Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2016 – 08:18 PM EDT

PDB ID	:	5EUJ
Title	:	PYRUVATE DECARBOXYLASE FROM ZYMOBACTER PALMAE
Authors	:	BUDDRUS, L.; CRENNELL, S.; LEAK, D.J.; DANSON, M.J.; ANDREWS, E.S.V.; ARCUS, V.L.
Deposited on	:	2015-11-18
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

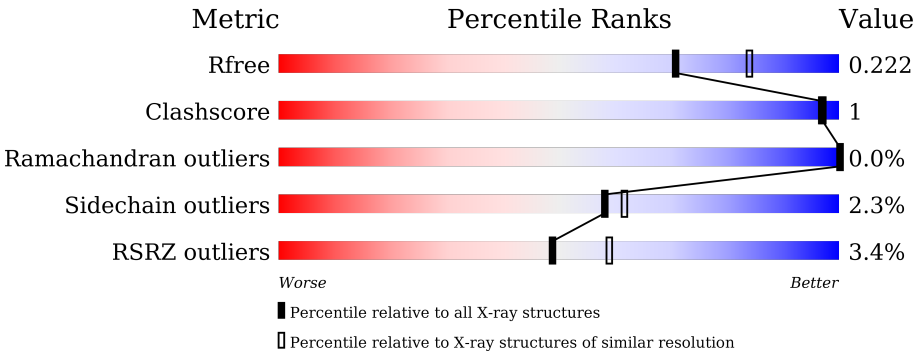
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	573	2% 91% 5% ·
1	B	573	2% 92% 5% ·
1	C	573	% 92% 5% ·
1	D	573	% 92% · ·
1	E	573	% 92% 5% ·
1	F	573	91% 5% ·

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Mol	Chain	Length	Quality of chain
1	G	573	2% 91% 6%
1	H	573	2% 91% 6%
1	I	573	2% 93%
1	J	573	% 91% 5%
1	K	573	2% 92% 5%
1	L	573	% 91% 5%
1	M	573	% 91% 6%
1	N	573	% 92% 5%
1	O	573	2% 92%
1	P	573	2% 92% 5%
1	Q	573	3% 94%
1	R	573	2% 92% 5%
1	S	573	2% 93%
1	T	573	% 92%
1	U	573	13% 91% 6%
1	V	573	13% 91% 5%
1	W	573	20% 92% 5%
1	X	573	2% 92%

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
4	EDO	A	603	-	-	-	X
4	EDO	F	601	-	-	-	X
4	EDO	I	603	-	-	-	X
4	EDO	N	603	-	-	-	X
4	EDO	Q	603	-	-	-	X
4	EDO	R	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 107004 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 Pyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	5	0
			4250	2665	737	823	25			
1	B	555	Total	C	N	O	S	0	4	0
			4237	2658	733	821	25			
1	C	555	Total	C	N	O	S	0	6	0
			4260	2670	742	823	25			
1	D	555	Total	C	N	O	S	0	5	0
			4245	2662	734	824	25			
1	E	556	Total	C	N	O	S	0	4	0
			4244	2662	734	823	25			
1	F	555	Total	C	N	O	S	0	9	0
			4285	2685	745	830	25			
1	G	555	Total	C	N	O	S	0	7	0
			4266	2675	739	827	25			
1	H	555	Total	C	N	O	S	0	6	0
			4252	2666	736	824	26			
1	I	556	Total	C	N	O	S	0	6	0
			4259	2670	737	827	25			
1	J	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	K	555	Total	C	N	O	S	0	7	0
			4266	2673	740	828	25			
1	L	555	Total	C	N	O	S	0	9	0
			4284	2683	745	831	25			
1	M	555	Total	C	N	O	S	0	7	0
			4262	2673	737	827	25			
1	N	555	Total	C	N	O	S	0	7	0
			4265	2672	740	828	25			
1	O	555	Total	C	N	O	S	0	3	0
			4229	2653	732	819	25			
1	P	555	Total	C	N	O	S	0	7	0
			4264	2673	738	828	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	555	Total	C	N	O	S	0	5	0
			4246	2663	734	824	25			
1	R	555	Total	C	N	O	S	0	8	0
			4270	2675	738	832	25			
1	S	555	Total	C	N	O	S	0	2	0
			4221	2649	731	816	25			
1	T	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	U	555	Total	C	N	O	S	0	4	0
