Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 09:44 AM EDT

PDB ID	:	3HHQ
Title	:	Crystal structure of apo dUT1p from Saccharomyces cerevisiae
Authors	:	Singer, A.U.; Evdokimova, E.; Kudritska, M.; Dong, A.; Edwards, A.M.; Yakunin, A.F.; Savchenko, A.
Deposited on	:	2009-05-15
Resolution	:	2.00 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:

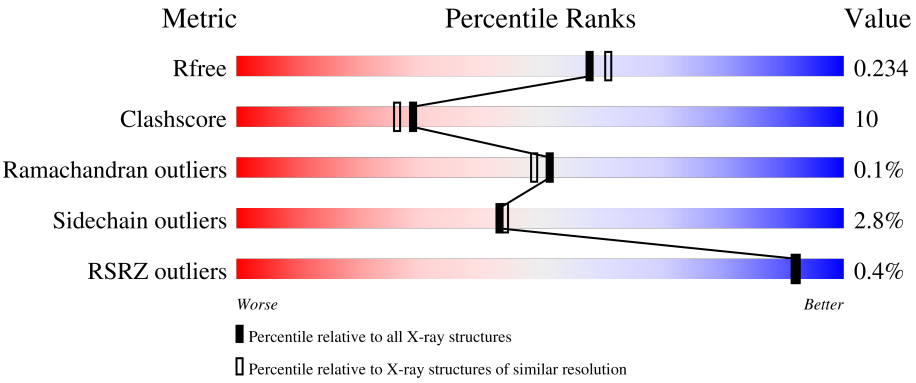
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	65% 10% 25%
1	B	167	60% 13% 23%
1	C	167	63% 13% 23%
1	D	167	59% 16% 25%
1	E	167	65% 11% 23%

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Mol	Chain	Length	Quality of chain
1	F	167	62% 11% 25%
1	G	167	58% 17% 24%
1	H	167	62% 12% 25%
1	I	167	62% 13% 24%
1	J	167	59% 16% 25%
1	K	167	59% 16% 24%
1	L	167	65% 10% 24%
1	M	167	60% 17% 22%
1	N	167	61% 11% 25%
1	O	167	63% 13% 24%
1	P	167	62% 13% 25%
1	Q	167	65% 9% 25%
1	R	167	66% 10% 24%
1	S	167	61% 14% 24%
1	T	167	65% 12% 23%
1	U	167	65% 11% 24%
1	V	167	62% 14% 24%
1	W	167	65% 12% 22%
1	X	167	66% 9% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	148	-	-	X	-
2	SO4	I	148	-	-	X	-
2	SO4	K	148	-	-	X	-
2	SO4	Q	148	-	-	X	-
2	SO4	S	148	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	V	148	-	-	X	-
2	SO4	V	149	-	-	X	-
5	EDO	D	151	-	-	X	-
5	EDO	D	152	-	-	X	-
5	EDO	G	151	-	-	X	-
5	EDO	J	150	-	-	X	-
5	EDO	K	150	-	-	X	-
5	EDO	K	152	-	-	X	-
5	EDO	M	151	-	-	X	-
5	EDO	Q	150	-	-	X	-
5	EDO	Q	151	-	-	X	-
5	EDO	S	151	-	-	X	-
5	EDO	T	154	-	-	X	-
5	EDO	V	156	-	-	X	-
6	PEG	H	149	-	-	X	-
6	PEG	X	148	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25087 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 Deoxyuridine 5'-triphosphate nucleotidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	2	0
			953	602	167	182	2			
1	B	128	Total	C	N	O	S	0	0	0
			951	598	164	187	2			
1	C	128	Total	C	N	O	S	0	4	0
			973	612	171	187	3			
1	D	125	Total	C	N	O	S	0	4	0
			964	607	169	185	3			
1	E	128	Total	C	N	O	S	0	0	0
			950	598	165	185	2			
1	F	126	Total	C	N	O	S	0	5	0
			973	614	170	187	2			
1	G	127	Total	C	N	O	S	0	2	0
			959	603	166	187	3			
1	H	126	Total	C	N	O	S	0	1	0
			943	593	166	182	2			
1	I	127	Total	C	N	O	S	0	3	0
			958	605	165	186	2			
1	J	126	Total	C	N	O	S	0	1	0
			947	596	167	182	2			
1	K	127	Total	C	N	O	S	0	4	0
			985	621	173	189	2			
1	L	127	Total	C	N	O	S	0	2	0
			952	601	165	184	2			
1	M	130	Total	C	N	O	S	0	3	0
			993	624	174	193	2			
1	N	125	Total	C	N	O	S	0	1	0
			940	594	163	181	2			
1	O	127	Total	C	N	O	S	0	3	0
			970	609	170	188	3			
1	P	125	Total	C	N	O	S	0	0	0
			928	585	161	180	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	125	Total	C	N	O	S	0	2	0
			947	597	166	182	2			
1	R	127	Total	C	N	O	S	0	2	0
			957	601	166	188	2			
1	S	127	Total	C	N	O	S	0	1	0
			949	598	165	183	3			
1	T	128	Total	C	N	O	S	0	0	0
			946	595	164	185	2			
1	U	127	Total	C	N	O	S	0	0	0
			945	595	164	184	2			
1	V	127	Total	C	N	O	S	0	1	0
			952	598	167	185	2			
1	W	130	Total	C	N	O	S	0	0	0
			964	605	167	190	2			
1	X	126	Total	C	N	O	S	0	3	0
			959	602	168	186	3			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P33317
A	-18	GLY	-	expression tag	UNP P33317
A	-17	SER	-	expression tag	UNP P33317
A	-16	SER	-	expression tag	UNP P33317
A	-15	HIS	-	expression tag	UNP P33317
A	-14	HIS	-	expression tag	UNP P33317
A	-13	HIS	-	expression tag	UNP P33317
A	-12	HIS	-	expression tag	UNP P33317
A	-11	HIS	-	expression tag	UNP P33317
A	-10	HIS	-	expression tag	UNP P33317
A	-9	SER	-	expression tag	UNP P33317
A	-8	SER	-	expression tag	UNP P33317
A	-7	GLY	-	expression tag	UNP P33317
A	-6	LEU	-	expression tag	UNP P33317
A	-5	VAL	-	expression tag	UNP P33317
A	-4	PRO	-	expression tag	UNP P33317
A	-3	ARG	-	expression tag	UNP P33317
A	-2	GLY	-	expression tag	UNP P33317
A	-1	SER	-	expression tag	UNP P33317
A	0	HIS	-	expression tag	UNP P33317
B	-19	MET	-	expression tag	UNP P33317
B	-18	GLY	-	expression tag	UNP P33317
B	-17	SER	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P33317
B	-15	HIS	-	expression tag	UNP P33317
B	-14	HIS	-	expression tag	UNP P33317
B	-13	HIS	-	expression tag	UNP P33317
B	-12	HIS	-	expression tag	UNP P33317
B	-11	HIS	-	expression tag	UNP P33317
B	-10	HIS	-	expression tag	UNP P33317
B	-9	SER	-	expression tag	UNP P33317
B	-8	SER	-	expression tag	UNP P33317
B	-7	GLY	-	expression tag	UNP P33317
B	-6	LEU	-	expression tag	UNP P33317
B	-5	VAL	-	expression tag	UNP P33317
B	-4	PRO	-	expression tag	UNP P33317
B	-3	ARG	-	expression tag	UNP P33317
B	-2	GLY	-	expression tag	UNP P33317
B	-1	SER	-	expression tag	UNP P33317
B	0	HIS	-	expression tag	UNP P33317
C	-19	MET	-	expression tag	UNP P33317
C	-18	GLY	-	expression tag	UNP P33317
C	-17	SER	-	expression tag	UNP P33317
C	-16	SER	-	expression tag	UNP P33317
C	-15	HIS	-	expression tag	UNP P33317
C	-14	HIS	-	expression tag	UNP P33317
C	-13	HIS	-	expression tag	UNP P33317
C	-12	HIS	-	expression tag	UNP P33317
C	-11	HIS	-	expression tag	UNP P33317
C	-10	HIS	-	expression tag	UNP P33317
C	-9	SER	-	expression tag	UNP P33317
C	-8	SER	-	expression tag	UNP P33317
C	-7	GLY	-	expression tag	UNP P33317
C	-6	LEU	-	expression tag	UNP P33317
C	-5	VAL	-	expression tag	UNP P33317
C	-4	PRO	-	expression tag	UNP P33317
C	-3	ARG	-	expression tag	UNP P33317
C	-2	GLY	-	expression tag	UNP P33317
C	-1	SER	-	expression tag	UNP P33317
C	0	HIS	-	expression tag	UNP P33317
D	-19	MET	-	expression tag	UNP P33317
D	-18	GLY	-	expression tag	UNP P33317
D	-17	SER	-	expression tag	UNP P33317
D	-16	SER	-	expression tag	UNP P33317
D	-15	HIS	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	HIS	-	expression tag	UNP P33317
D	-13	HIS	-	expression tag	UNP P33317
D	-12	HIS	-	expression tag	UNP P33317
D	-11	HIS	-	expression tag	UNP P33317
D	-10	HIS	-	expression tag	UNP P33317
D	-9	SER	-	expression tag	UNP P33317
D	-8	SER	-	expression tag	UNP P33317
D	-7	GLY	-	expression tag	UNP P33317
D	-6	LEU	-	expression tag	UNP P33317
D	-5	VAL	-	expression tag	UNP P33317
D	-4	PRO	-	expression tag	UNP P33317
D	-3	ARG	-	expression tag	UNP P33317
D	-2	GLY	-	expression tag	UNP P33317
D	-1	SER	-	expression tag	UNP P33317
D	0	HIS	-	expression tag	UNP P33317
E	-19	MET	-	expression tag	UNP P33317
E	-18	GLY	-	expression tag	UNP P33317
E	-17	SER	-	expression tag	UNP P33317
E	-16	SER	-	expression tag	UNP P33317
E	-15	HIS	-	expression tag	UNP P33317
E	-14	HIS	-	expression tag	UNP P33317
E	-13	HIS	-	expression tag	UNP P33317
E	-12	HIS	-	expression tag	UNP P33317
E	-11	HIS	-	expression tag	UNP P33317
E	-10	HIS	-	expression tag	UNP P33317
E	-9	SER	-	expression tag	UNP P33317
E	-8	SER	-	expression tag	UNP P33317
E	-7	GLY	-	expression tag	UNP P33317
E	-6	LEU	-	expression tag	UNP P33317
E	-5	VAL	-	expression tag	UNP P33317
E	-4	PRO	-	expression tag	UNP P33317
E	-3	ARG	-	expression tag	UNP P33317
E	-2	GLY	-	expression tag	UNP P33317
E	-1	SER	-	expression tag	UNP P33317
E	0	HIS	-	expression tag	UNP P33317
F	-19	MET	-	expression tag	UNP P33317
F	-18	GLY	-	expression tag	UNP P33317
F	-17	SER	-	expression tag	UNP P33317
F	-16	SER	-	expression tag	UNP P33317
F	-15	HIS	-	expression tag	UNP P33317
F	-14	HIS	-	expression tag	UNP P33317
F	-13	HIS	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	HIS	-	expression tag	UNP P33317
F	-11	HIS	-	expression tag	UNP P33317
F	-10	HIS	-	expression tag	UNP P33317
F	-9	SER	-	expression tag	UNP P33317
F	-8	SER	-	expression tag	UNP P33317
F	-7	GLY	-	expression tag	UNP P33317
F	-6	LEU	-	expression tag	UNP P33317
F	-5	VAL	-	expression tag	UNP P33317
F	-4	PRO	-	expression tag	UNP P33317
F	-3	ARG	-	expression tag	UNP P33317
F	-2	GLY	-	expression tag	UNP P33317
F	-1	SER	-	expression tag	UNP P33317
F	0	HIS	-	expression tag	UNP P33317
G	-19	MET	-	expression tag	UNP P33317
G	-18	GLY	-	expression tag	UNP P33317
G	-17	SER	-	expression tag	UNP P33317
G	-16	SER	-	expression tag	UNP P33317
G	-15	HIS	-	expression tag	UNP P33317
G	-14	HIS	-	expression tag	UNP P33317
G	-13	HIS	-	expression tag	UNP P33317
G	-12	HIS	-	expression tag	UNP P33317
G	-11	HIS	-	expression tag	UNP P33317
G	-10	HIS	-	expression tag	UNP P33317
G	-9	SER	-	expression tag	UNP P33317
G	-8	SER	-	expression tag	UNP P33317
G	-7	GLY	-	expression tag	UNP P33317
G	-6	LEU	-	expression tag	UNP P33317
G	-5	VAL	-	expression tag	UNP P33317
G	-4	PRO	-	expression tag	UNP P33317
G	-3	ARG	-	expression tag	UNP P33317
G	-2	GLY	-	expression tag	UNP P33317
G	-1	SER	-	expression tag	UNP P33317
G	0	HIS	-	expression tag	UNP P33317
H	-19	MET	-	expression tag	UNP P33317
H	-18	GLY	-	expression tag	UNP P33317
H	-17	SER	-	expression tag	UNP P33317
H	-16	SER	-	expression tag	UNP P33317
H	-15	HIS	-	expression tag	UNP P33317
H	-14	HIS	-	expression tag	UNP P33317
H	-13	HIS	-	expression tag	UNP P33317
H	-12	HIS	-	expression tag	UNP P33317
H	-11	HIS	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	HIS	-	expression tag	UNP P33317
H	-9	SER	-	expression tag	UNP P33317
H	-8	SER	-	expression tag	UNP P33317
H	-7	GLY	-	expression tag	UNP P33317
H	-6	LEU	-	expression tag	UNP P33317
H	-5	VAL	-	expression tag	UNP P33317
H	-4	PRO	-	expression tag	UNP P33317
H	-3	ARG	-	expression tag	UNP P33317
H	-2	GLY	-	expression tag	UNP P33317
H	-1	SER	-	expression tag	UNP P33317
H	0	HIS	-	expression tag	UNP P33317
I	-19	MET	-	expression tag	UNP P33317
I	-18	GLY	-	expression tag	UNP P33317
I	-17	SER	-	expression tag	UNP P33317
I	-16	SER	-	expression tag	UNP P33317
I	-15	HIS	-	expression tag	UNP P33317
I	-14	HIS	-	expression tag	UNP P33317
I	-13	HIS	-	expression tag	UNP P33317
I	-12	HIS	-	expression tag	UNP P33317
I	-11	HIS	-	expression tag	UNP P33317
I	-10	HIS	-	expression tag	UNP P33317
I	-9	SER	-	expression tag	UNP P33317
I	-8	SER	-	expression tag	UNP P33317
I	-7	GLY	-	expression tag	UNP P33317
I	-6	LEU	-	expression tag	UNP P33317
I	-5	VAL	-	expression tag	UNP P33317
I	-4	PRO	-	expression tag	UNP P33317
I	-3	ARG	-	expression tag	UNP P33317
I	-2	GLY	-	expression tag	UNP P33317
I	-1	SER	-	expression tag	UNP P33317
I	0	HIS	-	expression tag	UNP P33317
J	-19	MET	-	expression tag	UNP P33317
J	-18	GLY	-	expression tag	UNP P33317
J	-17	SER	-	expression tag	UNP P33317
J	-16	SER	-	expression tag	UNP P33317
J	-15	HIS	-	expression tag	UNP P33317
J	-14	HIS	-	expression tag	UNP P33317
J	-13	HIS	-	expression tag	UNP P33317
J	-12	HIS	-	expression tag	UNP P33317
J	-11	HIS	-	expression tag	UNP P33317
J	-10	HIS	-	expression tag	UNP P33317
J	-9	SER	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	SER	-	expression tag	UNP P33317
J	-7	GLY	-	expression tag	UNP P33317
J	-6	LEU	-	expression tag	UNP P33317
J	-5	VAL	-	expression tag	UNP P33317
J	-4	PRO	-	expression tag	UNP P33317
J	-3	ARG	-	expression tag	UNP P33317
J	-2	GLY	-	expression tag	UNP P33317
J	-1	SER	-	expression tag	UNP P33317
J	0	HIS	-	expression tag	UNP P33317
K	-19	MET	-	expression tag	UNP P33317
K	-18	GLY	-	expression tag	UNP P33317
K	-17	SER	-	expression tag	UNP P33317
K	-16	SER	-	expression tag	UNP P33317
K	-15	HIS	-	expression tag	UNP P33317
K	-14	HIS	-	expression tag	UNP P33317
K	-13	HIS	-	expression tag	UNP P33317
K	-12	HIS	-	expression tag	UNP P33317
K	-11	HIS	-	expression tag	UNP P33317
K	-10	HIS	-	expression tag	UNP P33317
K	-9	SER	-	expression tag	UNP P33317
K	-8	SER	-	expression tag	UNP P33317
K	-7	GLY	-	expression tag	UNP P33317
K	-6	LEU	-	expression tag	UNP P33317
K	-5	VAL	-	expression tag	UNP P33317
K	-4	PRO	-	expression tag	UNP P33317
K	-3	ARG	-	expression tag	UNP P33317
K	-2	GLY	-	expression tag	UNP P33317
K	-1	SER	-	expression tag	UNP P33317
K	0	HIS	-	expression tag	UNP P33317
L	-19	MET	-	expression tag	UNP P33317
L	-18	GLY	-	expression tag	UNP P33317
L	-17	SER	-	expression tag	UNP P33317
L	-16	SER	-	expression tag	UNP P33317
L	-15	HIS	-	expression tag	UNP P33317
L	-14	HIS	-	expression tag	UNP P33317
L	-13	HIS	-	expression tag	UNP P33317
L	-12	HIS	-	expression tag	UNP P33317
L	-11	HIS	-	expression tag	UNP P33317
L	-10	HIS	-	expression tag	UNP P33317
L	-9	SER	-	expression tag	UNP P33317
L	-8	SER	-	expression tag	UNP P33317
L	-7	GLY	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-6	LEU	-	expression tag	UNP P33317
L	-5	VAL	-	expression tag	UNP P33317
L	-4	PRO	-	expression tag	UNP P33317
L	-3	ARG	-	expression tag	UNP P33317
L	-2	GLY	-	expression tag	UNP P33317
L	-1	SER	-	expression tag	UNP P33317
L	0	HIS	-	expression tag	UNP P33317
M	-19	MET	-	expression tag	UNP P33317
M	-18	GLY	-	expression tag	UNP P33317
M	-17	SER	-	expression tag	UNP P33317
M	-16	SER	-	expression tag	UNP P33317
M	-15	HIS	-	expression tag	UNP P33317
M	-14	HIS	-	expression tag	UNP P33317
M	-13	HIS	-	expression tag	UNP P33317
M	-12	HIS	-	expression tag	UNP P33317
M	-11	HIS	-	expression tag	UNP P33317
M	-10	HIS	-	expression tag	UNP P33317
M	-9	SER	-	expression tag	UNP P33317
M	-8	SER	-	expression tag	UNP P33317
M	-7	GLY	-	expression tag	UNP P33317
M	-6	LEU	-	expression tag	UNP P33317
M	-5	VAL	-	expression tag	UNP P33317
M	-4	PRO	-	expression tag	UNP P33317
M	-3	ARG	-	expression tag	UNP P33317
M	-2	GLY	-	expression tag	UNP P33317
M	-1	SER	-	expression tag	UNP P33317
M	0	HIS	-	expression tag	UNP P33317
N	-19	MET	-	expression tag	UNP P33317
N	-18	GLY	-	expression tag	UNP P33317
N	-17	SER	-	expression tag	UNP P33317
N	-16	SER	-	expression tag	UNP P33317
N	-15	HIS	-	expression tag	UNP P33317
N	-14	HIS	-	expression tag	UNP P33317
N	-13	HIS	-	expression tag	UNP P33317
N	-12	HIS	-	expression tag	UNP P33317
N	-11	HIS	-	expression tag	UNP P33317
N	-10	HIS	-	expression tag	UNP P33317
N	-9	SER	-	expression tag	UNP P33317
N	-8	SER	-	expression tag	UNP P33317
N	-7	GLY	-	expression tag	UNP P33317
N	-6	LEU	-	expression tag	UNP P33317
N	-5	VAL	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-4	PRO	-	expression tag	UNP P33317
N	-3	ARG	-	expression tag	UNP P33317
N	-2	GLY	-	expression tag	UNP P33317
N	-1	SER	-	expression tag	UNP P33317
N	0	HIS	-	expression tag	UNP P33317
O	-19	MET	-	expression tag	UNP P33317
O	-18	GLY	-	expression tag	UNP P33317
O	-17	SER	-	expression tag	UNP P33317
O	-16	SER	-	expression tag	UNP P33317
O	-15	HIS	-	expression tag	UNP P33317
O	-14	HIS	-	expression tag	UNP P33317
O	-13	HIS	-	expression tag	UNP P33317
O	-12	HIS	-	expression tag	UNP P33317
O	-11	HIS	-	expression tag	UNP P33317
O	-10	HIS	-	expression tag	UNP P33317
O	-9	SER	-	expression tag	UNP P33317
O	-8	SER	-	expression tag	UNP P33317
O	-7	GLY	-	expression tag	UNP P33317
O	-6	LEU	-	expression tag	UNP P33317
O	-5	VAL	-	expression tag	UNP P33317
O	-4	PRO	-	expression tag	UNP P33317
O	-3	ARG	-	expression tag	UNP P33317
O	-2	GLY	-	expression tag	UNP P33317
O	-1	SER	-	expression tag	UNP P33317
O	0	HIS	-	expression tag	UNP P33317
P	-19	MET	-	expression tag	UNP P33317
P	-18	GLY	-	expression tag	UNP P33317
P	-17	SER	-	expression tag	UNP P33317
P	-16	SER	-	expression tag	UNP P33317
P	-15	HIS	-	expression tag	UNP P33317
P	-14	HIS	-	expression tag	UNP P33317
P	-13	HIS	-	expression tag	UNP P33317
P	-12	HIS	-	expression tag	UNP P33317
P	-11	HIS	-	expression tag	UNP P33317
P	-10	HIS	-	expression tag	UNP P33317
P	-9	SER	-	expression tag	UNP P33317
P	-8	SER	-	expression tag	UNP P33317
P	-7	GLY	-	expression tag	UNP P33317
P	-6	LEU	-	expression tag	UNP P33317
P	-5	VAL	-	expression tag	UNP P33317
P	-4	PRO	-	expression tag	UNP P33317
P	-3	ARG	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-2	GLY	-	expression tag	UNP P33317
P	-1	SER	-	expression tag	UNP P33317
P	0	HIS	-	expression tag	UNP P33317
Q	-19	MET	-	expression tag	UNP P33317
Q	-18	GLY	-	expression tag	UNP P33317
Q	-17	SER	-	expression tag	UNP P33317
Q	-16	SER	-	expression tag	UNP P33317
Q	-15	HIS	-	expression tag	UNP P33317
Q	-14	HIS	-	expression tag	UNP P33317
Q	-13	HIS	-	expression tag	UNP P33317
Q	-12	HIS	-	expression tag	UNP P33317
Q	-11	HIS	-	expression tag	UNP P33317
Q	-10	HIS	-	expression tag	UNP P33317
Q	-9	SER	-	expression tag	UNP P33317
Q	-8	SER	-	expression tag	UNP P33317
Q	-7	GLY	-	expression tag	UNP P33317
Q	-6	LEU	-	expression tag	UNP P33317
Q	-5	VAL	-	expression tag	UNP P33317
Q	-4	PRO	-	expression tag	UNP P33317
Q	-3	ARG	-	expression tag	UNP P33317
Q	-2	GLY	-	expression tag	UNP P33317
Q	-1	SER	-	expression tag	UNP P33317
Q	0	HIS	-	expression tag	UNP P33317
R	-19	MET	-	expression tag	UNP P33317
R	-18	GLY	-	expression tag	UNP P33317
R	-17	SER	-	expression tag	UNP P33317
R	-16	SER	-	expression tag	UNP P33317
R	-15	HIS	-	expression tag	UNP P33317
R	-14	HIS	-	expression tag	UNP P33317
R	-13	HIS	-	expression tag	UNP P33317
R	-12	HIS	-	expression tag	UNP P33317
R	-11	HIS	-	expression tag	UNP P33317
R	-10	HIS	-	expression tag	UNP P33317
R	-9	SER	-	expression tag	UNP P33317
R	-8	SER	-	expression tag	UNP P33317
R	-7	GLY	-	expression tag	UNP P33317
R	-6	LEU	-	expression tag	UNP P33317
R	-5	VAL	-	expression tag	UNP P33317
R	-4	PRO	-	expression tag	UNP P33317
R	-3	ARG	-	expression tag	UNP P33317
R	-2	GLY	-	expression tag	UNP P33317
R	-1	SER	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
R	0	HIS	-	expression tag	UNP P33317
S	-19	MET	-	expression tag	UNP P33317
S	-18	GLY	-	expression tag	UNP P33317
S	-17	SER	-	expression tag	UNP P33317
S	-16	SER	-	expression tag	UNP P33317
S	-15	HIS	-	expression tag	UNP P33317
S	-14	HIS	-	expression tag	UNP P33317
S	-13	HIS	-	expression tag	UNP P33317
S	-12	HIS	-	expression tag	UNP P33317
S	-11	HIS	-	expression tag	UNP P33317
S	-10	HIS	-	expression tag	UNP P33317
S	-9	SER	-	expression tag	UNP P33317
S	-8	SER	-	expression tag	UNP P33317
S	-7	GLY	-	expression tag	UNP P33317
S	-6	LEU	-	expression tag	UNP P33317
S	-5	VAL	-	expression tag	UNP P33317
S	-4	PRO	-	expression tag	UNP P33317
S	-3	ARG	-	expression tag	UNP P33317
S	-2	GLY	-	expression tag	UNP P33317
S	-1	SER	-	expression tag	UNP P33317
S	0	HIS	-	expression tag	UNP P33317
T	-19	MET	-	expression tag	UNP P33317
T	-18	GLY	-	expression tag	UNP P33317
T	-17	SER	-	expression tag	UNP P33317
T	-16	SER	-	expression tag	UNP P33317
T	-15	HIS	-	expression tag	UNP P33317
T	-14	HIS	-	expression tag	UNP P33317
T	-13	HIS	-	expression tag	UNP P33317
T	-12	HIS	-	expression tag	UNP P33317
T	-11	HIS	-	expression tag	UNP P33317
T	-10	HIS	-	expression tag	UNP P33317
T	-9	SER	-	expression tag	UNP P33317
T	-8	SER	-	expression tag	UNP P33317
T	-7	GLY	-	expression tag	UNP P33317
T	-6	LEU	-	expression tag	UNP P33317
T	-5	VAL	-	expression tag	UNP P33317
T	-4	PRO	-	expression tag	UNP P33317
T	-3	ARG	-	expression tag	UNP P33317
T	-2	GLY	-	expression tag	UNP P33317
T	-1	SER	-	expression tag	UNP P33317
T	0	HIS	-	expression tag	UNP P33317
U	-19	MET	-	expression tag	UNP P33317

