comment	Reference
X	154	ALA	-	expression tag	UNP Q59Z17

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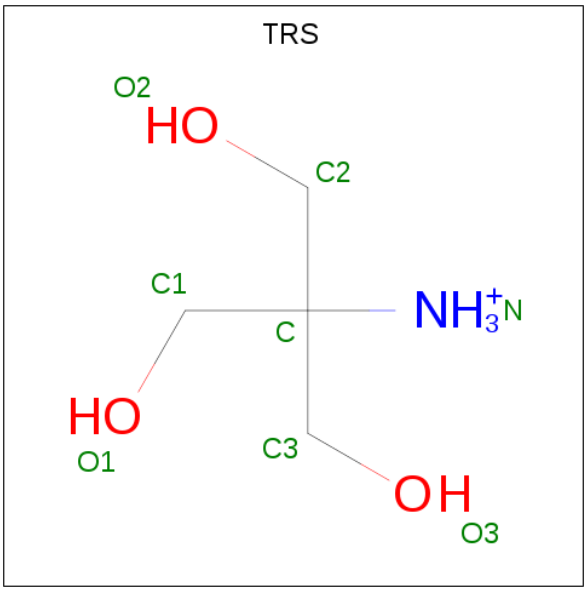
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0
2	T	1	Total O S 5 4 1	0	0
2	U	1	Total O S 5 4 1	0	0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

- 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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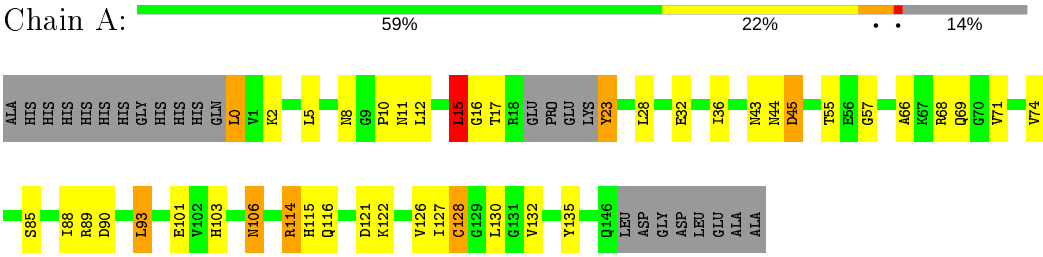
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	17	Total O 17 17	0	0
4	F	10	Total O 10 10	0	0
4	G	9	Total O 9 9	0	0
4	H	4	Total O 4 4	0	0
4	I	11	Total O 11 11	0	0
4	J	4	Total O 4 4	0	0
4	K	5	Total O 5 5	0	0
4	L	4	Total O 4 4	0	0
4	M	4	Total O 4 4	0	0
4	N	11	Total O 11 11	0	0
4	O	2	Total O 2 2	0	0
4	P	8	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 and DNA 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.

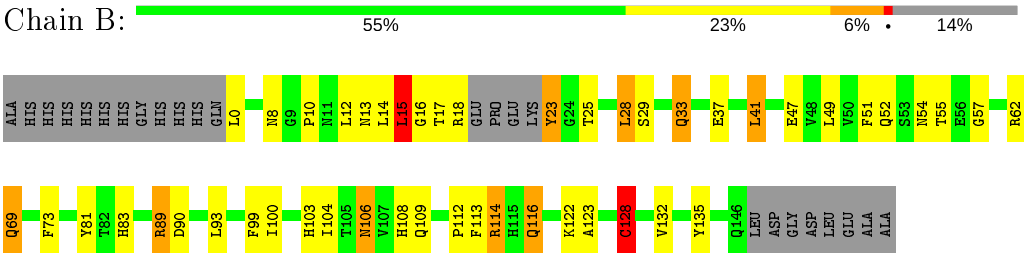
- Molecule 1: 3-dehydroquinase, type II

Chain A:



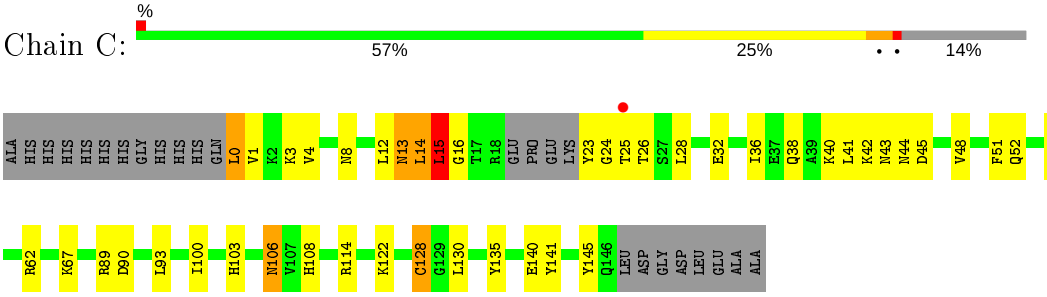
- Molecule 1: 3-dehydroquinase, type II

Chain B:



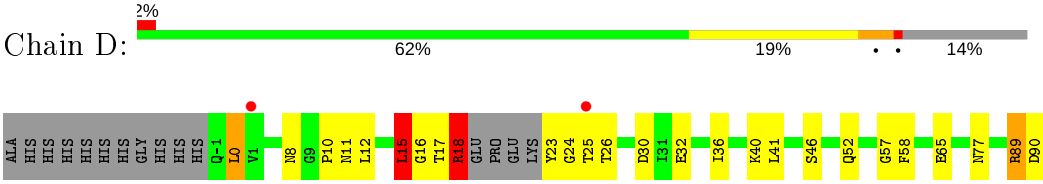
- Molecule 1: 3-dehydroquinase, type II

Chain C:



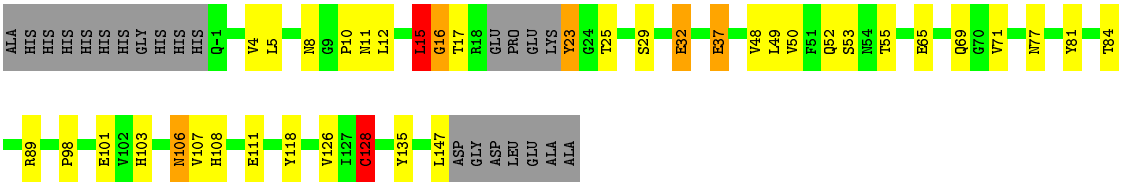
- Molecule 1: 3-dehydroquinase, type II

Chain D:



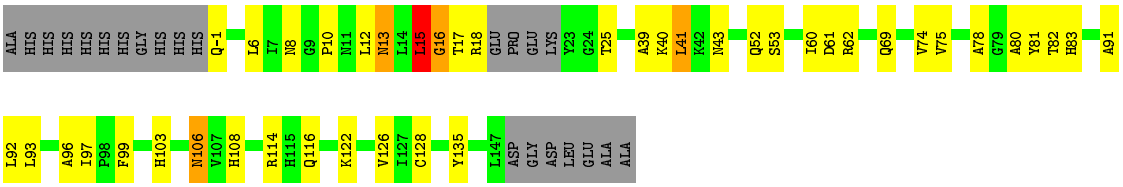
• Molecule 1: 3-dehydroquinase, type II

Chain E:



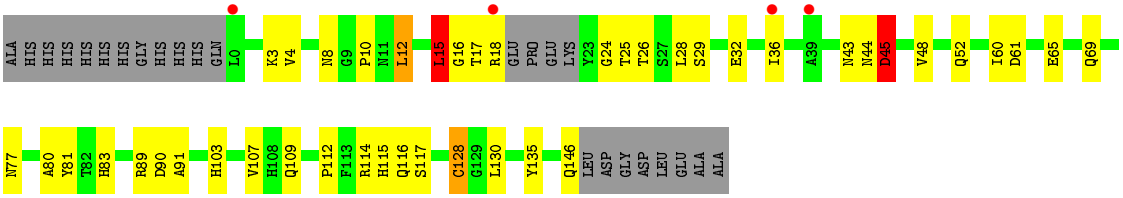
• Molecule 1: 3-dehydroquinase, type II

Chain F:



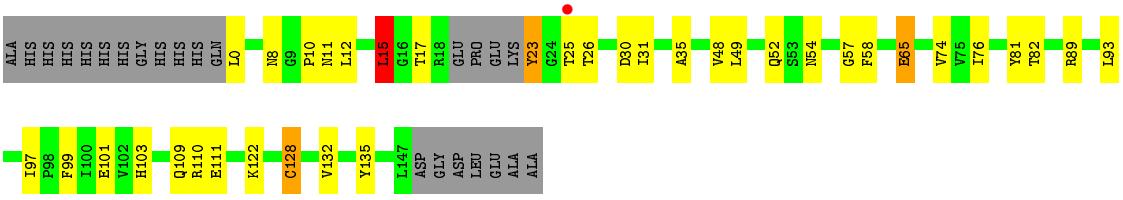
• Molecule 1: 3-dehydroquinase, type II

Chain G:



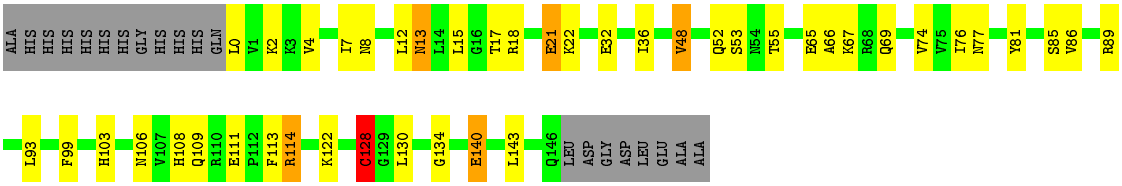
• Molecule 1: 3-dehydroquinase, type II

Chain H:



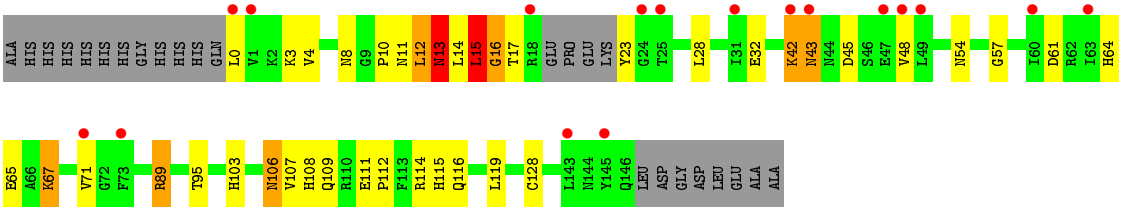
• Molecule 1: 3-dehydroquinase, type II

Chain I:



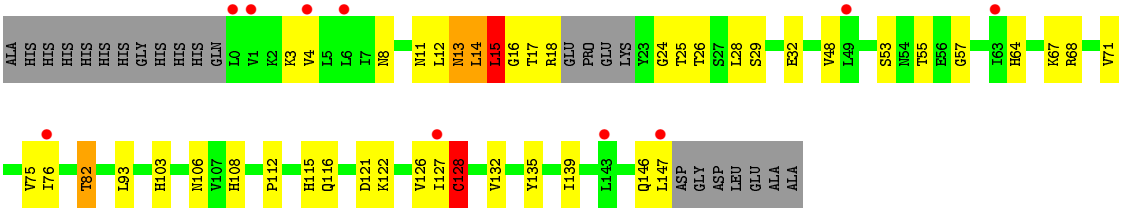
• Molecule 1: 3-dehydroquinase, type II

Chain J:



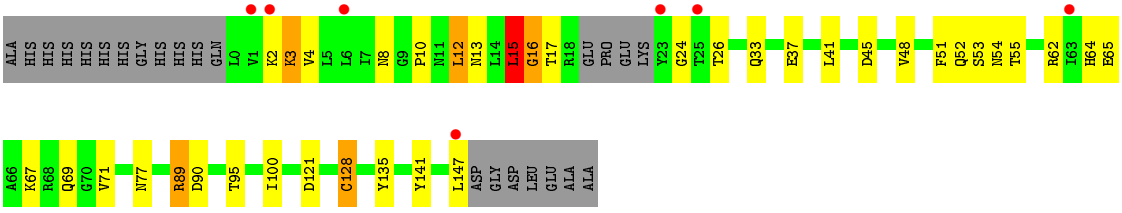
• Molecule 1: 3-dehydroquinase, type II

Chain K:



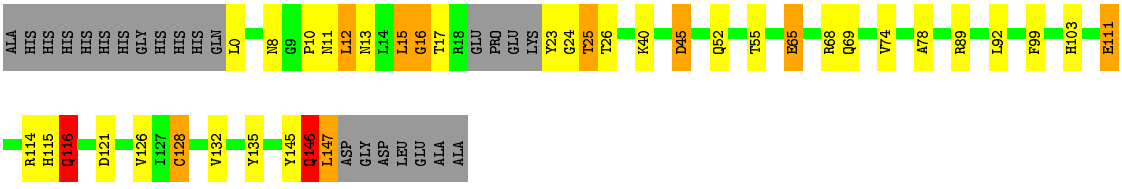
• Molecule 1: 3-dehydroquinase, type II

Chain L:



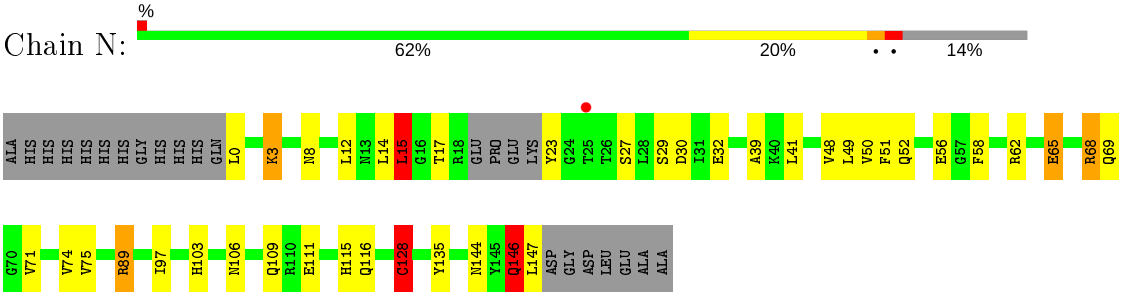
• Molecule 1: 3-dehydroquinase, type II

Chain M:



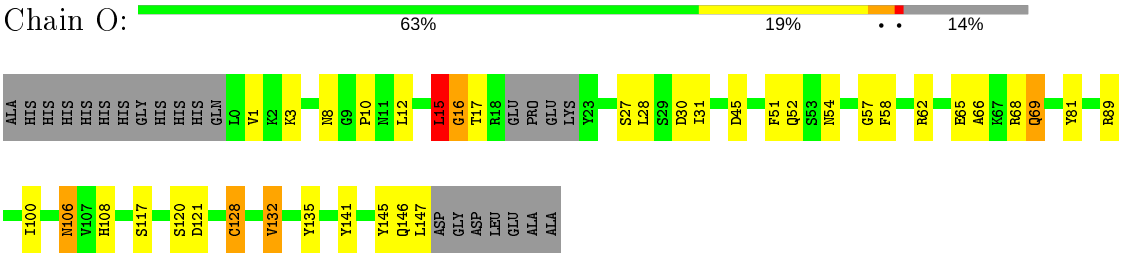
• Molecule 1: 3-dehydroquinase, type II

Chain N:



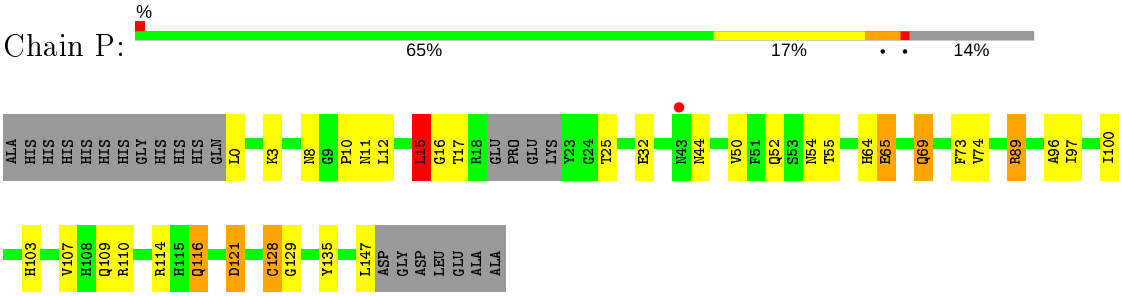
• Molecule 1: 3-dehydroquinase, type II

Chain O:



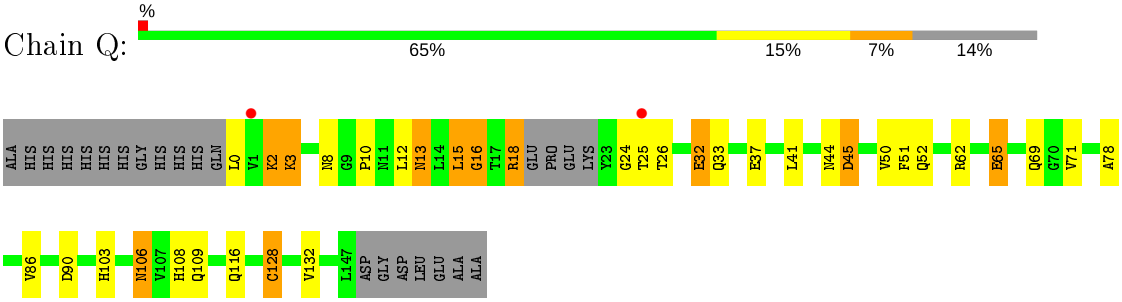
• Molecule 1: 3-dehydroquinase, type II

Chain P:



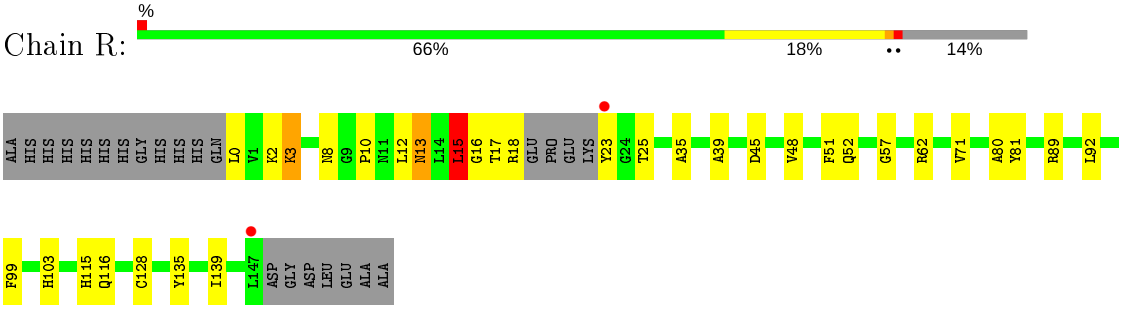
• Molecule 1: 3-dehydroquinase, type II

Chain Q:



• Molecule 1: 3-dehydroquinase, type II

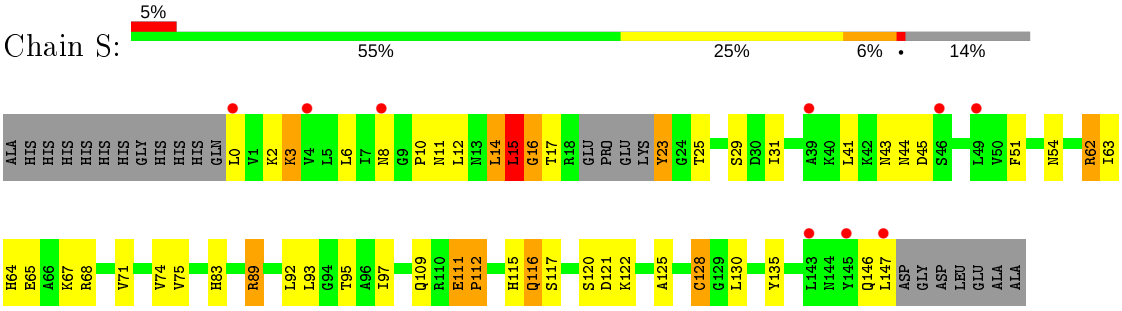
Chain R:



• Molecule 1: 3-dehydroquinase, type II

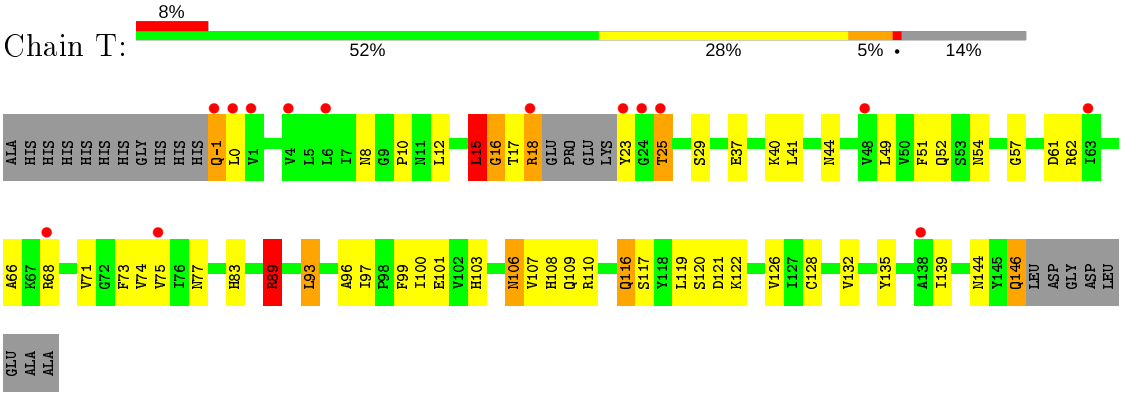
• Molecule 1: 3-dehydroquinase, type II

Chain S:



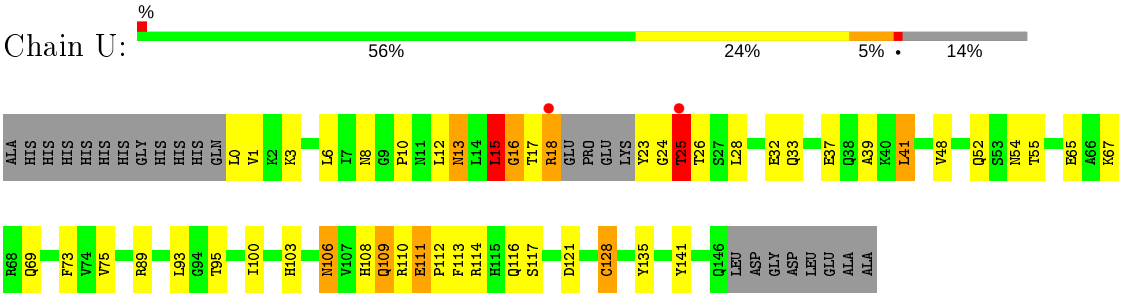
• Molecule 1: 3-dehydroquinase, type II

Chain T:



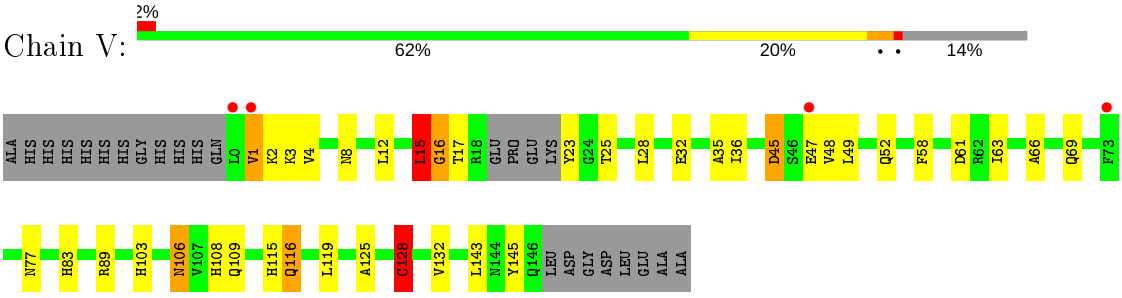
• Molecule 1: 3-dehydroquinase, type II

Chain U:



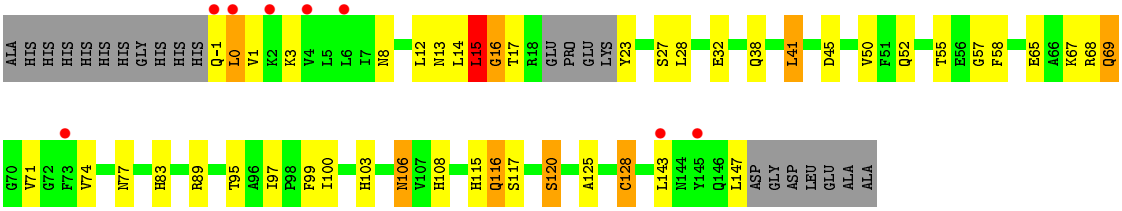
• Molecule 1: 3-dehydroquinase, type II

Chain V:



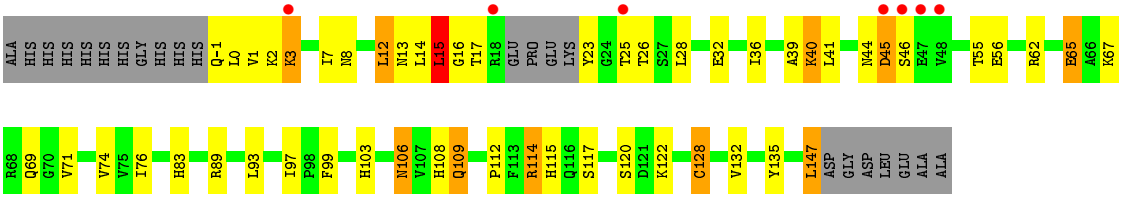
• Molecule 1: 3-dehydroquinase, type II

Chain W:



- Molecule 1: 3-dehydroquinase, type II

Chain X:



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

The worst 5 of 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

The worst 5 of 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

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

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

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

The worst 5 of 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:NE2	1:N:146:GLN:HA	1.68	1.07
1:J:12:LEU:O	1:J:15:LEU:HD22	1.54	1.07
1:N:146:GLN:HE21	1:N:146:GLN:HA	0.94	1.06
1:T:103:HIS:HB2	1:T:128:CYS:HB2	1.44	0.99
1:W:103:HIS:HB2	1:W:128:CYS:HB2	1.46	0.98