			4239	2659	733	822	25			
1	V	555	Total	C	N	O	S	0	4	0
			4238	2658	733	822	25			
1	W	555	Total	C	N	O	S	0	3	0
			4230	2654	732	819	25			
1	X	555	Total	C	N	O	S	0	3	0
			4228	2653	732	818	25			

There are 456 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ALA	ARG	conflict	UNP Q8KTX6
A	245	ALA	GLU	conflict	UNP Q8KTX6
A	557	LEU	-	expression tag	UNP Q8KTX6
A	558	VAL	-	expression tag	UNP Q8KTX6
A	559	PRO	-	expression tag	UNP Q8KTX6
A	560	ARG	-	expression tag	UNP Q8KTX6
A	561	GLY	-	expression tag	UNP Q8KTX6
A	562	SER	-	expression tag	UNP Q8KTX6
A	563	GLY	-	expression tag	UNP Q8KTX6
A	564	GLY	-	expression tag	UNP Q8KTX6
A	565	GLY	-	expression tag	UNP Q8KTX6
A	566	LEU	-	expression tag	UNP Q8KTX6
A	567	GLU	-	expression tag	UNP Q8KTX6
A	568	HIS	-	expression tag	UNP Q8KTX6
A	569	HIS	-	expression tag	UNP Q8KTX6
A	570	HIS	-	expression tag	UNP Q8KTX6
A	571	HIS	-	expression tag	UNP Q8KTX6
A	572	HIS	-	expression tag	UNP Q8KTX6
A	573	HIS	-	expression tag	UNP Q8KTX6
B	134	ALA	ARG	conflict	UNP Q8KTX6
B	245	ALA	GLU	conflict	UNP Q8KTX6
B	557	LEU	-	expression tag	UNP Q8KTX6
B	558	VAL	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	-	expression tag	UNP Q8KTX6
B	560	ARG	-	expression tag	UNP Q8KTX6
B	561	GLY	-	expression tag	UNP Q8KTX6
B	562	SER	-	expression tag	UNP Q8KTX6
B	563	GLY	-	expression tag	UNP Q8KTX6
B	564	GLY	-	expression tag	UNP Q8KTX6
B	565	GLY	-	expression tag	UNP Q8KTX6
B	566	LEU	-	expression tag	UNP Q8KTX6
B	567	GLU	-	expression tag	UNP Q8KTX6
B	568	HIS	-	expression tag	UNP Q8KTX6
B	569	HIS	-	expression tag	UNP Q8KTX6
B	570	HIS	-	expression tag	UNP Q8KTX6
B	571	HIS	-	expression tag	UNP Q8KTX6
B	572	HIS	-	expression tag	UNP Q8KTX6
B	573	HIS	-	expression tag	UNP Q8KTX6
C	134	ALA	ARG	conflict	UNP Q8KTX6
C	245	ALA	GLU	conflict	UNP Q8KTX6
C	557	LEU	-	expression tag	UNP Q8KTX6
C	558	VAL	-	expression tag	UNP Q8KTX6
C	559	PRO	-	expression tag	UNP Q8KTX6
C	560	ARG	-	expression tag	UNP Q8KTX6
C	561	GLY	-	expression tag	UNP Q8KTX6
C	562	SER	-	expression tag	UNP Q8KTX6
C	563	GLY	-	expression tag	UNP Q8KTX6
C	564	GLY	-	expression tag	UNP Q8KTX6
C	565	GLY	-	expression tag	UNP Q8KTX6
C	566	LEU	-	expression tag	UNP Q8KTX6
C	567	GLU	-	expression tag	UNP Q8KTX6
C	568	HIS	-	expression tag	UNP Q8KTX6
C	569	HIS	-	expression tag	UNP Q8KTX6
C	570	HIS	-	expression tag	UNP Q8KTX6
C	571	HIS	-	expression tag	UNP Q8KTX6
C	572	HIS	-	expression tag	UNP Q8KTX6
C	573	HIS	-	expression tag	UNP Q8KTX6