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-18	GLY	-	expression tag	UNP P33317
U	-17	SER	-	expression tag	UNP P33317
U	-16	SER	-	expression tag	UNP P33317
U	-15	HIS	-	expression tag	UNP P33317
U	-14	HIS	-	expression tag	UNP P33317
U	-13	HIS	-	expression tag	UNP P33317
U	-12	HIS	-	expression tag	UNP P33317
U	-11	HIS	-	expression tag	UNP P33317
U	-10	HIS	-	expression tag	UNP P33317
U	-9	SER	-	expression tag	UNP P33317
U	-8	SER	-	expression tag	UNP P33317
U	-7	GLY	-	expression tag	UNP P33317
U	-6	LEU	-	expression tag	UNP P33317
U	-5	VAL	-	expression tag	UNP P33317
U	-4	PRO	-	expression tag	UNP P33317
U	-3	ARG	-	expression tag	UNP P33317
U	-2	GLY	-	expression tag	UNP P33317
U	-1	SER	-	expression tag	UNP P33317
U	0	HIS	-	expression tag	UNP P33317
V	-19	MET	-	expression tag	UNP P33317
V	-18	GLY	-	expression tag	UNP P33317
V	-17	SER	-	expression tag	UNP P33317
V	-16	SER	-	expression tag	UNP P33317
V	-15	HIS	-	expression tag	UNP P33317
V	-14	HIS	-	expression tag	UNP P33317
V	-13	HIS	-	expression tag	UNP P33317
V	-12	HIS	-	expression tag	UNP P33317
V	-11	HIS	-	expression tag	UNP P33317
V	-10	HIS	-	expression tag	UNP P33317
V	-9	SER	-	expression tag	UNP P33317
V	-8	SER	-	expression tag	UNP P33317
V	-7	GLY	-	expression tag	UNP P33317
V	-6	LEU	-	expression tag	UNP P33317
V	-5	VAL	-	expression tag	UNP P33317
V	-4	PRO	-	expression tag	UNP P33317
V	-3	ARG	-	expression tag	UNP P33317
V	-2	GLY	-	expression tag	UNP P33317
V	-1	SER	-	expression tag	UNP P33317
V	0	HIS	-	expression tag	UNP P33317
W	-19	MET	-	expression tag	UNP P33317
W	-18	GLY	-	expression tag	UNP P33317
W	-17	SER	-	expression tag	UNP P33317

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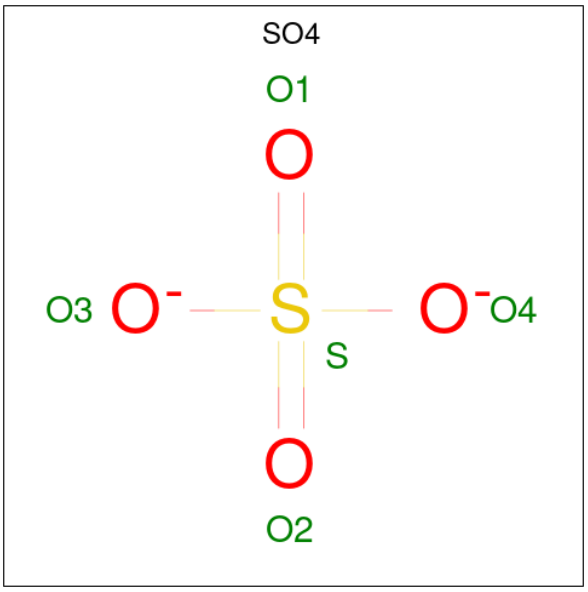
Chain	Residue	Modelled	Actual	Comment	Reference
W	-16	SER	-	expression tag	UNP P33317
W	-15	HIS	-	expression tag	UNP P33317
W	-14	HIS	-	expression tag	UNP P33317
W	-13	HIS	-	expression tag	UNP P33317
W	-12	HIS	-	expression tag	UNP P33317
W	-11	HIS	-	expression tag	UNP P33317
W	-10	HIS	-	expression tag	UNP P33317
W	-9	SER	-	expression tag	UNP P33317
W	-8	SER	-	expression tag	UNP P33317
W	-7	GLY	-	expression tag	UNP P33317
W	-6	LEU	-	expression tag	UNP P33317
W	-5	VAL	-	expression tag	UNP P33317
W	-4	PRO	-	expression tag	UNP P33317
W	-3	ARG	-	expression tag	UNP P33317
W	-2	GLY	-	expression tag	UNP P33317
W	-1	SER	-	expression tag	UNP P33317
W	0	HIS	-	expression tag	UNP P33317
X	-19	MET	-	expression tag	UNP P33317
X	-18	GLY	-	expression tag	UNP P33317
X	-17	SER	-	expression tag	UNP P33317
X	-16	SER	-	expression tag	UNP P33317
X	-15	HIS	-	expression tag	UNP P33317
X	-14	HIS	-	expression tag	UNP P33317
X	-13	HIS	-	expression tag	UNP P33317
X	-12	HIS	-	expression tag	UNP P33317
X	-11	HIS	-	expression tag	UNP P33317
X	-10	HIS	-	expression tag	UNP P33317
X	-9	SER	-	expression tag	UNP P33317
X	-8	SER	-	expression tag	UNP P33317
X	-7	GLY	-	expression tag	UNP P33317
X	-6	LEU	-	expression tag	UNP P33317
X	-5	VAL	-	expression tag	UNP P33317
X	-4	PRO	-	expression tag	UNP P33317
X	-3	ARG	-	expression tag	UNP P33317
X	-2	GLY	-	expression tag	UNP P33317
X	-1	SER	-	expression tag	UNP P33317
X	0	HIS	-	expression tag	UNP P33317

- 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	B	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	F	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	G	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	M	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	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	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	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	V	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	W	1	Total O S 5 4 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	L	1	Total Na 1 1	0	0
3	M	1	Total Na 1 1	0	0
3	N	1	Total Na 1 1	0	0
3	O	2	Total Na 2 2	0	0
3	P	1	Total Na 1 1	0	0
3	S	1	Total Na 1 1	0	0
3	T	2	Total Na 2 2	0	0
3	V	2	Total Na 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	2	Total Cl 2 2	0	0
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	I	1	Total Cl 1 1	0	0
4	J	1	Total Cl 1 1	0	0
4	L	2	Total Cl 2 2	0	0