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	17	THR
1	O	106	ASN
1	W	106	ASN
1	L	128	CYS
1	N	15	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	8	ASN
1	M	115	HIS
1	W	83	HIS
1	K	13	ASN
1	L	8	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	I	155	-	4,4,4	0.42	0	6,6,6	1.42	1 (16%)
2	SO4	K	155	-	4,4,4	0.17	0	6,6,6	0.67	0
2	SO4	H	155	-	4,4,4	0.45	0	6,6,6	0.79	0
2	SO4	U	155	-	4,4,4	0.28	0	6,6,6	1.49	1 (16%)
2	SO4	V	155	-	4,4,4	0.22	0	6,6,6	0.53	0
2	SO4	E	155	-	4,4,4	0.25	0	6,6,6	1.02	0
2	SO4	B	155	-	4,4,4	0.46	0	6,6,6	1.60	2 (33%)
3	TRS	J	156	-	7,7,7	0.59	0	9,9,9	0.70	0
2	SO4	C	155	-	4,4,4	0.40	0	6,6,6	0.81	0
2	SO4	O	155	-	4,4,4	0.34	0	6,6,6	0.96	0
3	TRS	W	156	-	7,7,7	0.67	0	9,9,9	1.01	0
2	SO4	W	155	-	4,4,4	0.31	0	6,6,6	0.91	0
2	SO4	N	155	-	4,4,4	0.17	0	6,6,6	1.05	0
2	SO4	X	155	-	4,4,4	0.40	0	6,6,6	0.74	0
2	SO4	G	155	-	4,4,4	0.56	0	6,6,6	1.13	1 (16%)
2	SO4	D	155	-	4,4,4	0.47	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	155	-	4,4,4	0.47	0	6,6,6	1.18	1 (16%)
2	SO4	M	155	-	4,4,4	0.52	0	6,6,6	0.93	0
2	SO4	J	155	-	4,4,4	0.46	0	6,6,6	0.79	0
3	TRS	D	156	-	7,7,7	0.60	0	9,9,9	1.57	3 (33%)
2	SO4	R	155	-	4,4,4	0.23	0	6,6,6	1.32	1 (16%)
2	SO4	S	155	-	4,4,4	0.43	0	6,6,6	1.01	0
2	SO4	P	155	-	4,4,4	0.27	0	6,6,6	0.85	0
3	TRS	P	156	-	7,7,7	0.55	0	9,9,9	1.68	3 (33%)
2	SO4	F	155	-	4,4,4	0.44	0	6,6,6	1.60	1 (16%)
2	SO4	T	155	-	4,4,4	0.30	0	6,6,6	1.04	0
2	SO4	Q	155	-	4,4,4	0.55	0	6,6,6	1.21	1 (16%)
2	SO4	A	156	-	4,4,4	0.49	0	6,6,6	0.80	0
3	TRS	G	156	-	7,7,7	0.72	0	9,9,9	1.27	1 (11%)
3	TRS	T	156	-	7,7,7	0.46	0	9,9,9	0.97	0
3	TRS	A	157	-	7,7,7	0.65	0	9,9,9	1.17	1 (11%)
3	TRS	N	156	-	7,7,7	0.34	0	9,9,9	0.53	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	W	156	-	-	4/9/9/9	-
3	TRS	D	156	-	-	9/9/9/9	-
3	TRS	P	156	-	-	5/9/9/9	-
3	TRS	G	156	-	-	0/9/9/9	-
3	TRS	T	156	-	-	1/9/9/9	-
3	TRS	A	157	-	-	1/9/9/9	-
3	TRS	J	156	-	-	0/9/9/9	-
3	TRS	N	156	-	-	3/9/9/9	-

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	155	SO4	O3-S-O1	3.11	125.55	109.31
3	P	156	TRS	C3-C-N	2.78	116.29	107.98
2	I	155	SO4	O4-S-O1	2.70	123.38	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	157	TRS	O1-C1-C	-2.67	102.55	111.00
2	B	155	SO4	O4-S-O3	-2.63	97.85	109.06

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	W	156	TRS	N-C-C3-O3
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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

The worst 5 of 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

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	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	X	155	5/5	0.83	0.19	107,109,111,113	0
2	SO4	H	155	5/5	0.83	0.21	101,103,105,108	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
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	W	155	5/5	0.86	0.26	110,113,114,115	0
2	SO4	C	155	5/5	0.86	0.23	111,112,114,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	V	155	5/5	0.92	0.13	110,111,112,112	0
2	SO4	G	155	5/5	0.92	0.21	86,90,93,95	0
2	SO4	R	155	5/5	0.93	0.22	96,98,99,100	0
2	SO4	D	155	5/5	0.93	0.19	95,95,97,100	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
3	TRS	W	156	8/8	0.95	0.17	52,55,56,56	0
2	SO4	B	155	5/5	0.95	0.19	84,84,90,91	0
3	TRS	J	156	8/8	0.95	0.23	45,49,50,50	0
2	SO4	A	156	5/5	0.95	0.28	88,89,91,91	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.