D	134	ALA	ARG	conflict	UNP Q8KTX6
D	245	ALA	GLU	conflict	UNP Q8KTX6
D	557	LEU	-	expression tag	UNP Q8KTX6
D	558	VAL	-	expression tag	UNP Q8KTX6
D	559	PRO	-	expression tag	UNP Q8KTX6
D	560	ARG	-	expression tag	UNP Q8KTX6
D	561	GLY	-	expression tag	UNP Q8KTX6
D	562	SER	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	563	GLY	-	expression tag	UNP Q8KTX6
D	564	GLY	-	expression tag	UNP Q8KTX6
D	565	GLY	-	expression tag	UNP Q8KTX6
D	566	LEU	-	expression tag	UNP Q8KTX6
D	567	GLU	-	expression tag	UNP Q8KTX6
D	568	HIS	-	expression tag	UNP Q8KTX6
D	569	HIS	-	expression tag	UNP Q8KTX6
D	570	HIS	-	expression tag	UNP Q8KTX6
D	571	HIS	-	expression tag	UNP Q8KTX6
D	572	HIS	-	expression tag	UNP Q8KTX6
D	573	HIS	-	expression tag	UNP Q8KTX6
E	134	ALA	ARG	conflict	UNP Q8KTX6
E	245	ALA	GLU	conflict	UNP Q8KTX6
E	557	LEU	-	expression tag	UNP Q8KTX6
E	558	VAL	-	expression tag	UNP Q8KTX6
E	559	PRO	-	expression tag	UNP Q8KTX6
E	560	ARG	-	expression tag	UNP Q8KTX6
E	561	GLY	-	expression tag	UNP Q8KTX6
E	562	SER	-	expression tag	UNP Q8KTX6
E	563	GLY	-	expression tag	UNP Q8KTX6
E	564	GLY	-	expression tag	UNP Q8KTX6
E	565	GLY	-	expression tag	UNP Q8KTX6
E	566	LEU	-	expression tag	UNP Q8KTX6
E	567	GLU	-	expression tag	UNP Q8KTX6
E	568	HIS	-	expression tag	UNP Q8KTX6
E	569	HIS	-	expression tag	UNP Q8KTX6
E	570	HIS	-	expression tag	UNP Q8KTX6
E	571	HIS	-	expression tag	UNP Q8KTX6
E	572	HIS	-	expression tag	UNP Q8KTX6
E	573	HIS	-	expression tag	UNP Q8KTX6
F	134	ALA	ARG	conflict	UNP Q8KTX6
F	245	ALA	GLU	conflict	UNP Q8KTX6
F	557	LEU	-	expression tag	UNP Q8KTX6
F	558	VAL	-	expression tag	UNP Q8KTX6
F	559	PRO	-	expression tag	UNP Q8KTX6
F	560	ARG	-	expression tag	UNP Q8KTX6
F	561	GLY	-	expression tag	UNP Q8KTX6
F	562	SER	-	expression tag	UNP Q8KTX6
F	563	GLY	-	expression tag	UNP Q8KTX6
F	564	GLY	-	expression tag	UNP Q8KTX6
F	565	GLY	-	expression tag	UNP Q8KTX6
F	566	LEU	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	567	GLU	-	expression tag	UNP Q8KTX6
F	568	HIS	-	expression tag	UNP Q8KTX6
F	569	HIS	-	expression tag	UNP Q8KTX6
F	570	HIS	-	expression tag	UNP Q8KTX6
F	571	HIS	-	expression tag	UNP Q8KTX6
F	572	HIS	-	expression tag	UNP Q8KTX6
F	573	HIS	-	expression tag	UNP Q8KTX6
G	134	ALA	ARG	conflict	UNP Q8KTX6
G	245	ALA	GLU	conflict	UNP Q8KTX6
G	557	LEU	-	expression tag	UNP Q8KTX6
G	558	VAL	-	expression tag	UNP Q8KTX6
G	559	PRO	-	expression tag	UNP Q8KTX6
G	560	ARG	-	expression tag	UNP Q8KTX6