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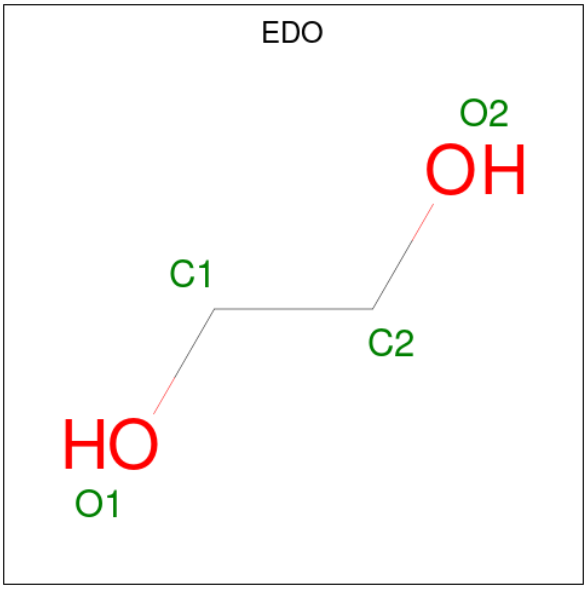
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	2	Total Cl 2 2	0	0
4	Q	1	Total Cl 1 1	0	0
4	R	1	Total Cl 1 1	0	0
4	T	1	Total Cl 1 1	0	0
4	U	1	Total Cl 1 1	0	0
4	V	1	Total Cl 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	Q	1	Total	C	O	0	0
			4	2	2		
5	Q	1	Total	C	O	0	0
			4	2	2		
5	Q	1	Total	C	O	0	0
			4	2	2		
5	Q	1	Total	C	O	0	0
			4	2	2		
5	R	1	Total	C	O	0	0
			4	2	2		
5	R	1	Total	C	O	0	0
			4	2	2		
5	S	1	Total	C	O	0	0
			4	2	2		

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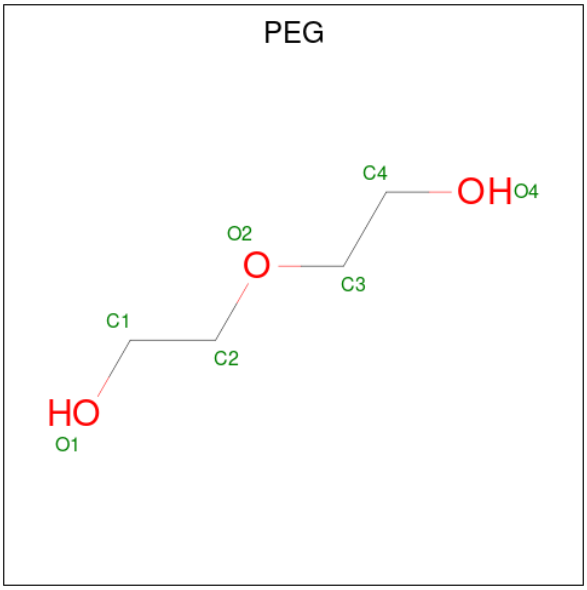
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	T	1	Total C O 4 2 2	0	0
5	T	1	Total C O 4 2 2	0	0
5	T	1	Total C O 4 2 2	0	0
5	U	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	W	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 7 4 3	0	0
6	J	1	Total C O 7 4 3	0	0
6	J	1	Total C O 7 4 3	0	0

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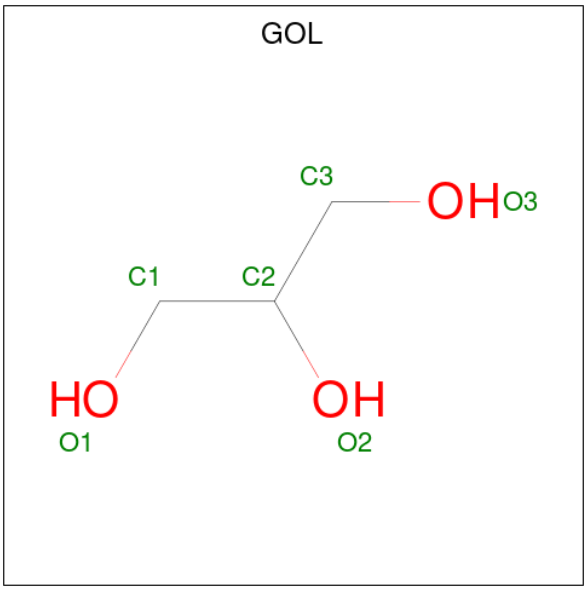
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	1	Total C O 7 4 3	0	0
6	M	1	Total C O 7 4 3	0	0
6	X	1	Total C O 7 4 3	0	0
6	X	1	Total C O 7 4 3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	U	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	67	Total O 67 67	0	0
8	B	88	Total O 88 88	0	0
8	C	58	Total O 58 58	0	0
8	D	87	Total O 87 87	0	0

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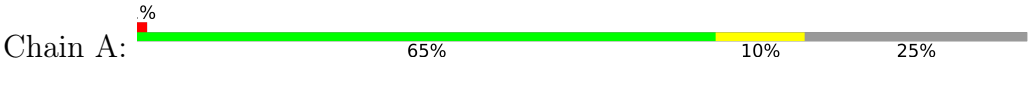
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	65	Total O 65 65	0	0
8	F	74	Total O 74 74	0	0
8	G	59	Total O 59 59	0	0
8	H	59	Total O 59 59	0	0
8	I	80	Total O 80 80	0	0
8	J	57	Total O 57 57	0	0
8	K	74	Total O 74 74	0	0
8	L	69	Total O 69 69	0	0
8	M	63	Total O 63 63	0	0
8	N	64	Total O 64 64	0	0
8	O	81	Total O 81 81	0	0
8	P	75	Total O 75 75	0	0
8	Q	76	Total O 76 76	0	0
8	R	76	Total O 76 76	0	0
8	S	63	Total O 63 63	0	0
8	T	77	Total O 77 77	0	0
8	U	85	Total O 85 85	0	0
8	V	84	Total O 84 84	0	0
8	W	81	Total O 81 81	0	0
8	X	70	Total O 70 70	0	0

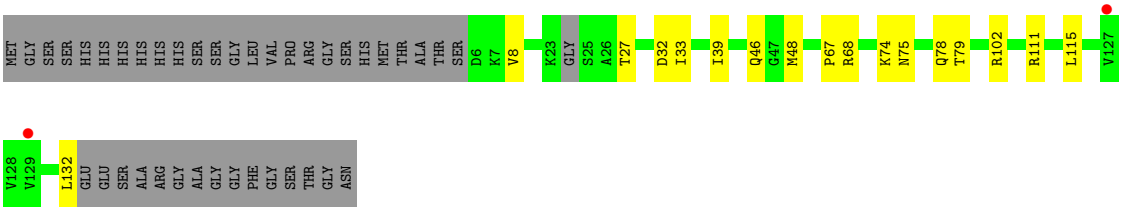
3 Residue-property plots

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

• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

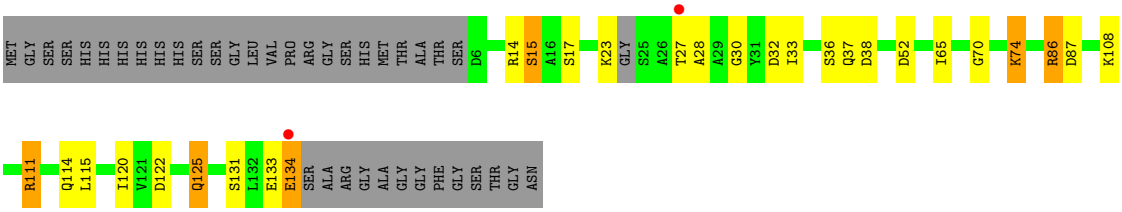
Chain A:





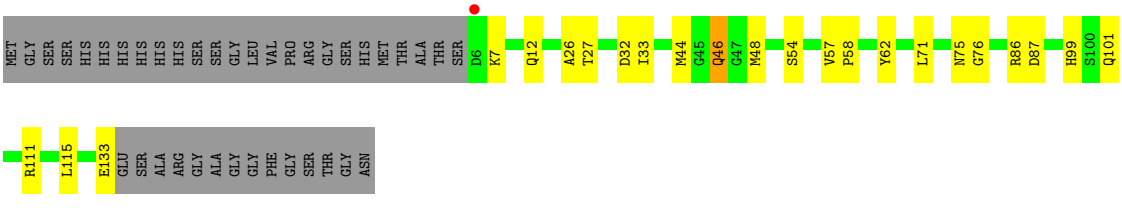
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain B:



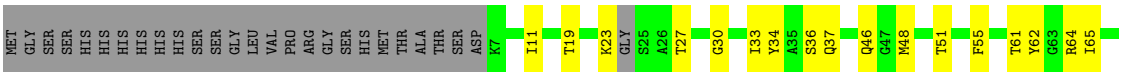
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

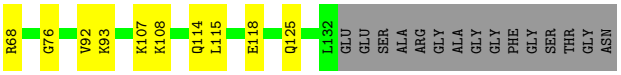
Chain C:



• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

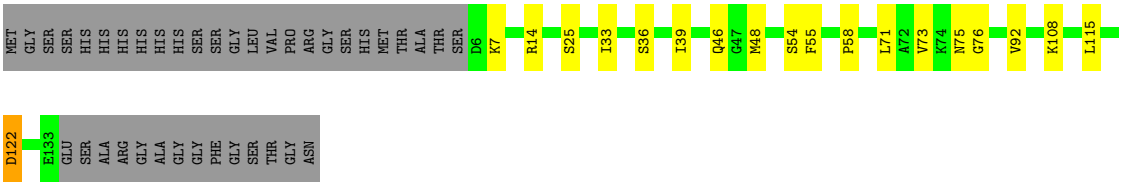
Chain D:





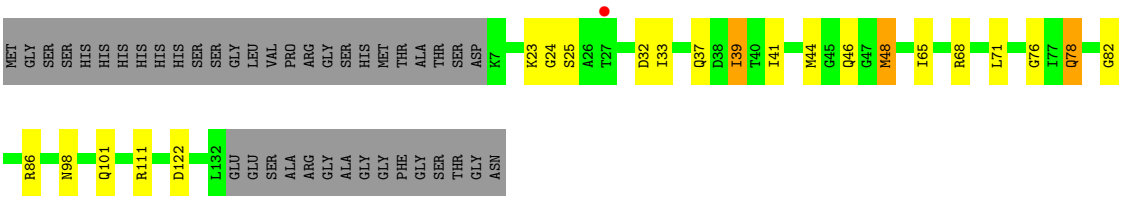
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain E:



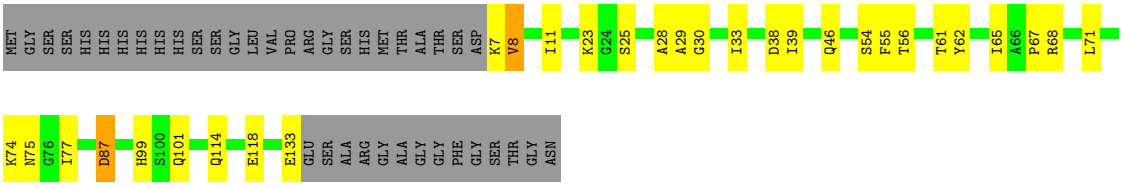
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain F:



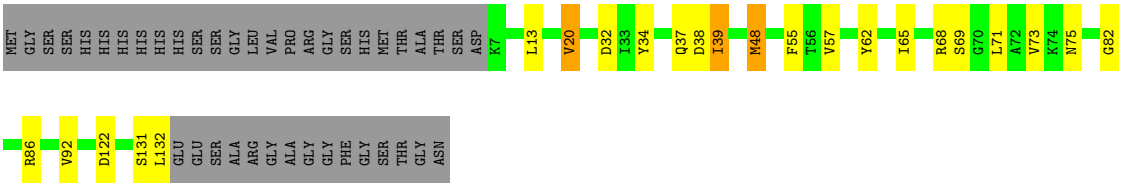
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain G:



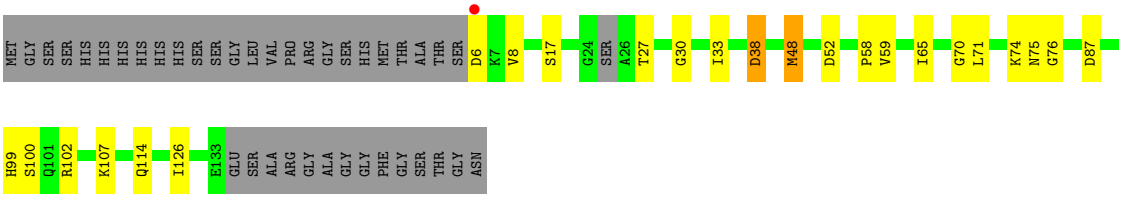
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain H:



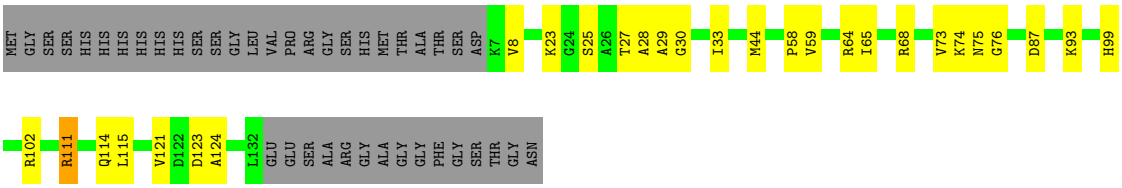
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain I:



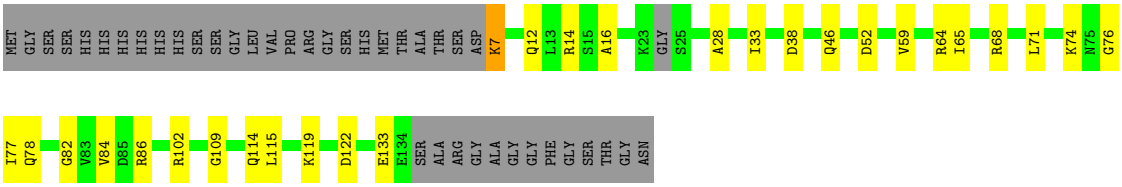
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain J:



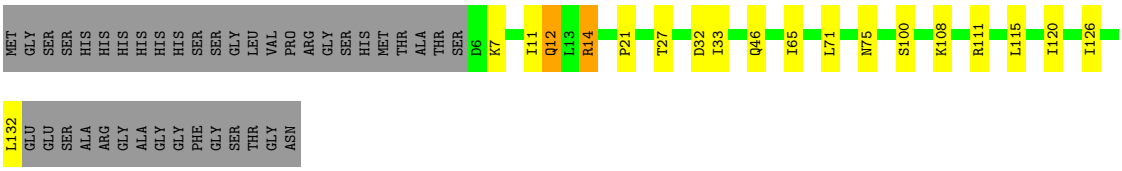
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain K:



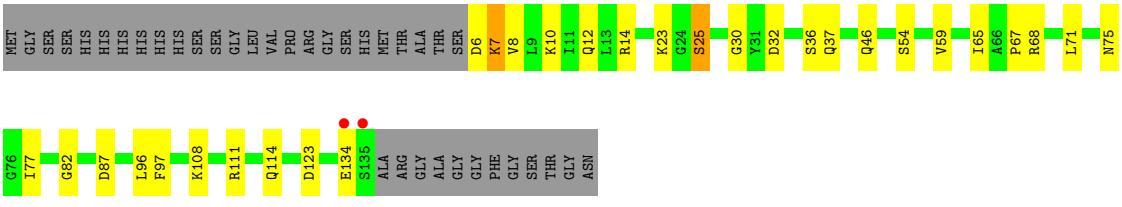
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain L:



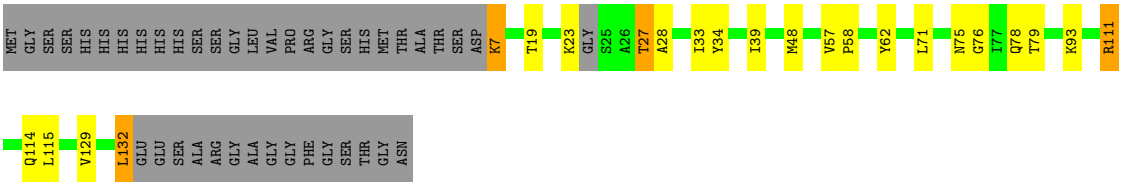
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain M:



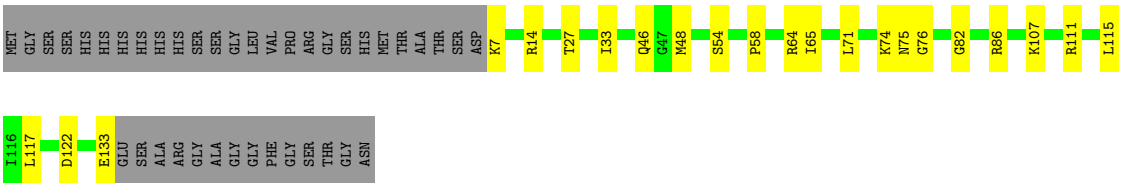
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain N:



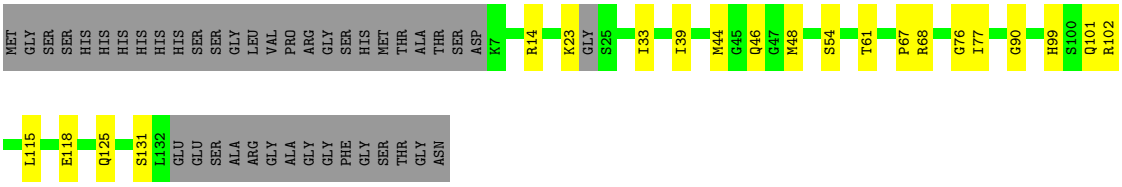
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain O:



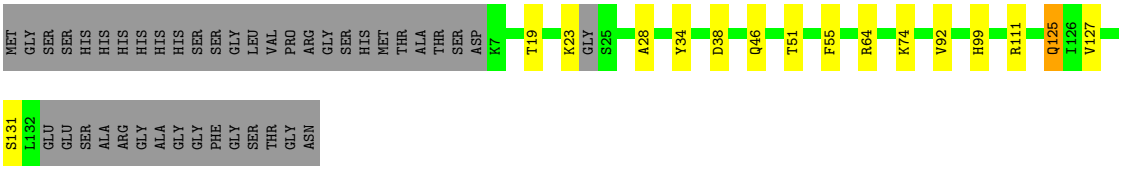
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain P:



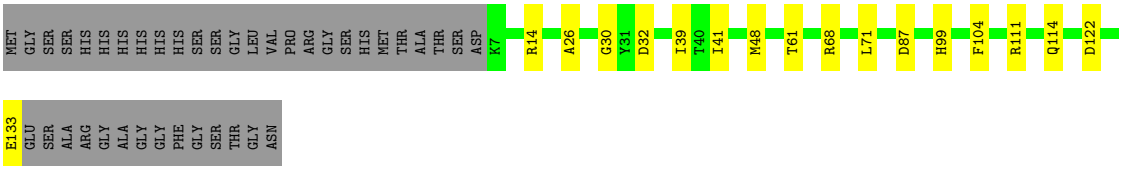
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain Q:



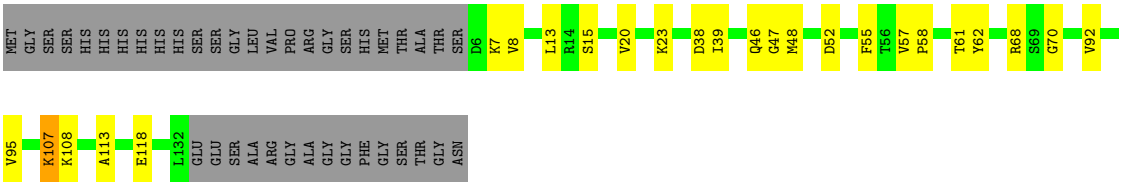
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain R:

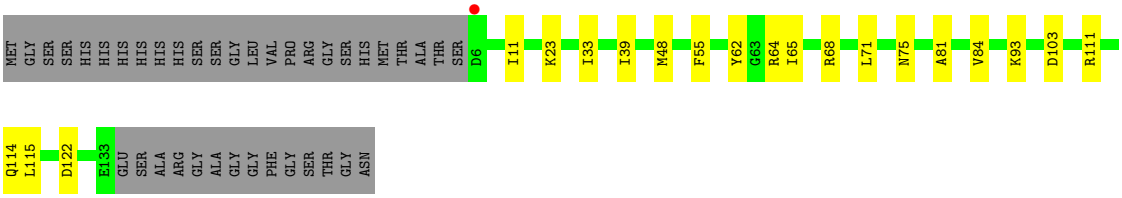


• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

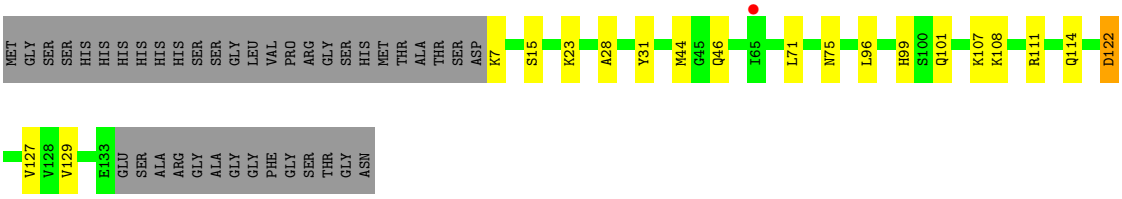
Chain S:



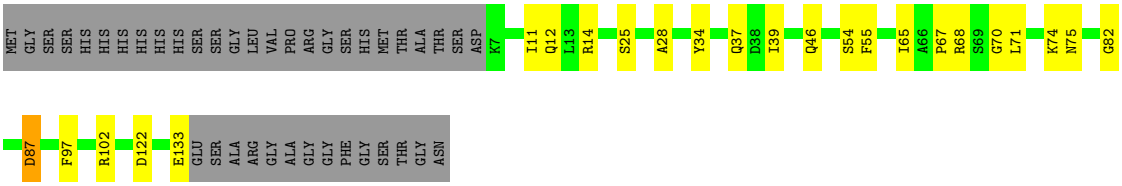
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase



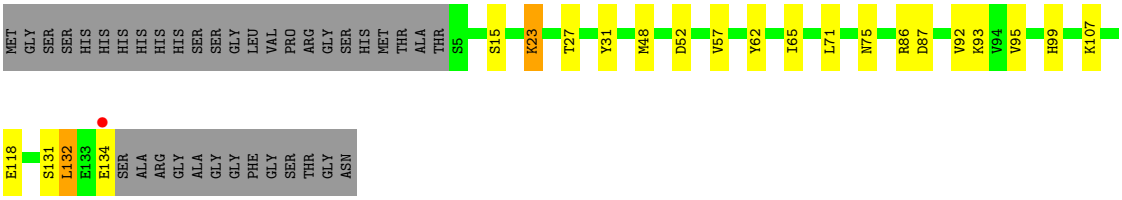
• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase



• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

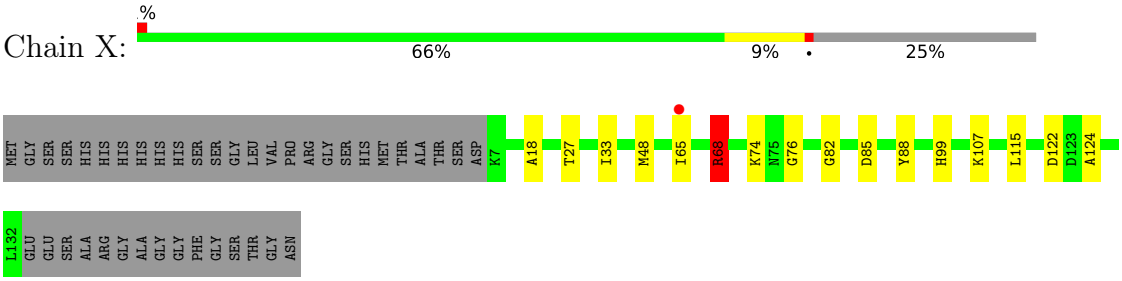


• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase



• Molecule 1: Deoxyuridine 5'-triphosphate nucleotidohydrolase

Chain X:


%
66%
9%
25%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR ALA THR SER ASP K7 A18 T27 I33 M48 I65 R68 K74 N75 G76 G82 D85 Y88 H99 K107 L115 D122 D123 A124
L132 GLU GLU SER ALA ARG GLY ALA GLY GLY PHE GLY SER THR GLY ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.46Å 95.47Å 97.59Å 98.79° 97.42° 107.13°	Depositor
Resolution (Å)	40.62 – 2.00 40.61 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.7 (40.62-2.00) 86.1 (40.61-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.236 0.173 , 0.234	Depositor DCC
R_{free} test set	9588 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 21.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.168 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25087	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: CL, GOL, NA, EDO, SO4, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.97	0/966	0.91	0/1307
1	B	0.98	1/961 (0.1%)	1.01	5/1302 (0.4%)
1	C	0.85	0/993	0.86	0/1344
1	D	0.98	0/974	0.94	0/1318
1	E	0.88	0/961	0.92	1/1302 (0.1%)
1	F	0.93	0/984	0.88	1/1335 (0.1%)
1	G	0.90	0/970	0.91	1/1313 (0.1%)
1	H	0.99	2/954 (0.2%)	0.89	0/1293
1	I	0.95	0/971	0.94	3/1316 (0.2%)
1	J	0.96	0/958	0.96	2/1297 (0.2%)
1	K	0.96	0/998	0.93	3/1349 (0.2%)
1	L	0.85	0/966	0.86	1/1309 (0.1%)
1	M	0.90	1/1004 (0.1%)	0.95	2/1358 (0.1%)
1	N	0.95	0/950	0.92	0/1286
1	O	0.99	0/981	0.91	1/1327 (0.1%)
1	P	0.97	1/938 (0.1%)	0.91	0/1271
1	Q	0.99	0/957	0.92	1/1296 (0.1%)
1	R	0.82	0/968	0.86	3/1311 (0.2%)
1	S	0.92	0/960	0.88	0/1300
1	T	1.00	1/957 (0.1%)	0.95	3/1298 (0.2%)
1	U	1.01	0/956	0.96	1/1295 (0.1%)
1	V	0.98	0/963	0.97	2/1305 (0.2%)
1	W	0.99	1/975 (0.1%)	0.93	1/1321 (0.1%)
1	X	1.05	0/970	0.98	2/1314 (0.2%)
All	All	0.95	7/23235 (0.0%)	0.92	33/31467 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	R	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	20	VAL	CB-CG2	-5.80	1.40	1.52
1	W	95	VAL	CB-CG1	5.78	1.65	1.52
1	B	111	ARG	CG-CD	-5.71	1.37	1.51
1	T	62	TYR	CD1-CE1	-5.70	1.30	1.39
1	M	97	PHE	CE1-CZ	5.13	1.47	1.37
1	H	34	TYR	CD1-CE1	-5.11	1.31	1.39
1	P	90	GLY	C-O	5.11	1.31	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	122	ASP	CB-CG-OD2	7.80	125.32	118.30
1	M	123	ASP	CB-CG-OD2	7.34	124.91	118.30
1	K	38	ASP	CB-CG-OD1	6.61	124.25	118.30
1	K	52	ASP	CB-CG-OD2	6.31	123.98	118.30
1	I	87	ASP	CB-CG-OD2	6.29	123.96	118.30
1	O	111	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	52	ASP	CB-CG-OD1	6.04	123.74	118.30
1	T	64	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	K	14	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	G	87	ASP	CB-CG-OD2	5.74	123.46	118.30
1	T	64	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	M	7	LYS	N-CA-C	-5.65	95.74	111.00
1	J	102	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	71	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	Q	38	ASP	CB-CG-OD1	5.55	123.30	118.30
1	T	103	ASP	CB-CG-OD2	5.55	123.30	118.30
1	J	87	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	14	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	V	87	ASP	CB-CG-OD2	5.47	123.22	118.30
1	X	68[A]	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	X	68[B]	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	I	38	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	V	122	ASP	CB-CG-OD2	5.38	123.14	118.30
1	U	122	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	86	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	14	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	R	122	ASP	CB-CG-OD2	5.31	123.08	118.30
1	W	87	ASP	CB-CG-OD2	5.22	123.00	118.30
1	R	14	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	87	ASP	CB-CG-OD2	5.13	122.92	118.30
1	I	38	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	38	ASP	CB-CG-OD1	5.05	122.85	118.30
1	R	87	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	29	ALA	Peptide
1	R	61	THR	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	953	0	989	21	0
1	B	951	0	967	17	1
1	C	973	0	1004	27	0
1	D	964	0	990	32	0
1	E	950	0	976	12	0
1	F	973	0	1003	26	0
1	G	959	0	986	31	0
1	H	943	0	969	17	0
1	I	958	0	982	17	0
1	J	947	0	980	36	0
1	K	985	0	1021	41	0
1	L	952	0	985	10	0
1	M	993	0	1021	35	0
1	N	940	0	974	19	0
1	O	970	0	998	20	0
1	P	928	0	953	15	0
1	Q	947	0	975	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	957	0	982	14	0
1	S	949	0	978	22	0
1	T	946	0	965	21	0
1	U	945	0	974	11	0
1	V	952	0	975	23	0
1	W	964	0	985	14	0
1	X	959	0	980	15	0
2	A	10	0	0	0	0
2	B	10	0	0	3	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	15	0	0	1	0
2	G	15	0	0	1	0
2	H	5	0	0	0	0
2	I	5	0	0	3	0
2	J	5	0	0	0	0
2	K	10	0	0	3	0
2	M	10	0	0	0	0
2	N	10	0	0	0	0
2	O	5	0	0	0	0
2	P	10	0	0	0	0
2	Q	5	0	0	4	0
2	R	5	0	0	0	0
2	S	10	0	0	2	0
2	T	5	0	0	0	0
2	U	5	0	0	0	0
2	V	15	0	0	4	0
2	W	10	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	2	0	0	0	0
3	P	1	0	0	0	0
3	S	1	0	0	0	0
3	T	2	0	0	0	0
3	V	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	L	2	0	0	0	0
4	N	2	0	0	1	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
5	D	8	0	12	14	0
5	E	4	0	6	1	0
5	F	4	0	6	0	0
5	G	4	0	6	6	0
5	J	8	0	12	8	0
5	K	12	0	18	15	0
5	M	16	0	24	7	0
5	N	4	0	6	3	0
5	O	12	0	17	3	0
5	P	4	0	6	3	0
5	Q	16	0	24	12	0
5	R	8	0	12	0	0
5	S	4	0	6	4	0
5	T	12	0	18	7	0
5	U	4	0	6	0	0
5	V	12	0	18	6	0
5	W	4	0	6	0	0
6	H	7	0	10	6	0
6	J	14	0	20	5	0
6	K	7	0	10	1	0
6	M	7	0	10	0	0
6	X	14	0	20	6	0
7	U	6	0	8	0	0
8	A	67	0	0	2	0
8	B	88	0	0	0	0
8	C	58	0	0	2	0
8	D	87	0	0	0	0
8	E	65	0	0	0	0
8	F	74	0	0	3	0
8	G	59	0	0	0	0
8	H	59	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	80	0	0	2	0
8	J	57	0	0	0	0
8	K	74	0	0	2	0
8	L	69	0	0	0	0
8	M	63	0	0	3	0
8	N	64	0	0	3	0
8	O	81	0	0	0	0
8	P	75	0	0	3	0
8	Q	76	0	0	1	1
8	R	76	0	0	2	0
8	S	63	0	0	2	0
8	T	77	0	0	1	0
8	U	85	0	0	1	0
8	V	84	0	0	0	0
8	W	81	0	0	0	0
8	X	70	0	0	1	0
All	All	25087	0	23893	452	1

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 10.

All (452) 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:C:46:GLN:HE21	1:C:48[B]:MET:HE1	1.21	1.06
1:V:87:ASP:OD1	1:X:27:THR:HG23	1.61	1.01
1:M:68:ARG:HB2	1:M:71[B]:LEU:HD13	1.40	1.00
1:P:77:ILE:HG22	5:P:151:EDO:H11	1.42	0.99
1:X:85:ASP:OD1	6:X:148:PEG:H21	1.60	0.99
1:K:102:ARG:HD2	5:K:152:EDO:H22	1.41	0.98
1:Q:34:TYR:HB2	5:Q:151:EDO:H12	1.43	0.98
1:S:68:ARG:HD2	8:S:1047:HOH:O	1.64	0.97
1:Q:34:TYR:O	5:Q:151:EDO:H21	1.65	0.96
1:G:74:LYS:HA	1:K:74:LYS:HE2	1.44	0.96
1:K:64:ARG:HG3	5:K:151:EDO:H11	1.47	0.96
1:M:67:PRO:HG3	5:M:152:EDO:H21	1.45	0.96
1:Q:19:THR:O	5:Q:151:EDO:H11	1.66	0.95
1:Q:99:HIS:HE1	1:R:99:HIS:NE2	1.64	0.94
1:O:107:LYS:HE2	1:V:37:GLN:HE21	1.32	0.93
1:C:46:GLN:HE21	1:C:48[B]:MET:CE	1.82	0.92
1:T:68:ARG:HD3	8:T:1366:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:ARG:HD2	5:J:150:EDO:H12	1.54	0.90
1:Q:99:HIS:CE1	1:R:99:HIS:NE2	2.40	0.90
1:K:102:ARG:HB3	5:K:152:EDO:H21	1.52	0.89
1:H:39:ILE:HB	6:H:149:PEG:H42	1.55	0.89
1:D:34:TYR:O	5:D:151:EDO:H22	1.72	0.88
1:O:7:LYS:HB3	1:O:58:PRO:HB3	1.54	0.88
1:D:46:GLN:HE22	1:F:76:GLY:HA2	1.38	0.88
1:M:87:ASP:OD1	1:O:27:THR:HG23	1.73	0.88
1:K:7:LYS:HZ2	1:K:59:VAL:HG23	1.36	0.87
1:C:7:LYS:HA	1:C:58:PRO:HB3	1.58	0.86
1:C:26:ALA:HB2	1:M:8:VAL:HG21	1.58	0.84
1:J:111[B]:ARG:HH21	1:J:111[B]:ARG:CG	1.90	0.84
1:J:33:ILE:HD11	1:J:115:LEU:HB2	1.61	0.83
1:P:68:ARG:HD2	8:P:1186:HOH:O	1.79	0.82
1:S:68:ARG:NH2	5:S:151:EDO:H11	1.95	0.81
1:K:76:GLY:HA2	1:L:46:GLN:HE22	1.43	0.81
1:T:33:ILE:HD11	1:T:115:LEU:HB2	1.59	0.81
1:A:46:GLN:HE22	1:C:76:GLY:HA2	1.44	0.81
1:D:65:ILE:O	5:D:152:EDO:H11	1.80	0.80
1:V:25:SER:HB3	1:V:28:ALA:HB2	1.64	0.80
1:O:64:ARG:HG3	5:O:153:EDO:H22	1.63	0.79
1:M:71[B]:LEU:HD12	1:M:71[B]:LEU:H	1.47	0.79
1:C:46:GLN:NE2	1:C:48[B]:MET:HE1	1.95	0.79
1:K:64:ARG:CG	5:K:151:EDO:H11	2.13	0.79
1:D:76:GLY:HA2	1:E:46:GLN:HE22	1.47	0.78
1:A:132:LEU:CD1	1:C:54:SER:HB3	2.13	0.78
1:D:19:THR:H	5:D:151:EDO:H21	1.48	0.78
1:G:46:GLN:HE22	1:I:76:GLY:HA2	1.48	0.78
5:V:152:EDO:H21	5:V:153:EDO:H12	1.65	0.77
1:M:68:ARG:HB2	1:M:71[B]:LEU:CD1	2.14	0.77
1:D:64:ARG:HG3	5:D:152:EDO:C2	2.14	0.77
1:K:7:LYS:NZ	1:K:59:VAL:HG23	2.00	0.77
1:C:44:MET:HE2	1:C:101:GLN:NE2	2.00	0.76
1:S:48[B]:MET:HE1	1:S:95:VAL:HG13	1.65	0.76
1:K:71:LEU:HB2	5:K:150:EDO:H22	1.67	0.76
1:P:76:GLY:HA2	1:Q:46:GLN:HE22	1.50	0.76
1:D:64:ARG:NH2	5:D:152:EDO:O1	2.19	0.76
1:P:33:ILE:HD11	1:P:115:LEU:HB2	1.68	0.76
1:F:44:MET:CE	1:F:101:GLN:NE2	2.49	0.75
1:C:44:MET:HE1	8:C:1928:HOH:O	1.87	0.75
1:D:64:ARG:HG3	5:D:152:EDO:H21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:ARG:NH2	1:J:111[A]:ARG:NH2	2.34	0.74
1:H:32:ASP:OD1	1:H:68[A]:ARG:NH1	2.20	0.74
1:J:93:LYS:H	6:J:152:PEG:H41	1.53	0.74
1:A:132:LEU:HD11	1:C:54:SER:HB3	1.69	0.74
1:J:111[B]:ARG:HH21	1:J:111[B]:ARG:HG3	1.51	0.74
1:K:102:ARG:HD2	5:K:152:EDO:C2	2.16	0.74
1:J:64:ARG:CD	5:J:150:EDO:H12	2.18	0.73
1:K:71:LEU:HB2	5:K:150:EDO:C2	2.19	0.72
1:K:33[A]:ILE:HD11	1:K:115:LEU:HB2	1.71	0.72
1:J:27:THR:HG22	1:K:86[A]:ARG:NH1	2.04	0.71
1:C:44:MET:CE	1:C:101:GLN:NE2	2.53	0.71
1:H:38:ASP:O	6:H:149:PEG:H12	1.89	0.71
1:F:44:MET:HE2	1:F:101:GLN:NE2	2.06	0.71
1:G:67:PRO:CB	5:G:151:EDO:H11	2.20	0.71
1:N:23:LYS:NZ	1:O:122:ASP:O	2.23	0.70
1:P:99:HIS:HE1	2:Q:148:SO4:O1	1.73	0.70
1:D:23:LYS:NZ	1:E:122:ASP:O	2.25	0.70
1:J:64:ARG:HG3	5:J:150:EDO:C1	2.21	0.69
1:W:31:TYR:OH	1:X:124:ALA:HB3	1.91	0.69
1:M:68:ARG:N	5:M:151:EDO:H22	2.07	0.69
1:V:46:GLN:HE22	1:X:76:GLY:HA2	1.57	0.69
1:G:68:ARG:O	5:G:151:EDO:H12	1.92	0.69
1:S:48[B]:MET:CE	1:S:95:VAL:HG13	2.22	0.69
1:J:64:ARG:HG3	5:J:150:EDO:H11	1.73	0.69
1:X:85:ASP:OD1	6:X:148:PEG:C2	2.37	0.69
1:F:44:MET:HE2	1:F:101:GLN:HE21	1.58	0.69
1:A:27:THR:HG22	1:B:86:ARG:NH2	2.06	0.69
1:R:68:ARG:HD3	8:R:802:HOH:O	1.95	0.67
1:W:57:VAL:O	1:W:86:ARG:NH2	2.27	0.67
1:Q:64:ARG:HG3	5:Q:150:EDO:H22	1.77	0.67
1:A:33[A]:ILE:HD11	1:A:115:LEU:HB2	1.77	0.66
1:N:39:ILE:HD12	1:N:48:MET:O	1.94	0.66
1:D:30:GLY:HA3	1:D:114:GLN:HE21	1.61	0.66
1:K:12:GLN:HE21	1:L:132:LEU:HG	1.60	0.66
1:M:6:ASP:N	1:M:59:VAL:H	1.93	0.66
1:C:32:ASP:HB3	1:C:111:ARG:HG2	1.76	0.66
1:N:27:THR:HG22	1:O:86[A]:ARG:CZ	2.26	0.66
8:P:1978:HOH:O	1:Q:131:SER:HB2	1.96	0.65
2:Q:148:SO4:O2	1:R:99:HIS:HE1	1.79	0.65
1:Q:64:ARG:CG	5:Q:150:EDO:H22	2.27	0.65
1:T:68:ARG:NH2	1:T:111:ARG:NH2	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:114:GLN:OE1	5:T:152:EDO:H21	1.97	0.65
1:G:33:ILE:CD1	1:G:65:ILE:HD12	2.26	0.64
5:E:150:EDO:H11	1:K:16:ALA:HB3	1.78	0.64
1:O:82:GLY:HA3	5:O:153:EDO:H11	1.79	0.64
1:O:107:LYS:HE2	1:V:37:GLN:NE2	2.10	0.64
1:L:71:LEU:HA	1:L:75:ASN:HD22	1.63	0.63
1:J:76:GLY:HA2	1:K:46:GLN:HE22	1.62	0.63
1:F:44:MET:CE	1:F:101:GLN:HE21	2.11	0.63
1:M:30:GLY:HA3	1:M:114:GLN:HE21	1.62	0.63
1:O:107:LYS:CE	1:V:37:GLN:HE21	2.08	0.63
1:S:70:GLY:HA3	5:S:151:EDO:H12	1.80	0.63
1:F:44:MET:HE3	1:F:101:GLN:NE2	2.12	0.62
1:J:59:VAL:H	6:J:153:PEG:H31	1.64	0.62
1:D:51:THR:O	5:D:151:EDO:O2	2.17	0.62
1:F:37:GLN:HB3	8:F:1349:HOH:O	1.98	0.62
1:A:39:ILE:HD12	1:A:48:MET:O	1.99	0.62
1:V:68[A]:ARG:HB2	5:V:156:EDO:H12	1.81	0.62
1:C:26:ALA:CB	1:M:8:VAL:HG21	2.26	0.62
1:M:67:PRO:CG	5:M:152:EDO:H21	2.25	0.62
2:B:148:SO4:O1	1:C:99:HIS:HE1	1.82	0.61
1:K:82:GLY:HA3	5:K:151:EDO:H12	1.81	0.61
1:N:79:THR:OG1	5:N:153:EDO:H21	1.99	0.61
1:G:77:ILE:HG22	5:G:151:EDO:H21	1.81	0.61
1:C:44:MET:CE	1:C:101:GLN:HE21	2.13	0.61
1:G:101:GLN:HG3	5:K:152:EDO:C1	2.31	0.60
1:R:68:ARG:CD	8:R:802:HOH:O	2.48	0.60
1:X:88:TYR:HB2	6:X:148:PEG:H12	1.83	0.60
1:B:27:THR:HG23	1:C:87:ASP:HB3	1.83	0.60
1:G:87:ASP:HB3	1:I:27:THR:CG2	2.31	0.60
1:H:37:GLN:HB3	6:H:149:PEG:H21	1.83	0.60
1:K:76:GLY:CA	1:L:46:GLN:HE22	2.11	0.60
1:M:68:ARG:NH2	8:M:933:HOH:O	2.35	0.60
1:A:79:THR:HG23	8:A:1821:HOH:O	2.01	0.60
1:A:67:PRO:HD3	1:A:79:THR:HG22	1.83	0.60
1:J:99:HIS:HE1	2:K:148:SO4:O4	1.85	0.60
1:D:37[A]:GLN:OE1	1:J:73:VAL:HG11	2.02	0.60
1:S:39:ILE:HD12	1:S:48[A]:MET:O	2.02	0.60
1:B:36:SER:O	1:B:108:LYS:HE2	2.02	0.59
1:J:99:HIS:CE1	2:K:148:SO4:O4	2.55	0.59
1:T:65:ILE:HD11	1:T:84:VAL:CG2	2.32	0.59
6:H:149:PEG:H11	1:K:109:GLY:CA	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:65:ILE:HD11	1:T:84:VAL:HG21	1.84	0.59
1:D:19:THR:H	5:D:151:EDO:C2	2.13	0.59
1:E:76:GLY:HA2	1:F:46:GLN:HE22	1.66	0.59
1:M:71[B]:LEU:HD12	1:M:71[B]:LEU:N	2.18	0.59
1:M:71[B]:LEU:HA	1:M:75:ASN:HD22	1.68	0.59
1:F:33[A]:ILE:HD11	1:F:65[A]:ILE:HD13	1.85	0.59
1:N:39:ILE:CD1	1:N:48:MET:O	2.51	0.59
1:O:64:ARG:HD2	5:O:153:EDO:H21	1.85	0.59
1:E:73:VAL:HG22	1:F:48:MET:HE1	1.83	0.58
1:T:65:ILE:HD13	5:T:154:EDO:H22	1.84	0.58
1:G:23:LYS:NZ	1:H:122:ASP:O	2.35	0.58
1:K:65[A]:ILE:HD12	1:K:84:VAL:HG23	1.85	0.58
1:K:82:GLY:H	6:K:153:PEG:H42	1.68	0.58
1:H:13:LEU:HD21	1:H:20:VAL:HG22	1.85	0.58
1:M:68:ARG:N	5:M:151:EDO:C2	2.65	0.58
1:L:33[A]:ILE:HD11	1:L:115:LEU:HB2	1.85	0.58
1:V:102:ARG:NH2	2:V:149:SO4:O1	2.37	0.58
1:M:14[A]:ARG:HD2	1:M:54:SER:OG	2.04	0.58
1:V:133:GLU:HA	1:V:133:GLU:OE1	2.04	0.58
1:G:77:ILE:CG2	5:G:151:EDO:H21	2.34	0.57
1:K:65[A]:ILE:CD1	1:K:84:VAL:HG23	2.33	0.57
1:P:99:HIS:CE1	2:Q:148:SO4:O1	2.54	0.57
1:K:102:ARG:CB	5:K:152:EDO:H21	2.29	0.57
1:L:11:ILE:HD13	1:L:21:PRO:HD2	1.86	0.57
1:C:26:ALA:HB2	1:M:8:VAL:CG2	2.31	0.57
1:J:27:THR:HG22	1:K:86[A]:ARG:CZ	2.34	0.57
1:E:7:LYS:HB3	1:E:58:PRO:HB3	1.87	0.57
1:G:30:GLY:HA3	1:G:114:GLN:HE21	1.68	0.57
1:C:57:VAL:O	1:C:86:ARG:NH1	2.32	0.57
1:K:65[A]:ILE:CD1	1:K:84:VAL:CG2	2.83	0.57
1:K:65[A]:ILE:HD11	1:K:84:VAL:HG21	1.86	0.56
1:S:7:LYS:HA	1:S:58:PRO:HB3	1.86	0.56
1:W:27:THR:O	1:W:27:THR:HG22	2.05	0.56
1:B:33:ILE:CD1	1:B:65:ILE:HD12	2.35	0.56
1:D:34:TYR:O	5:D:151:EDO:C2	2.50	0.56
1:A:74:LYS:HG3	1:A:75:ASN:ND2	2.20	0.56
1:B:33:ILE:HD11	1:B:115:LEU:HB2	1.87	0.56
1:B:33:ILE:HD13	1:B:65:ILE:HD12	1.87	0.56
1:F:33[A]:ILE:HD13	1:F:65[A]:ILE:HD12	1.88	0.56
2:S:148:SO4:O2	1:U:99:HIS:CE1	2.58	0.56
1:T:23:LYS:NZ	1:U:122:ASP:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:LYS:HZ2	1:K:59:VAL:H	1.53	0.56
1:I:6:ASP:HB3	1:I:8:VAL:H	1.70	0.56
1:V:67:PRO:CB	5:V:156:EDO:H21	2.36	0.56
1:C:26:ALA:CB	1:M:8:VAL:CG2	2.84	0.55
1:O:33:ILE:HD11	1:O:115:LEU:HB2	1.89	0.55
1:T:81:ALA:HB3	5:T:154:EDO:H11	1.88	0.55
1:C:33:ILE:HD11	1:C:115:LEU:HB2	1.88	0.55
1:G:7:LYS:HG2	1:G:8:VAL:H	1.72	0.55
1:J:30:GLY:HA3	1:J:114:GLN:HE21	1.72	0.55
1:P:44:MET:HE3	1:P:101:GLN:NE2	2.22	0.55
1:U:44:MET:CE	1:U:101:GLN:HE22	2.20	0.55
1:N:79:THR:OG1	5:N:153:EDO:C2	2.55	0.55
1:S:68:ARG:CD	8:S:1047:HOH:O	2.38	0.54
1:E:14:ARG:HD2	1:E:54:SER:OG	2.07	0.54
1:P:76:GLY:CA	1:Q:46:GLN:HE22	2.19	0.54
1:A:74:LYS:NZ	1:A:75:ASN:HD21	2.06	0.54
1:C:12:GLN:HB3	1:C:54:SER:HB2	1.89	0.54
1:G:33:ILE:HD11	1:G:65:ILE:HD12	1.88	0.54
6:H:149:PEG:H11	1:K:109:GLY:HA2	1.90	0.54
1:M:68:ARG:H	5:M:151:EDO:C2	2.21	0.54
1:P:39:ILE:HD12	1:P:48:MET:O	2.07	0.54
1:S:68:ARG:CZ	5:S:151:EDO:H11	2.37	0.54
1:F:39:ILE:HD12	1:F:48:MET:O	2.08	0.54
2:B:148:SO4:O1	1:C:99:HIS:CE1	2.61	0.53
1:M:71[A]:LEU:HA	1:M:75:ASN:HD22	1.73	0.53
1:N:33:ILE:HD11	1:N:115:LEU:HB3	1.90	0.53
1:S:55:PHE:CE1	1:S:92:VAL:HG21	2.43	0.53
1:G:67:PRO:HB3	5:G:151:EDO:H11	1.91	0.53
1:G:77:ILE:HG22	5:G:151:EDO:C2	2.39	0.53
1:K:65[A]:ILE:HD11	1:K:84:VAL:CG2	2.39	0.53
1:J:64:ARG:CG	5:J:150:EDO:H12	2.38	0.53
1:J:59:VAL:H	6:J:153:PEG:C3	2.21	0.53
1:S:23:LYS:NZ	1:T:122:ASP:O	2.42	0.53
1:J:111[B]:ARG:CG	1:J:111[B]:ARG:NH2	2.60	0.53
1:J:64:ARG:CG	5:J:150:EDO:C1	2.86	0.53
1:K:114:GLN:NE2	8:K:580:HOH:O	2.40	0.53
1:T:68:ARG:NH2	1:T:111:ARG:HH22	2.06	0.53
1:T:65:ILE:CD1	1:T:84:VAL:CG2	2.87	0.52
1:G:29:ALA:HB2	1:H:62:TYR:HB3	1.92	0.52
1:P:77:ILE:CG2	5:P:151:EDO:H11	2.28	0.52
1:T:71:LEU:HA	1:T:75:ASN:HD22	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33[A]:ILE:HD11	1:F:65[A]:ILE:CD1	2.40	0.52
1:O:107:LYS:CE	1:V:37:GLN:NE2	2.71	0.52
1:J:65:ILE:O	5:J:150:EDO:H22	2.10	0.52
1:N:7:LYS:HB3	1:N:58:PRO:HB3	1.92	0.52
1:N:33:ILE:HD11	1:N:115:LEU:CB	2.40	0.52
1:D:34:TYR:HB2	5:D:151:EDO:H22	1.91	0.52
1:D:46:GLN:HE22	1:F:76:GLY:CA	2.16	0.52
1:E:55:PHE:CE1	1:E:92:VAL:HG21	2.45	0.52
1:U:71:LEU:HA	1:U:75:ASN:HD22	1.75	0.52
2:Q:148:SO4:O2	1:R:99:HIS:CE1	2.62	0.52
1:R:68:ARG:NH2	1:R:111:ARG:HH21	2.08	0.52
1:V:71:LEU:HA	1:V:75:ASN:HD22	1.75	0.52
1:I:6:ASP:O	1:I:58:PRO:HB3	2.09	0.52
1:J:23:LYS:HE2	1:J:28:ALA:O	2.09	0.52
1:J:111[B]:ARG:HH21	1:J:111[B]:ARG:HG2	1.70	0.52
1:D:48:MET:SD	1:D:93:LYS:HD3	2.50	0.52
1:K:77:ILE:CG2	5:K:150:EDO:H21	2.40	0.52
1:D:33:ILE:CD1	1:D:65:ILE:HD12	2.39	0.51
1:G:23:LYS:HE2	1:G:28:ALA:O	2.11	0.51
2:V:148:SO4:O3	1:X:99:HIS:HE1	1.93	0.51
1:N:34:TYR:CE1	1:N:111:ARG:HD2	2.45	0.51
1:C:44:MET:HE3	1:C:101:GLN:NE2	2.26	0.51
1:V:65:ILE:HB	1:V:82:GLY:HA2	1.93	0.51
1:D:93:LYS:HE3	8:K:2113:HOH:O	2.11	0.51
8:C:1580:HOH:O	1:J:44:MET:HE2	2.11	0.51
1:F:78:GLN:NE2	8:F:431:HOH:O	2.44	0.51
1:I:6:ASP:HB3	1:I:8:VAL:HB	1.92	0.50
1:W:48:MET:HE3	1:W:93:LYS:HZ2	1.74	0.50
1:D:55:PHE:CE1	1:D:92:VAL:HG21	2.46	0.50
1:M:37:GLN:NE2	1:X:107:LYS:HE2	2.26	0.50
1:F:44:MET:HE3	1:F:101:GLN:HE22	1.75	0.50
1:N:76:GLY:HA2	1:O:46:GLN:HE22	1.76	0.50
1:R:32:ASP:HB3	1:R:111:ARG:HD3	1.93	0.50
1:V:68[B]:ARG:N	5:V:156:EDO:H21	2.27	0.50
1:F:33[A]:ILE:CD1	1:F:65[A]:ILE:HD12	2.42	0.50
1:G:87:ASP:HB3	1:I:27:THR:HG23	1.93	0.50
1:M:14[B]:ARG:NH2	8:M:1096:HOH:O	2.27	0.50
2:S:148:SO4:O2	1:U:99:HIS:HE1	1.95	0.50
1:N:19:THR:O	4:N:151:CL:CL	2.67	0.50
1:V:11:ILE:HD13	1:V:55:PHE:HB3	1.94	0.50
1:C:71:LEU:HA	1:C:75:ASN:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:LEU:HA	1:N:75:ASN:HD22	1.77	0.50
1:D:76:GLY:CA	1:E:46:GLN:HE22	2.22	0.49
1:M:67:PRO:CA	5:M:151:EDO:H22	2.42	0.49
1:T:39:ILE:HD12	1:T:48:MET:O	2.12	0.49
1:O:14:ARG:HD2	1:O:54:SER:OG	2.12	0.49
1:A:74:LYS:O	1:A:102:ARG:NH1	2.45	0.49
1:F:33[A]:ILE:CD1	1:F:65[A]:ILE:CD1	2.90	0.49
5:N:153:EDO:H12	8:N:157:HOH:O	2.12	0.49
1:A:32:ASP:OD1	1:A:68[B]:ARG:NH2	2.43	0.49
1:A:67:PRO:HD3	1:A:79:THR:CG2	2.42	0.49
1:T:93:LYS:O	5:T:154:EDO:H21	2.12	0.49
1:F:86[A]:ARG:NH1	1:F:122:ASP:OD1	2.45	0.49
1:J:58:PRO:HA	6:J:153:PEG:H32	1.94	0.49
1:M:68:ARG:CZ	8:M:933:HOH:O	2.60	0.49
1:V:68[A]:ARG:N	5:V:156:EDO:H21	2.28	0.49
1:X:65:ILE:HB	1:X:82:GLY:HA2	1.95	0.49
1:F:24:GLY:N	8:F:2267:HOH:O	2.36	0.49
1:J:76:GLY:CA	1:K:46:GLN:HE22	2.25	0.49
1:J:111[B]:ARG:HG3	1:J:111[B]:ARG:NH2	2.26	0.49
1:P:44:MET:CE	1:P:101:GLN:NE2	2.76	0.49
1:I:75:ASN:HA	1:I:102:ARG:HH22	1.77	0.48
1:A:132:LEU:HD11	1:C:54:SER:CB	2.40	0.48
1:G:68:ARG:NH1	2:G:150:SO4:O3	2.46	0.48
1:K:68[B]:ARG:NH2	2:K:149:SO4:O1	2.45	0.48
1:M:46:GLN:HE22	1:O:76:GLY:HA2	1.79	0.48
6:X:149:PEG:H12	8:X:157:HOH:O	2.13	0.48
1:G:99:HIS:CE1	2:I:148:SO4:O3	2.65	0.48
1:B:15:SER:HB3	1:B:17:SER:H	1.77	0.48
1:H:65:ILE:HB	1:H:82:GLY:HA2	1.96	0.48
1:K:102:ARG:CD	5:K:152:EDO:H22	2.29	0.48
1:R:26:ALA:HB2	1:S:8:VAL:HG21	1.96	0.48
1:I:38:ASP:OD1	1:I:107:LYS:HA	2.13	0.48
1:Q:34:TYR:O	5:Q:151:EDO:C2	2.49	0.48
1:Q:51:THR:HB	5:Q:151:EDO:H22	1.96	0.48
1:M:12:GLN:HB2	1:N:132:LEU:HD13	1.96	0.48
1:Q:34:TYR:CB	5:Q:151:EDO:H12	2.31	0.48
1:D:64:ARG:CG	5:D:152:EDO:H21	2.41	0.47
1:G:54:SER:HB3	1:H:132:LEU:HD11	1.96	0.47
1:H:39:ILE:HD12	1:H:48:MET:O	2.13	0.47
1:M:32:ASP:HB3	1:M:111:ARG:HD2	1.96	0.47
1:N:23:LYS:HE2	1:N:28:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:23:LYS:NZ	1:X:122:ASP:O	2.40	0.47
1:B:32:ASP:HB3	1:B:111:ARG:HD2	1.96	0.47
1:G:99:HIS:HE1	2:I:148:SO4:O3	1.97	0.47
1:S:46:GLN:HE21	1:S:48[B]:MET:HE1	1.79	0.47
1:K:65[A]:ILE:HB	1:K:82:GLY:HA2	1.97	0.47
1:K:68[B]:ARG:HD3	1:K:71:LEU:CD1	2.44	0.47
1:O:107:LYS:NZ	1:V:37:GLN:NE2	2.63	0.47
1:T:65:ILE:HD12	1:T:84:VAL:HG23	1.97	0.47
1:W:131:SER:O	1:W:134:GLU:HG2	2.13	0.47
1:J:68:ARG:NH2	1:J:111[A]:ARG:CZ	2.77	0.47
1:I:71:LEU:HA	1:I:75:ASN:HD22	1.80	0.47
1:V:14:ARG:NH1	1:V:54:SER:OG	2.43	0.47
1:D:19:THR:N	5:D:151:EDO:H21	2.24	0.47
1:A:74:LYS:HZ2	1:A:75:ASN:HD21	1.62	0.46
1:D:64:ARG:HG3	5:D:152:EDO:H22	1.96	0.46
1:H:69:SER:O	1:H:73:VAL:HG23	2.16	0.46
1:R:30:GLY:HA3	1:R:114:GLN:HE21	1.81	0.46
1:B:133:GLU:O	1:B:134:GLU:CB	2.64	0.46
1:H:55:PHE:CE1	1:H:92:VAL:HG21	2.51	0.46
1:J:121:VAL:CG1	1:J:124:ALA:HB2	2.46	0.46
1:K:122:ASP:OD2	1:K:122:ASP:N	2.49	0.46
1:L:12:GLN:NE2	1:L:14:ARG:HG2	2.30	0.46
1:G:38:ASP:HB2	1:S:38:ASP:O	2.16	0.46
1:G:101:GLN:HG3	5:K:152:EDO:C2	2.46	0.46
1:G:29:ALA:HB2	1:H:62:TYR:CB	2.45	0.46
1:Q:55:PHE:CE1	1:Q:92:VAL:HG21	2.51	0.46
1:V:46:GLN:NE2	1:V:97:PHE:HE2	2.13	0.46
1:D:34:TYR:HB2	5:D:151:EDO:C2	2.46	0.45
1:F:32:ASP:HB3	1:F:111:ARG:HG2	1.98	0.45
1:G:33:ILE:HD11	1:G:65:ILE:CD1	2.45	0.45
1:O:74:LYS:HD3	1:X:74:LYS:HE2	1.98	0.45
1:I:6:ASP:N	1:I:59:VAL:H	2.14	0.45
1:U:23:LYS:HB3	1:U:28:ALA:HB3	1.98	0.45
1:F:41:ILE:HG22	1:F:98:ASN:HB2	1.98	0.45
1:I:30:GLY:HA3	1:I:114:GLN:HE21	1.82	0.45
1:I:52:ASP:OD1	8:I:1843:HOH:O	2.21	0.45
1:A:27:THR:HG22	1:B:86:ARG:HH21	1.80	0.45
1:B:120:ILE:CD1	1:B:122:ASP:HB3	2.46	0.45
1:K:65[B]:ILE:HB	1:K:82:GLY:HA2	1.99	0.45
1:P:44:MET:CE	1:P:101:GLN:HE21	2.29	0.45
1:W:62:TYR:CE1	1:W:118:GLU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:77:ILE:CG2	1:M:96:LEU:HD22	2.47	0.45
1:T:11:ILE:HD13	1:T:55:PHE:HB3	1.99	0.45
1:M:23:LYS:HE3	1:M:25:SER:O	2.17	0.45
1:X:88:TYR:CD1	6:X:148:PEG:H12	2.52	0.45
1:J:123:ASP:OD2	1:L:7:LYS:HD3	2.16	0.44
1:N:114:GLN:NE2	8:N:650:HOH:O	2.48	0.44
1:A:8:VAL:HG22	1:B:125:GLN:HG2	1.98	0.44
1:G:61:THR:HA	1:G:118:GLU:O	2.17	0.44
1:V:70:GLY:O	1:V:74:LYS:HG3	2.17	0.44
1:Q:19:THR:O	5:Q:151:EDO:C1	2.53	0.44
1:Q:125:GLN:HB2	8:Q:812:HOH:O	2.18	0.44
1:F:65[B]:ILE:HB	1:F:82:GLY:HA2	1.98	0.44
1:Q:64:ARG:HD2	5:Q:150:EDO:H11	1.99	0.44
1:F:48:MET:HE3	1:F:48:MET:HB2	1.76	0.43
1:V:12:GLN:HB2	1:W:132:LEU:HD13	2.00	0.43
1:J:64:ARG:HG3	5:J:150:EDO:H12	1.95	0.43
1:P:14:ARG:HD2	1:P:54:SER:OG	2.18	0.43
1:R:39:ILE:HD12	1:R:48:MET:O	2.18	0.43
1:M:67:PRO:HG3	5:M:152:EDO:C2	2.33	0.43
1:R:71:LEU:HD22	1:R:104:PHE:CZ	2.52	0.43
1:X:33:ILE:HD11	1:X:115:LEU:HB2	2.00	0.43
1:F:68:ARG:NH2	2:F:150:SO4:O3	2.52	0.43
1:K:77:ILE:HB	5:K:150:EDO:H21	2.01	0.43
1:O:71:LEU:HA	1:O:75:ASN:HD22	1.83	0.43
1:U:46:GLN:HA	1:U:96:LEU:O	2.18	0.43
1:W:71:LEU:HA	1:W:75:ASN:HD22	1.82	0.43
1:J:93:LYS:O	6:J:152:PEG:H21	2.19	0.43
1:D:11:ILE:HD13	1:D:55:PHE:HB3	2.01	0.43
1:O:65:ILE:HB	1:O:82:GLY:HA2	2.00	0.43
1:U:111:ARG:NH2	8:U:634:HOH:O	2.51	0.43
1:R:41:ILE:HD13	1:R:41:ILE:N	2.34	0.43
1:E:36:SER:O	1:E:108:LYS:HG3	2.18	0.43
1:G:56:THR:OG1	1:H:132:LEU:HD22	2.19	0.43
1:I:114:GLN:NE2	8:I:398:HOH:O	2.46	0.43
1:U:107:LYS:O	1:U:108:LYS:C	2.57	0.43
1:O:58:PRO:HD2	1:O:117:LEU:HD22	2.01	0.42
1:D:36:SER:O	1:D:108:LYS:HE2	2.19	0.42
1:M:65:ILE:HB	1:M:82:GLY:HA2	2.01	0.42
1:G:11:ILE:HD13	1:G:55:PHE:HB3	2.01	0.42
1:R:39:ILE:CD1	1:R:48:MET:O	2.68	0.42
1:T:114:GLN:OE1	5:T:152:EDO:C2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:GLY:O	1:I:74:LYS:HG3	2.18	0.42
1:B:30:GLY:HA3	1:B:114:GLN:HE21	1.84	0.42
1:H:37:GLN:OE1	6:H:149:PEG:H31	2.20	0.42
1:H:57:VAL:O	1:H:86:ARG:NH2	2.52	0.42
1:T:65:ILE:HD13	5:T:154:EDO:C2	2.48	0.42
1:B:70:GLY:O	1:B:74:LYS:HB2	2.20	0.42
1:D:33:ILE:HD11	1:D:115:LEU:HB2	2.00	0.42
1:A:8:VAL:HG22	1:B:125:GLN:CG	2.49	0.42
1:A:132:LEU:HD12	1:C:54:SER:HB3	1.95	0.42
1:S:57:VAL:HG21	1:S:62:TYR:HA	2.02	0.42
1:X:68[A]:ARG:HB3	1:X:68[A]:ARG:HH21	1.84	0.42
1:J:74:LYS:HZ1	1:J:75:ASN:HD21	1.67	0.42
1:M:36:SER:O	1:M:108[B]:LYS:HG2	2.20	0.42
1:Q:23:LYS:HE2	1:Q:28:ALA:O	2.20	0.42
1:K:77:ILE:HG22	5:K:150:EDO:C1	2.50	0.41
1:N:39:ILE:HD11	8:N:2005:HOH:O	2.18	0.41
1:T:65:ILE:CD1	5:T:154:EDO:H22	2.49	0.41
1:D:61:THR:HA	1:D:118:GLU:O	2.20	0.41
1:E:33:ILE:HD11	1:E:115:LEU:HB2	2.02	0.41
2:V:148:SO4:O1	1:W:99:HIS:HE1	2.03	0.41
1:W:65:ILE:HD11	1:W:92:VAL:CG1	2.50	0.41
1:S:47:GLY:O	1:S:48[B]:MET:HE2	2.20	0.41
1:J:33:ILE:CD1	1:J:115:LEU:HB2	2.41	0.41
1:S:38:ASP:OD1	1:S:107:LYS:HA	2.20	0.41
1:S:61:THR:HA	1:S:118:GLU:O	2.19	0.41
1:V:102:ARG:NH2	2:V:149:SO4:S	2.94	0.41
1:A:78:GLN:HG2	2:B:148:SO4:O2	2.21	0.41
1:Q:74:LYS:HG3	5:Q:153:EDO:C2	2.50	0.41
1:W:48:MET:CE	1:W:93:LYS:NZ	2.83	0.41
1:X:18:ALA:O	6:X:149:PEG:H21	2.20	0.41
1:W:15:SER:OG	1:W:52:ASP:OD2	2.20	0.41
1:C:57:VAL:HG21	1:C:62:TYR:HA	2.03	0.41
1:I:48:MET:HE3	1:I:48:MET:HB2	1.79	0.41
1:L:32:ASP:HB3	1:L:111:ARG:HG2	2.02	0.41
1:M:10:LYS:HD2	1:N:129:VAL:HG11	2.02	0.41
1:V:68[B]:ARG:H	5:V:156:EDO:C1	2.33	0.41
1:B:23:LYS:HG3	1:B:30:GLY:O	2.20	0.41
1:D:62:TYR:CE1	1:D:118:GLU:HB2	2.55	0.41
1:E:71:LEU:HA	1:E:75:ASN:HD22	1.86	0.41
1:G:71:LEU:HA	1:G:75:ASN:HD22	1.85	0.41
1:P:61:THR:HA	1:P:118:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:67:PRO:HB3	5:P:151:EDO:H12	2.02	0.41
1:S:13:LEU:HD21	1:S:20:VAL:HG22	2.03	0.41
1:S:108:LYS:HD3	1:S:108:LYS:C	2.41	0.41
1:U:31:TYR:O	1:U:114:GLN:HA	2.21	0.41
1:W:107:LYS:HA	1:W:107:LYS:HD3	1.94	0.41
1:D:68[B]:ARG:NH1	2:D:148:SO4:O3	2.54	0.41
1:I:99:HIS:CE1	2:I:148:SO4:O4	2.74	0.41
1:N:57:VAL:HG21	1:N:62:TYR:HA	2.02	0.41
1:D:107:LYS:O	1:D:108:LYS:C	2.59	0.40
1:G:62:TYR:CE1	1:G:118:GLU:HB2	2.56	0.40
1:S:68:ARG:HH22	5:S:151:EDO:H11	1.80	0.40
1:A:68[A]:ARG:NH1	8:A:1188:HOH:O	2.53	0.40
1:F:41:ILE:CG2	1:F:98:ASN:HB2	2.52	0.40
1:H:71:LEU:HA	1:H:75:ASN:HD22	1.85	0.40
8:P:1195:HOH:O	5:Q:150:EDO:H12	2.21	0.40
1:S:15:SER:OG	1:S:52:ASP:OD2	2.30	0.40
1:T:65:ILE:CD1	1:T:84:VAL:HG23	2.52	0.40
1:U:127:VAL:HG12	1:U:129:VAL:HG13	2.02	0.40
1:E:39:ILE:HD12	1:E:39:ILE:HA	1.86	0.40
1:I:33[A]:ILE:CD1	1:I:65:ILE:HD12	2.51	0.40
1:J:68:ARG:NH2	1:J:111[A]:ARG:HH22	2.17	0.40
1:M:8:VAL:HG12	1:M:10:LYS:HG2	2.03	0.40
1:B:23:LYS:HE2	1:B:28:ALA:O	2.22	0.40
1:K:119:LYS:HE3	1:L:120:ILE:O	2.22	0.40
1:M:6:ASP:CB	1:M:8:VAL:HB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:NE2	8:Q:1169:HOH:O[1_455]	2.17	0.03