G	561	GLY	-	expression tag	UNP Q8KTX6
G	562	SER	-	expression tag	UNP Q8KTX6
G	563	GLY	-	expression tag	UNP Q8KTX6
G	564	GLY	-	expression tag	UNP Q8KTX6
G	565	GLY	-	expression tag	UNP Q8KTX6
G	566	LEU	-	expression tag	UNP Q8KTX6
G	567	GLU	-	expression tag	UNP Q8KTX6
G	568	HIS	-	expression tag	UNP Q8KTX6
G	569	HIS	-	expression tag	UNP Q8KTX6
G	570	HIS	-	expression tag	UNP Q8KTX6
G	571	HIS	-	expression tag	UNP Q8KTX6
G	572	HIS	-	expression tag	UNP Q8KTX6
G	573	HIS	-	expression tag	UNP Q8KTX6
H	134	ALA	ARG	conflict	UNP Q8KTX6
H	245	ALA	GLU	conflict	UNP Q8KTX6
H	557	LEU	-	expression tag	UNP Q8KTX6
H	558	VAL	-	expression tag	UNP Q8KTX6
H	559	PRO	-	expression tag	UNP Q8KTX6
H	560	ARG	-	expression tag	UNP Q8KTX6
H	561	GLY	-	expression tag	UNP Q8KTX6
H	562	SER	-	expression tag	UNP Q8KTX6
H	563	GLY	-	expression tag	UNP Q8KTX6
H	564	GLY	-	expression tag	UNP Q8KTX6
H	565	GLY	-	expression tag	UNP Q8KTX6
H	566	LEU	-	expression tag	UNP Q8KTX6
H	567	GLU	-	expression tag	UNP Q8KTX6
H	568	HIS	-	expression tag	UNP Q8KTX6
H	569	HIS	-	expression tag	UNP Q8KTX6
H	570	HIS	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	571	HIS	-	expression tag	UNP Q8KTX6
H	572	HIS	-	expression tag	UNP Q8KTX6
H	573	HIS	-	expression tag	UNP Q8KTX6
I	134	ALA	ARG	conflict	UNP Q8KTX6
I	245	ALA	GLU	conflict	UNP Q8KTX6
I	557	LEU	-	expression tag	UNP Q8KTX6
I	558	VAL	-	expression tag	UNP Q8KTX6
I	559	PRO	-	expression tag	UNP Q8KTX6
I	560	ARG	-	expression tag	UNP Q8KTX6
I	561	GLY	-	expression tag	UNP Q8KTX6
I	562	SER	-	expression tag	UNP Q8KTX6
I	563	GLY	-	expression tag	UNP Q8KTX6
I	564	GLY	-	expression tag	UNP Q8KTX6
I	565	GLY	-	expression tag	UNP Q8KTX6
I	566	LEU	-	expression tag	UNP Q8KTX6
I	567	GLU	-	expression tag	UNP Q8KTX6
I	568	HIS	-	expression tag	UNP Q8KTX6
I	569	HIS	-	expression tag	UNP Q8KTX6
I	570	HIS	-	expression tag	UNP Q8KTX6
I	571	HIS	-	expression tag	UNP Q8KTX6
I	572	HIS	-	expression tag	UNP Q8KTX6
I	573	HIS	-	expression tag	UNP Q8KTX6
J	134	ALA	ARG	conflict	UNP Q8KTX6
J	245	ALA	GLU	conflict	UNP Q8KTX6
J	557	LEU	-	expression tag	UNP Q8KTX6
J	558	VAL	-	expression tag	UNP Q8KTX6
J	559	PRO	-	expression tag	UNP Q8KTX6
J	560	ARG	-	expression tag	UNP Q8KTX6
J	561	GLY	-	expression tag	UNP Q8KTX6
J	562	SER	-	expression tag	UNP Q8KTX6
J	563	GLY	-	expression tag	UNP Q8KTX6
J	564	GLY	-	expression tag	UNP Q8KTX6
J	565	GLY	-	expression tag	UNP Q8KTX6
J	566	LEU	-	expression tag	UNP Q8KTX6
J	567	GLU	-	expression tag	UNP Q8KTX6
J	568	HIS	-	expression tag	UNP Q8KTX6
J	569	HIS	-	expression tag	UNP Q8KTX6
J	570	HIS	-	expression tag	UNP Q8KTX6
J	571	HIS	-	expression tag	UNP Q8KTX6
J	572	HIS	-	expression tag	UNP Q8KTX6
J	573	HIS	-	expression tag	UNP Q8KTX6
K	134	ALA	ARG	conflict	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	245	ALA	GLU	conflict	UNP Q8KTX6
K	557	LEU	-	expression tag	UNP Q8KTX6
K	558	VAL	-	expression tag	UNP Q8KTX6
K	559	PRO	-	expression tag	UNP Q8KTX6
K	560	ARG	-	expression tag	UNP Q8KTX6
K	561	GLY	-	expression tag	UNP Q8KTX6
K	562	SER	-	expression tag	UNP Q8KTX6
K	563	GLY	-	expression tag	UNP Q8KTX6
K	564	GLY	-	expression tag	UNP Q8KTX6
K	565	GLY	-	expression tag	UNP Q8KTX6
K	566	LEU	-	expression tag	UNP Q8KTX6
K	567	GLU	-	expression tag	UNP Q8KTX6
K	568	HIS	-	expression tag	UNP Q8KTX6
K	569	HIS	-	expression tag	UNP Q8KTX6
K	570	HIS	-	expression tag	UNP Q8KTX6
K	571	HIS	-	expression tag	UNP Q8KTX6
K	572	HIS	-	expression tag	UNP Q8KTX6
K	573	HIS	-	expression tag	UNP Q8KTX6
L	134	ALA	ARG	conflict	UNP Q8KTX6
L	245	ALA	GLU	conflict	UNP Q8KTX6
L	557	LEU	-	expression tag	UNP Q8KTX6
L	558	VAL	-	expression tag	UNP Q8KTX6
L	559	PRO	-	expression tag	UNP Q8KTX6
L	560	ARG	-	expression tag	UNP Q8KTX6
L	561	GLY	-	expression tag	UNP Q8KTX6
L	562	SER	-	expression tag	UNP Q8KTX6
L	563	GLY	-	expression tag	UNP Q8KTX6
L	564	GLY	-	expression tag	UNP Q8KTX6
L	565	GLY	-	expression tag	UNP Q8KTX6
L	566	LEU	-	expression tag	UNP Q8KTX6
L	567	GLU	-	expression tag	UNP Q8KTX6
L	568	HIS	-	expression tag	UNP Q8KTX6
L	569	HIS	-	expression tag	UNP Q8KTX6
L	570	HIS	-	expression tag	UNP Q8KTX6
L	571	HIS	-	expression tag	UNP Q8KTX6
L	572	HIS	-	expression tag	UNP Q8KTX6
L	573	HIS	-	expression tag	UNP Q8KTX6
M	134	ALA	ARG	conflict	UNP Q8KTX6
M	245	ALA	GLU	conflict	UNP Q8KTX6
M	557	LEU	-	expression tag	UNP Q8KTX6
M	558	VAL	-	expression tag	UNP Q8KTX6
M	559	PRO	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	560	ARG	-	expression tag	UNP Q8KTX6
M	561	GLY	-	expression tag	UNP Q8KTX6
M	562	SER	-	expression tag	UNP Q8KTX6
M	563	GLY	-	expression tag	UNP Q8KTX6
M	564	GLY	-	expression tag	UNP Q8KTX6
M	565	GLY	-	expression tag	UNP Q8KTX6
M	566	LEU	-	expression tag	UNP Q8KTX6
M	567	GLU	-	expression tag	UNP Q8KTX6
M	568	HIS	-	expression tag	UNP Q8KTX6
M	569	HIS	-	expression tag	UNP Q8KTX6
M	570	HIS	-	expression tag	UNP Q8KTX6
M	571	HIS	-	expression tag	UNP Q8KTX6