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	124/167 (74%)	121 (98%)	3 (2%)	0	100	100
1	B	124/167 (74%)	121 (98%)	3 (2%)	0	100	100
1	C	130/167 (78%)	129 (99%)	1 (1%)	0	100	100
1	D	125/167 (75%)	122 (98%)	3 (2%)	0	100	100
1	E	126/167 (75%)	124 (98%)	2 (2%)	0	100	100
1	F	129/167 (77%)	127 (98%)	2 (2%)	0	100	100
1	G	127/167 (76%)	125 (98%)	2 (2%)	0	100	100
1	H	125/167 (75%)	123 (98%)	2 (2%)	0	100	100
1	I	126/167 (75%)	120 (95%)	6 (5%)	0	100	100
1	J	125/167 (75%)	123 (98%)	2 (2%)	0	100	100
1	K	127/167 (76%)	123 (97%)	3 (2%)	1 (1%)	19	13
1	L	127/167 (76%)	125 (98%)	2 (2%)	0	100	100
1	M	131/167 (78%)	124 (95%)	6 (5%)	1 (1%)	19	13
1	N	122/167 (73%)	120 (98%)	2 (2%)	0	100	100
1	O	128/167 (77%)	127 (99%)	1 (1%)	0	100	100
1	P	121/167 (72%)	119 (98%)	2 (2%)	0	100	100
1	Q	123/167 (74%)	120 (98%)	3 (2%)	0	100	100
1	R	127/167 (76%)	126 (99%)	1 (1%)	0	100	100
1	S	126/167 (75%)	124 (98%)	1 (1%)	1 (1%)	19	13
1	T	126/167 (75%)	123 (98%)	3 (2%)	0	100	100
1	U	125/167 (75%)	123 (98%)	2 (2%)	0	100	100
1	V	126/167 (75%)	125 (99%)	1 (1%)	0	100	100
1	W	128/167 (77%)	122 (95%)	6 (5%)	0	100	100
1	X	127/167 (76%)	123 (97%)	4 (3%)	0	100	100
All	All	3025/4008 (76%)	2959 (98%)	63 (2%)	3 (0%)	51	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	7	LYS
1	K	28	ALA
1	S	113	ALA