M	572	HIS	-	expression tag	UNP Q8KTX6
M	573	HIS	-	expression tag	UNP Q8KTX6
N	134	ALA	ARG	conflict	UNP Q8KTX6
N	245	ALA	GLU	conflict	UNP Q8KTX6
N	557	LEU	-	expression tag	UNP Q8KTX6
N	558	VAL	-	expression tag	UNP Q8KTX6
N	559	PRO	-	expression tag	UNP Q8KTX6
N	560	ARG	-	expression tag	UNP Q8KTX6
N	561	GLY	-	expression tag	UNP Q8KTX6
N	562	SER	-	expression tag	UNP Q8KTX6
N	563	GLY	-	expression tag	UNP Q8KTX6
N	564	GLY	-	expression tag	UNP Q8KTX6
N	565	GLY	-	expression tag	UNP Q8KTX6
N	566	LEU	-	expression tag	UNP Q8KTX6
N	567	GLU	-	expression tag	UNP Q8KTX6
N	568	HIS	-	expression tag	UNP Q8KTX6
N	569	HIS	-	expression tag	UNP Q8KTX6
N	570	HIS	-	expression tag	UNP Q8KTX6
N	571	HIS	-	expression tag	UNP Q8KTX6
N	572	HIS	-	expression tag	UNP Q8KTX6
N	573	HIS	-	expression tag	UNP Q8KTX6
O	134	ALA	ARG	conflict	UNP Q8KTX6
O	245	ALA	GLU	conflict	UNP Q8KTX6
O	557	LEU	-	expression tag	UNP Q8KTX6
O	558	VAL	-	expression tag	UNP Q8KTX6
O	559	PRO	-	expression tag	UNP Q8KTX6
O	560	ARG	-	expression tag	UNP Q8KTX6
O	561	GLY	-	expression tag	UNP Q8KTX6
O	562	SER	-	expression tag	UNP Q8KTX6
O	563	GLY	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	564	GLY	-	expression tag	UNP Q8KTX6
O	565	GLY	-	expression tag	UNP Q8KTX6
O	566	LEU	-	expression tag	UNP Q8KTX6
O	567	GLU	-	expression tag	UNP Q8KTX6
O	568	HIS	-	expression tag	UNP Q8KTX6
O	569	HIS	-	expression tag	UNP Q8KTX6
O	570	HIS	-	expression tag	UNP Q8KTX6
O	571	HIS	-	expression tag	UNP Q8KTX6
O	572	HIS	-	expression tag	UNP Q8KTX6
O	573	HIS	-	expression tag	UNP Q8KTX6
P	134	ALA	ARG	conflict	UNP Q8KTX6
P	245	ALA	GLU	conflict	UNP Q8KTX6
P	557	LEU	-	expression tag	UNP Q8KTX6
P	558	VAL	-	expression tag	UNP Q8KTX6
P	559	PRO	-	expression tag	UNP Q8KTX6
P	560	ARG	-	expression tag	UNP Q8KTX6
P	561	GLY	-	expression tag	UNP Q8KTX6
P	562	SER	-	expression tag	UNP Q8KTX6
P	563	GLY	-	expression tag	UNP Q8KTX6
P	564	GLY	-	expression tag	UNP Q8KTX6
P	565	GLY	-	expression tag	UNP Q8KTX6
P	566	LEU	-	expression tag	UNP Q8KTX6
P	567	GLU	-	expression tag	UNP Q8KTX6
P	568	HIS	-	expression tag	UNP Q8KTX6
P	569	HIS	-	expression tag	UNP Q8KTX6
P	570	HIS	-	expression tag	UNP Q8KTX6
P	571	HIS	-	expression tag	UNP Q8KTX6
P	572	HIS	-	expression tag	UNP Q8KTX6
P	573	HIS	-	expression tag	UNP Q8KTX6
Q	134	ALA	ARG	conflict	UNP Q8KTX6
Q	245	ALA	GLU	conflict	UNP Q8KTX6
Q	557	LEU	-	expression tag	UNP Q8KTX6
Q	558	VAL	-	expression tag	UNP Q8KTX6
Q	559	PRO	-	expression tag	UNP Q8KTX6