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	103/131 (79%)	102 (99%)	1 (1%)	76	81
1	B	102/131 (78%)	97 (95%)	5 (5%)	25	21
1	C	105/131 (80%)	102 (97%)	3 (3%)	42	43
1	D	104/131 (79%)	102 (98%)	2 (2%)	57	61
1	E	102/131 (78%)	100 (98%)	2 (2%)	55	58
1	F	105/131 (80%)	100 (95%)	5 (5%)	25	22
1	G	104/131 (79%)	100 (96%)	4 (4%)	33	31
1	H	101/131 (77%)	98 (97%)	3 (3%)	41	41
1	I	103/131 (79%)	99 (96%)	4 (4%)	32	30
1	J	102/131 (78%)	98 (96%)	4 (4%)	32	30
1	K	107/131 (82%)	104 (97%)	3 (3%)	43	44
1	L	103/131 (79%)	97 (94%)	6 (6%)	20	15
1	M	107/131 (82%)	105 (98%)	2 (2%)	57	61
1	N	102/131 (78%)	96 (94%)	6 (6%)	19	15
1	O	105/131 (80%)	102 (97%)	3 (3%)	42	43
1	P	100/131 (76%)	95 (95%)	5 (5%)	24	20
1	Q	102/131 (78%)	98 (96%)	4 (4%)	32	30
1	R	104/131 (79%)	103 (99%)	1 (1%)	76	81
1	S	102/131 (78%)	101 (99%)	1 (1%)	76	81
1	T	101/131 (77%)	101 (100%)	0	100	100
1	U	102/131 (78%)	100 (98%)	2 (2%)	55	58
1	V	102/131 (78%)	100 (98%)	2 (2%)	55	58
1	W	104/131 (79%)	102 (98%)	2 (2%)	57	61
1	X	103/131 (79%)	99 (96%)	4 (4%)	32	30
All	All	2475/3144 (79%)	2401 (97%)	74 (3%)	43	41

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	B	15	SER
1	B	74	LYS
1	B	125	GLN
1	B	131	SER
1	B	134	GLU
1	C	27	THR
1	C	46	GLN
1	C	133	GLU
1	D	27	THR
1	D	125	GLN
1	E	25	SER
1	E	48	MET
1	F	23	LYS
1	F	25	SER
1	F	39	ILE
1	F	48	MET
1	F	78	GLN
1	G	8	VAL
1	G	25	SER
1	G	39	ILE
1	G	133	GLU
1	H	39	ILE
1	H	48	MET
1	H	131	SER
1	I	17	SER
1	I	48	MET
1	I	100	SER
1	I	126	ILE
1	J	8	VAL
1	J	25	SER
1	J	111[A]	ARG
1	J	111[B]	ARG
1	K	7	LYS
1	K	78	GLN
1	K	133	GLU
1	L	12	GLN
1	L	27	THR
1	L	65	ILE
1	L	100	SER
1	L	108	LYS
1	L	126	ILE
1	M	25	SER

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Mol	Chain	Res	Type
1	M	134	GLU
1	N	7	LYS
1	N	27	THR
1	N	78	GLN
1	N	93	LYS
1	N	111	ARG
1	N	132	LEU
1	O	48[A]	MET
1	O	48[B]	MET
1	O	133	GLU
1	P	23	LYS
1	P	46	GLN
1	P	102	ARG
1	P	125	GLN
1	P	131	SER
1	Q	111[A]	ARG
1	Q	111[B]	ARG
1	Q	125	GLN
1	Q	127	VAL
1	R	133	GLU
1	S	107	LYS
1	U	7	LYS
1	U	15	SER
1	V	34	TYR
1	V	39	ILE
1	W	23	LYS
1	W	132	LEU
1	X	48[A]	MET
1	X	48[B]	MET
1	X	68[A]	ARG
1	X	68[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	75	ASN
1	B	114	GLN
1	C	46	GLN
1	C	75	ASN
1	C	99	HIS
1	C	101	GLN

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Mol	Chain	Res	Type
1	D	46	GLN
1	D	114	GLN
1	D	125	GLN
1	E	37	GLN
1	E	46	GLN
1	E	75	ASN
1	E	114	GLN
1	F	46	GLN
1	F	78	GLN
1	F	101	GLN
1	F	114	GLN
1	G	46	GLN
1	G	75	ASN
1	G	99	HIS
1	G	114	GLN
1	H	75	ASN
1	H	99	HIS
1	I	37	GLN
1	I	75	ASN
1	I	114	GLN
1	J	37	GLN
1	J	75	ASN
1	J	99	HIS
1	J	114	GLN
1	K	12	GLN
1	K	46	GLN
1	K	78	GLN
1	K	114	GLN
1	L	12	GLN
1	L	46	GLN
1	L	75	ASN
1	M	46	GLN
1	M	75	ASN
1	M	114	GLN
1	N	75	ASN
1	N	78	GLN
1	N	114	GLN
1	O	75	ASN
1	P	37	GLN
1	P	99	HIS
1	P	101	GLN
1	P	125	GLN

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Mol	Chain	Res	Type
1	Q	46	GLN
1	Q	75	ASN
1	Q	99	HIS
1	R	75	ASN
1	R	114	GLN
1	R	125	GLN
1	S	37	GLN
1	S	75	ASN
1	T	75	ASN
1	T	99	HIS
1	U	37	GLN
1	U	75	ASN
1	U	99	HIS
1	U	101	GLN
1	V	37	GLN
1	V	46	GLN
1	V	75	ASN
1	W	75	ASN
1	W	99	HIS
1	W	114	GLN
1	X	37	GLN
1	X	75	ASN
1	X	99	HIS
1	X	101	GLN
1	X	114	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 108 ligands modelled in this entry, 31 are monoatomic - leaving 77 for Mogul analysis.

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	B	149	-	4,4,4	0.29	0	6,6,6	0.52	0
5	EDO	M	153	-	3,3,3	0.79	0	2,2,2	0.48	0
5	EDO	E	150	-	3,3,3	0.65	0	2,2,2	0.36	0
2	SO4	V	148	-	4,4,4	0.23	0	6,6,6	0.57	0
6	PEG	J	153	-	6,6,6	0.49	0	5,5,5	0.77	0
2	SO4	K	149	-	4,4,4	0.18	0	6,6,6	0.64	0
5	EDO	V	152	-	3,3,3	0.71	0	2,2,2	0.06	0
5	EDO	O	152	-	3,3,3	0.46	0	2,2,2	0.53	0
6	PEG	H	149	-	6,6,6	1.16	0	5,5,5	1.36	0
5	EDO	D	152	-	3,3,3	0.62	0	2,2,2	0.32	0
2	SO4	O	148	-	4,4,4	0.08	0	6,6,6	0.76	0
5	EDO	O	153	-	3,3,3	0.80	0	2,2,2	1.54	0
5	EDO	S	151	-	3,3,3	0.38	0	2,2,2	0.92	0
5	EDO	G	151	-	3,3,3	0.57	0	2,2,2	0.45	0
2	SO4	D	148	-	4,4,4	0.11	0	6,6,6	0.30	0
5	EDO	Q	152	-	3,3,3	0.55	0	2,2,2	0.44	0
5	EDO	Q	150	-	3,3,3	0.63	0	2,2,2	1.21	0
2	SO4	V	150	-	4,4,4	0.14	0	6,6,6	0.29	0
5	EDO	Q	153	-	3,3,3	0.46	0	2,2,2	0.55	0
2	SO4	M	149	-	4,4,4	0.19	0	6,6,6	0.49	0
5	EDO	R	151	-	3,3,3	0.85	0	2,2,2	0.40	0
2	SO4	F	149	-	4,4,4	0.13	0	6,6,6	0.32	0
5	EDO	Q	151	-	3,3,3	0.44	0	2,2,2	0.66	0
2	SO4	V	149	-	4,4,4	0.16	0	6,6,6	0.52	0
2	SO4	G	148	-	4,4,4	0.16	0	6,6,6	0.36	0
2	SO4	H	148	-	4,4,4	0.10	0	6,6,6	0.45	0
2	SO4	I	148	-	4,4,4	0.49	0	6,6,6	0.54	0
6	PEG	K	153	-	6,6,6	0.68	0	5,5,5	0.63	0
5	EDO	V	156	-	3,3,3	0.39	0	2,2,2	0.73	0
5	EDO	D	151	-	3,3,3	0.68	0	2,2,2	0.63	0
5	EDO	J	151	-	3,3,3	0.42	0	2,2,2	0.54	0
2	SO4	Q	148	-	4,4,4	0.28	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	148	-	4,4,4	0.17	0	6,6,6	0.55	0
2	SO4	U	148	-	4,4,4	0.19	0	6,6,6	0.22	0
6	PEG	M	155	-	6,6,6	1.16	0	5,5,5	0.83	0
5	EDO	K	151	-	3,3,3	0.36	0	2,2,2	0.60	0
2	SO4	G	150	-	4,4,4	0.15	0	6,6,6	0.14	0
5	EDO	M	154	-	3,3,3	0.75	0	2,2,2	0.33	0
5	EDO	M	152	-	3,3,3	0.37	0	2,2,2	0.55	0
2	SO4	A	149	-	4,4,4	0.12	0	6,6,6	0.30	0
2	SO4	N	148	-	4,4,4	0.19	0	6,6,6	0.32	0
5	EDO	U	150	-	3,3,3	0.49	0	2,2,2	0.50	0
2	SO4	E	148	-	4,4,4	0.13	0	6,6,6	0.32	0
5	EDO	T	152	-	3,3,3	0.54	0	2,2,2	0.87	0
2	SO4	W	148	-	4,4,4	0.22	0	6,6,6	0.37	0
2	SO4	N	149	-	4,4,4	0.15	0	6,6,6	0.32	0
2	SO4	W	149	-	4,4,4	0.22	0	6,6,6	0.20	0
2	SO4	B	148	-	4,4,4	0.39	0	6,6,6	0.47	0
5	EDO	K	152	-	3,3,3	0.64	0	2,2,2	0.47	0
5	EDO	R	150	-	3,3,3	0.53	0	2,2,2	0.38	0
2	SO4	T	148	-	4,4,4	0.16	0	6,6,6	0.34	0
5	EDO	V	153	-	3,3,3	0.55	0	2,2,2	0.42	0
7	GOL	U	151	-	5,5,5	0.22	0	5,5,5	0.86	0
2	SO4	J	148	-	4,4,4	0.13	0	6,6,6	0.59	0
2	SO4	R	148	-	4,4,4	0.15	0	6,6,6	0.32	0
2	SO4	K	148	-	4,4,4	0.66	0	6,6,6	0.59	0
6	PEG	X	149	-	6,6,6	0.45	0	5,5,5	0.37	0
2	SO4	S	149	-	4,4,4	0.27	0	6,6,6	0.50	0
5	EDO	J	150	-	3,3,3	0.43	0	2,2,2	0.44	0
2	SO4	G	149	-	4,4,4	0.22	0	6,6,6	0.57	0
2	SO4	M	148	-	4,4,4	0.59	0	6,6,6	0.84	0
2	SO4	P	149	-	4,4,4	0.15	0	6,6,6	0.30	0
5	EDO	T	153	-	3,3,3	0.69	0	2,2,2	0.55	0
2	SO4	F	148	-	4,4,4	0.27	0	6,6,6	0.73	0
6	PEG	J	152	-	6,6,6	0.67	0	5,5,5	0.44	0
5	EDO	P	151	-	3,3,3	0.53	0	2,2,2	0.93	0
5	EDO	O	150	-	3,3,3	0.63	0	2,2,2	0.06	0
2	SO4	S	148	-	4,4,4	0.36	0	6,6,6	0.64	0
5	EDO	F	153	-	3,3,3	0.76	0	2,2,2	0.49	0
2	SO4	P	148	-	4,4,4	0.19	0	6,6,6	0.47	0
5	EDO	T	154	-	3,3,3	1.18	0	2,2,2	0.86	0
5	EDO	K	150	-	3,3,3	0.54	0	2,2,2	0.67	0
5	EDO	N	153	-	3,3,3	0.48	0	2,2,2	0.74	0
5	EDO	W	150	-	3,3,3	0.53	0	2,2,2	0.20	0
2	SO4	F	150	-	4,4,4	0.28	0	6,6,6	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	M	151	-	3,3,3	0.45	0	2,2,2	0.37	0
6	PEG	X	148	-	6,6,6	0.62	0	5,5,5	1.01	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
5	EDO	T	153	-	-	1/1/1/1	-
5	EDO	M	153	-	-	0/1/1/1	-
6	PEG	J	152	-	-	3/4/4/4	-
5	EDO	E	150	-	-	1/1/1/1	-
6	PEG	J	153	-	-	4/4/4/4	-
5	EDO	P	151	-	-	1/1/1/1	-
6	PEG	K	153	-	-	2/4/4/4	-
5	EDO	O	150	-	-	0/1/1/1	-
5	EDO	V	156	-	-	0/1/1/1	-
5	EDO	V	152	-	-	0/1/1/1	-
5	EDO	U	150	-	-	1/1/1/1	-
5	EDO	D	151	-	-	1/1/1/1	-
5	EDO	O	152	-	-	1/1/1/1	-
5	EDO	T	152	-	-	0/1/1/1	-
6	PEG	H	149	-	-	2/4/4/4	-
5	EDO	F	153	-	-	1/1/1/1	-
5	EDO	J	151	-	-	0/1/1/1	-
5	EDO	D	152	-	-	1/1/1/1	-
5	EDO	O	153	-	-	0/1/1/1	-
5	EDO	S	151	-	-	1/1/1/1	-
5	EDO	T	154	-	-	1/1/1/1	-
5	EDO	G	151	-	-	1/1/1/1	-
5	EDO	K	150	-	-	1/1/1/1	-
5	EDO	N	153	-	-	1/1/1/1	-
5	EDO	Q	152	-	-	1/1/1/1	-
5	EDO	K	152	-	-	1/1/1/1	-
5	EDO	Q	150	-	-	0/1/1/1	-
6	PEG	M	155	-	-	4/4/4/4	-
5	EDO	R	150	-	-	1/1/1/1	-
5	EDO	K	151	-	-	1/1/1/1	-
5	EDO	Q	153	-	-	1/1/1/1	-
5	EDO	W	150	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	M	151	-	-	0/1/1/1	-
5	EDO	M	154	-	-	1/1/1/1	-
5	EDO	V	153	-	-	1/1/1/1	-
5	EDO	M	152	-	-	1/1/1/1	-
5	EDO	R	151	-	-	1/1/1/1	-
5	EDO	Q	151	-	-	0/1/1/1	-
7	GOL	U	151	-	-	2/4/4/4	-
6	PEG	X	148	-	-	1/4/4/4	-
6	PEG	X	149	-	-	0/4/4/4	-
5	EDO	J	150	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	U	151	GOL	O1-C1-C2-C3
6	M	155	PEG	O2-C3-C4-O4
6	J	152	PEG	O2-C3-C4-O4
6	J	153	PEG	O1-C1-C2-O2
6	J	153	PEG	O2-C3-C4-O4
5	E	150	EDO	O1-C1-C2-O2
6	H	149	PEG	O2-C3-C4-O4
5	D	151	EDO	O1-C1-C2-O2
5	D	152	EDO	O1-C1-C2-O2
5	J	150	EDO	O1-C1-C2-O2
5	K	150	EDO	O1-C1-C2-O2
5	K	152	EDO	O1-C1-C2-O2
5	M	152	EDO	O1-C1-C2-O2
5	N	153	EDO	O1-C1-C2-O2
5	O	152	EDO	O1-C1-C2-O2
5	T	154	EDO	O1-C1-C2-O2
5	V	153	EDO	O1-C1-C2-O2
6	H	149	PEG	O1-C1-C2-O2
6	X	148	PEG	O1-C1-C2-O2
6	M	155	PEG	O1-C1-C2-O2
5	P	151	EDO	O1-C1-C2-O2
5	Q	152	EDO	O1-C1-C2-O2
5	U	150	EDO	O1-C1-C2-O2
5	G	151	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	R	150	EDO	O1-C1-C2-O2
5	T	153	EDO	O1-C1-C2-O2
6	K	153	PEG	C1-C2-O2-C3
6	J	153	PEG	C1-C2-O2-C3
6	M	155	PEG	C1-C2-O2-C3
5	Q	153	EDO	O1-C1-C2-O2
6	J	152	PEG	C4-C3-O2-C2
7	U	151	GOL	O1-C1-C2-O2
6	J	152	PEG	C1-C2-O2-C3
5	K	151	EDO	O1-C1-C2-O2
6	J	153	PEG	C4-C3-O2-C2
6	M	155	PEG	C4-C3-O2-C2
5	R	151	EDO	O1-C1-C2-O2
6	K	153	PEG	C4-C3-O2-C2
5	F	153	EDO	O1-C1-C2-O2
5	W	150	EDO	O1-C1-C2-O2
5	M	154	EDO	O1-C1-C2-O2
5	S	151	EDO	O1-C1-C2-O2