Q	560	ARG	-	expression tag	UNP Q8KTX6
Q	561	GLY	-	expression tag	UNP Q8KTX6
Q	562	SER	-	expression tag	UNP Q8KTX6
Q	563	GLY	-	expression tag	UNP Q8KTX6
Q	564	GLY	-	expression tag	UNP Q8KTX6
Q	565	GLY	-	expression tag	UNP Q8KTX6
Q	566	LEU	-	expression tag	UNP Q8KTX6
Q	567	GLU	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	568	HIS	-	expression tag	UNP Q8KTX6
Q	569	HIS	-	expression tag	UNP Q8KTX6
Q	570	HIS	-	expression tag	UNP Q8KTX6
Q	571	HIS	-	expression tag	UNP Q8KTX6
Q	572	HIS	-	expression tag	UNP Q8KTX6
Q	573	HIS	-	expression tag	UNP Q8KTX6
R	134	ALA	ARG	conflict	UNP Q8KTX6
R	245	ALA	GLU	conflict	UNP Q8KTX6
R	557	LEU	-	expression tag	UNP Q8KTX6
R	558	VAL	-	expression tag	UNP Q8KTX6
R	559	PRO	-	expression tag	UNP Q8KTX6
R	560	ARG	-	expression tag	UNP Q8KTX6
R	561	GLY	-	expression tag	UNP Q8KTX6
R	562	SER	-	expression tag	UNP Q8KTX6
R	563	GLY	-	expression tag	UNP Q8KTX6
R	564	GLY	-	expression tag	UNP Q8KTX6
R	565	GLY	-	expression tag	UNP Q8KTX6
R	566	LEU	-	expression tag	UNP Q8KTX6
R	567	GLU	-	expression tag	UNP Q8KTX6
R	568	HIS	-	expression tag	UNP Q8KTX6
R	569	HIS	-	expression tag	UNP Q8KTX6
R	570	HIS	-	expression tag	UNP Q8KTX6
R	571	HIS	-	expression tag	UNP Q8KTX6
R	572	HIS	-	expression tag	UNP Q8KTX6
R	573	HIS	-	expression tag	UNP Q8KTX6
S	134	ALA	ARG	conflict	UNP Q8KTX6
S	245	ALA	GLU	conflict	UNP Q8KTX6
S	557	LEU	-	expression tag	UNP Q8KTX6
S	558	VAL	-	expression tag	UNP Q8KTX6
S	559	PRO	-	expression tag	UNP Q8KTX6
S	560	ARG	-	expression tag	UNP Q8KTX6
S	561	GLY	-	expression tag	UNP Q8KTX6
S	562	SER	-	expression tag	UNP Q8KTX6
S	563	GLY	-	expression tag	UNP Q8KTX6
S	564	GLY	-	expression tag	UNP Q8KTX6
S	565	GLY	-	expression tag	UNP Q8KTX6
S	566	LEU	-	expression tag	UNP Q8KTX6
S	567	GLU	-	expression tag	UNP Q8KTX6
S	568	HIS	-	expression tag	UNP Q8KTX6
S	569	HIS	-	expression tag	UNP Q8KTX6
S	570	HIS	-	expression tag	UNP Q8KTX6
S	571	HIS	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	572	HIS	-	expression tag	UNP Q8KTX6
S	573	HIS	-	expression tag	UNP Q8KTX6
T	134	ALA	ARG	conflict	UNP Q8KTX6
T	245	ALA	GLU	conflict	UNP Q8KTX6
T	557	LEU	-	expression tag	UNP Q8KTX6
T	558	VAL	-	expression tag	UNP Q8KTX6
T	559	PRO	-	expression tag	UNP Q8KTX6
T	560	ARG	-	expression tag	UNP Q8KTX6
T	561	GLY	-	expression tag	UNP Q8KTX6
T	562	SER	-	expression tag	UNP Q8KTX6
T	563	GLY	-	expression tag	UNP Q8KTX6
T	564	GLY	-	expression tag	UNP Q8KTX6