There are no ring outliers.

39 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	150	EDO	1	0
2	V	148	SO4	2	0
6	J	153	PEG	3	0
2	K	149	SO4	1	0
5	V	152	EDO	1	0
6	H	149	PEG	6	0
5	D	152	EDO	6	0
5	O	153	EDO	3	0
5	S	151	EDO	4	0
5	G	151	EDO	6	0
2	D	148	SO4	1	0
5	Q	150	EDO	4	0
5	Q	153	EDO	1	0
5	Q	151	EDO	7	0
2	V	149	SO4	2	0
2	I	148	SO4	3	0
6	K	153	PEG	1	0
5	V	156	EDO	5	0
5	D	151	EDO	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	148	SO4	4	0
5	K	151	EDO	3	0
2	G	150	SO4	1	0
5	M	152	EDO	3	0
5	T	152	EDO	2	0
2	B	148	SO4	3	0
5	K	152	EDO	7	0
5	V	153	EDO	1	0
2	K	148	SO4	2	0
6	X	149	PEG	2	0
5	J	150	EDO	8	0
6	J	152	PEG	2	0
5	P	151	EDO	3	0
2	S	148	SO4	2	0
5	T	154	EDO	5	0
5	K	150	EDO	5	0
5	N	153	EDO	3	0
2	F	150	SO4	1	0
5	M	151	EDO	4	0
6	X	148	PEG	4	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	126/167 (75%)	-0.40	2 (1%) 72 70	16, 21, 29, 39	0
1	B	128/167 (76%)	-0.43	2 (1%) 72 70	16, 21, 29, 42	0
1	C	128/167 (76%)	-0.25	1 (0%) 86 85	16, 21, 29, 38	0
1	D	125/167 (74%)	-0.51	0 100 100	16, 20, 28, 39	0
1	E	128/167 (76%)	-0.45	0 100 100	16, 21, 29, 36	0
1	F	126/167 (75%)	-0.44	1 (0%) 86 85	16, 20, 30, 35	0
1	G	127/167 (76%)	-0.46	0 100 100	15, 21, 28, 37	0
1	H	126/167 (75%)	-0.52	0 100 100	17, 20, 28, 31	0
1	I	127/167 (76%)	-0.52	1 (0%) 86 85	16, 21, 29, 38	0
1	J	126/167 (75%)	-0.47	0 100 100	17, 20, 28, 35	0
1	K	127/167 (76%)	-0.44	0 100 100	15, 20, 29, 41	0
1	L	127/167 (76%)	-0.45	0 100 100	16, 21, 29, 34	0
1	M	130/167 (77%)	-0.38	2 (1%) 73 72	15, 21, 33, 51	0
1	N	125/167 (74%)	-0.39	0 100 100	15, 21, 28, 38	0
1	O	127/167 (76%)	-0.50	0 100 100	16, 20, 28, 35	0
1	P	125/167 (74%)	-0.56	0 100 100	16, 21, 29, 37	0
1	Q	125/167 (74%)	-0.53	0 100 100	16, 20, 27, 38	0
1	R	127/167 (76%)	-0.50	0 100 100	15, 21, 29, 35	0
1	S	127/167 (76%)	-0.44	0 100 100	15, 21, 29, 37	0
1	T	128/167 (76%)	-0.49	1 (0%) 86 85	15, 21, 28, 37	0
1	U	127/167 (76%)	-0.47	1 (0%) 86 85	9, 20, 28, 38	2 (1%)
1	V	127/167 (76%)	-0.53	0 100 100	15, 21, 27, 40	0
1	W	130/167 (77%)	-0.45	1 (0%) 86 85	15, 21, 32, 37	0
1	X	126/167 (75%)	-0.45	1 (0%) 86 85	11, 21, 28, 37	2 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3045/4008 (75%)	-0.46	13 (0%)	92	92	9, 21, 29, 51	4 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	134	GLU	4.4
1	M	135	SER	4.0
1	C	6	ASP	3.3
1	A	127	VAL	3.2
1	X	65	ILE	3.2
1	T	6	ASP	2.7
1	B	27	THR	2.4
1	F	27[A]	THR	2.4
1	U	65	ILE	2.4
1	W	134	GLU	2.2
1	A	129	VAL	2.1
1	I	6	ASP	2.1
1	B	134	GLU	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, 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
5	EDO	E	150	4/4	0.74	0.23	51,51,52,52	0
4	CL	U	149	1/1	0.77	0.14	59,59,59,59	0
2	SO4	K	149	5/5	0.77	0.17	71,72,73,74	0
6	PEG	X	149	7/7	0.78	0.15	60,60,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	I	149	1/1	0.79	0.08	56,56,56,56	0
2	SO4	G	150	5/5	0.80	0.18	92,93,93,93	0
6	PEG	M	155	7/7	0.81	0.18	30,35,38,38	0
6	PEG	K	153	7/7	0.81	0.16	37,38,41,41	0
2	SO4	A	149	5/5	0.82	0.18	75,76,76,78	0
5	EDO	J	151	4/4	0.83	0.18	53,55,55,57	0
5	EDO	K	152	4/4	0.85	0.19	35,39,39,45	0
3	NA	V	154	1/1	0.85	0.10	45,45,45,45	0
5	EDO	F	153	4/4	0.85	0.16	31,33,33,35	0
4	CL	B	150	1/1	0.85	0.11	57,57,57,57	0
6	PEG	H	149	7/7	0.86	0.27	21,23,29,31	0
5	EDO	M	154	4/4	0.86	0.16	38,43,43,44	0
4	CL	E	149	1/1	0.87	0.07	75,75,75,75	0
2	SO4	D	148	5/5	0.87	0.19	94,95,95,95	0
4	CL	J	149	1/1	0.88	0.07	65,65,65,65	0
5	EDO	U	150	4/4	0.89	0.36	39,42,43,44	0
5	EDO	V	153	4/4	0.89	0.17	32,40,40,42	0
4	CL	L	150	1/1	0.89	0.09	54,54,54,54	0
6	PEG	J	153	7/7	0.89	0.24	33,42,43,44	0
4	CL	T	151	1/1	0.89	0.20	52,52,52,52	0
2	SO4	R	148	5/5	0.89	0.19	88,89,90,91	0
6	PEG	X	148	7/7	0.89	0.15	28,29,36,38	0
2	SO4	B	149	5/5	0.89	0.18	61,61,63,64	0
5	EDO	Q	153	4/4	0.90	0.29	34,34,37,37	0
5	EDO	T	153	4/4	0.90	0.17	29,30,32,33	0
2	SO4	W	149	5/5	0.90	0.14	90,90,91,91	0
3	NA	C	149	1/1	0.90	0.11	48,48,48,48	0
2	SO4	F	149	5/5	0.90	0.18	70,72,73,73	0
4	CL	D	150	1/1	0.91	0.15	58,58,58,58	0
5	EDO	R	150	4/4	0.91	0.14	34,38,39,40	0
5	EDO	R	151	4/4	0.91	0.18	27,34,34,35	0
7	GOL	U	151	6/6	0.91	0.16	25,28,32,37	0
2	SO4	P	148	5/5	0.92	0.11	74,74,74,75	0
5	EDO	S	151	4/4	0.92	0.10	42,43,44,44	0
2	SO4	P	149	5/5	0.92	0.15	75,76,77,78	0
2	SO4	F	150	5/5	0.92	0.18	57,59,60,60	0
5	EDO	M	153	4/4	0.93	0.09	23,27,27,31	0
2	SO4	G	149	5/5	0.93	0.16	51,52,55,56	0
5	EDO	T	154	4/4	0.93	0.21	17,27,29,32	0
4	CL	Q	149	1/1	0.93	0.14	69,69,69,69	0
4	CL	D	149	1/1	0.93	0.08	51,51,51,51	0
2	SO4	N	148	5/5	0.93	0.11	67,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	148	5/5	0.94	0.27	87,88,88,88	0
5	EDO	O	152	4/4	0.94	0.07	32,35,37,37	0
4	CL	R	149	1/1	0.94	0.06	47,47,47,47	0
6	PEG	J	152	7/7	0.94	0.18	31,35,38,40	0
3	NA	O	151	1/1	0.94	0.07	49,49,49,49	0
2	SO4	U	148	5/5	0.95	0.17	67,67,68,68	0
3	NA	F	152	1/1	0.95	0.08	30,30,30,30	0
5	EDO	Q	152	4/4	0.95	0.06	32,32,34,37	0
2	SO4	H	148	5/5	0.95	0.14	57,58,58,59	0
5	EDO	V	152	4/4	0.95	0.08	18,21,25,26	0
3	NA	V	151	1/1	0.95	0.07	29,29,29,29	0
4	CL	V	155	1/1	0.95	0.04	57,57,57,57	0
5	EDO	G	151	4/4	0.96	0.25	14,15,18,21	0
4	CL	L	148	1/1	0.96	0.07	58,58,58,58	0
5	EDO	D	151	4/4	0.96	0.28	15,20,21,25	0
5	EDO	M	152	4/4	0.96	0.21	13,17,22,22	0
5	EDO	D	152	4/4	0.96	0.25	9,18,18,24	0
2	SO4	V	150	5/5	0.96	0.12	68,69,70,70	0
2	SO4	W	148	5/5	0.96	0.15	64,65,66,66	0
5	EDO	P	151	4/4	0.96	0.23	15,19,21,22	0
5	EDO	Q	150	4/4	0.96	0.27	11,13,13,18	0
2	SO4	G	148	5/5	0.97	0.10	41,41,45,46	0
5	EDO	N	153	4/4	0.97	0.20	19,22,23,25	0
3	NA	L	149	1/1	0.97	0.13	27,27,27,27	0
5	EDO	O	153	4/4	0.97	0.25	11,16,21,22	0
5	EDO	J	150	4/4	0.97	0.31	21,25,28,28	0
5	EDO	V	156	4/4	0.97	0.20	19,21,21,22	0
5	EDO	W	150	4/4	0.97	0.10	24,31,32,33	0
2	SO4	N	149	5/5	0.97	0.13	59,60,61,61	0
5	EDO	Q	151	4/4	0.97	0.27	16,18,19,20	0
5	EDO	K	150	4/4	0.97	0.22	13,17,22,23	0
5	EDO	K	151	4/4	0.97	0.27	14,17,21,22	0
4	CL	N	152	1/1	0.97	0.07	48,48,48,48	0
2	SO4	S	149	5/5	0.97	0.10	48,51,51,52	0
2	SO4	M	149	5/5	0.97	0.10	35,36,39,40	0
5	EDO	T	152	4/4	0.97	0.25	15,18,21,22	0
3	NA	P	150	1/1	0.98	0.08	26,26,26,26	0
5	EDO	O	150	4/4	0.98	0.07	31,31,31,32	0
3	NA	S	150	1/1	0.98	0.16	24,24,24,24	0
3	NA	T	149	1/1	0.98	0.08	34,34,34,34	0
3	NA	T	150	1/1	0.98	0.09	23,23,23,23	0
4	CL	N	151	1/1	0.98	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	J	148	5/5	0.98	0.14	49,51,52,52	0
2	SO4	O	148	5/5	0.98	0.08	41,41,44,45	0
2	SO4	A	148	5/5	0.98	0.14	49,50,52,53	0
4	CL	C	148	1/1	0.98	0.07	48,48,48,48	0
5	EDO	M	151	4/4	0.98	0.24	13,19,19,21	0
3	NA	M	150	1/1	0.98	0.10	28,28,28,28	0
3	NA	N	150	1/1	0.98	0.15	36,36,36,36	0
2	SO4	T	148	5/5	0.98	0.10	45,46,48,49	0
2	SO4	Q	148	5/5	0.99	0.07	18,21,23,25	0
4	CL	F	151	1/1	0.99	0.14	41,41,41,41	0
2	SO4	B	148	5/5	0.99	0.06	18,18,20,22	0
3	NA	A	150	1/1	0.99	0.12	19,19,19,19	0
2	SO4	K	148	5/5	0.99	0.07	17,19,23,24	0
2	SO4	F	148	5/5	0.99	0.06	21,22,24,26	0
2	SO4	M	148	5/5	0.99	0.05	16,19,21,22	0
2	SO4	V	148	5/5	0.99	0.05	13,17,18,19	0
2	SO4	V	149	5/5	0.99	0.12	34,36,39,40	0
3	NA	O	149	1/1	0.99	0.13	22,22,22,22	0
2	SO4	I	148	5/5	0.99	0.05	16,19,21,22	0
2	SO4	S	148	5/5	1.00	0.05	12,13,16,22	0

6.5 Other polymers (i)

There are no such residues in this entry.