T	565	GLY	-	expression tag	UNP Q8KTX6
T	566	LEU	-	expression tag	UNP Q8KTX6
T	567	GLU	-	expression tag	UNP Q8KTX6
T	568	HIS	-	expression tag	UNP Q8KTX6
T	569	HIS	-	expression tag	UNP Q8KTX6
T	570	HIS	-	expression tag	UNP Q8KTX6
T	571	HIS	-	expression tag	UNP Q8KTX6
T	572	HIS	-	expression tag	UNP Q8KTX6
T	573	HIS	-	expression tag	UNP Q8KTX6
U	134	ALA	ARG	conflict	UNP Q8KTX6
U	245	ALA	GLU	conflict	UNP Q8KTX6
U	557	LEU	-	expression tag	UNP Q8KTX6
U	558	VAL	-	expression tag	UNP Q8KTX6
U	559	PRO	-	expression tag	UNP Q8KTX6
U	560	ARG	-	expression tag	UNP Q8KTX6
U	561	GLY	-	expression tag	UNP Q8KTX6
U	562	SER	-	expression tag	UNP Q8KTX6
U	563	GLY	-	expression tag	UNP Q8KTX6
U	564	GLY	-	expression tag	UNP Q8KTX6
U	565	GLY	-	expression tag	UNP Q8KTX6
U	566	LEU	-	expression tag	UNP Q8KTX6
U	567	GLU	-	expression tag	UNP Q8KTX6
U	568	HIS	-	expression tag	UNP Q8KTX6
U	569	HIS	-	expression tag	UNP Q8KTX6
U	570	HIS	-	expression tag	UNP Q8KTX6
U	571	HIS	-	expression tag	UNP Q8KTX6
U	572	HIS	-	expression tag	UNP Q8KTX6
U	573	HIS	-	expression tag	UNP Q8KTX6
V	134	ALA	ARG	conflict	UNP Q8KTX6
V	245	ALA	GLU	conflict	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
V	557	LEU	-	expression tag	UNP Q8KTX6
V	558	VAL	-	expression tag	UNP Q8KTX6
V	559	PRO	-	expression tag	UNP Q8KTX6
V	560	ARG	-	expression tag	UNP Q8KTX6
V	561	GLY	-	expression tag	UNP Q8KTX6
V	562	SER	-	expression tag	UNP Q8KTX6
V	563	GLY	-	expression tag	UNP Q8KTX6
V	564	GLY	-	expression tag	UNP Q8KTX6
V	565	GLY	-	expression tag	UNP Q8KTX6
V	566	LEU	-	expression tag	UNP Q8KTX6
V	567	GLU	-	expression tag	UNP Q8KTX6
V	568	HIS	-	expression tag	UNP Q8KTX6
V	569	HIS	-	expression tag	UNP Q8KTX6
V	570	HIS	-	expression tag	UNP Q8KTX6
V	571	HIS	-	expression tag	UNP Q8KTX6
V	572	HIS	-	expression tag	UNP Q8KTX6
V	573	HIS	-	expression tag	UNP Q8KTX6
W	134	ALA	ARG	conflict	UNP Q8KTX6
W	245	ALA	GLU	conflict	UNP Q8KTX6
W	557	LEU	-	expression tag	UNP Q8KTX6
W	558	VAL	-	expression tag	UNP Q8KTX6
W	559	PRO	-	expression tag	UNP Q8KTX6
W	560	ARG	-	expression tag	UNP Q8KTX6
W	561	GLY	-	expression tag	UNP Q8KTX6
W	562	SER	-	expression tag	UNP Q8KTX6
W	563	GLY	-	expression tag	UNP Q8KTX6
W	564	GLY	-	expression tag	UNP Q8KTX6
W	565	GLY	-	expression tag	UNP Q8KTX6
W	566	LEU	-	expression tag	UNP Q8KTX6
W	567	GLU	-	expression tag	UNP Q8KTX6
W	568	HIS	-	expression tag	UNP Q8KTX6
W	569	HIS	-	expression tag	UNP Q8KTX6
W	570	HIS	-	expression tag	UNP Q8KTX6
W	571	HIS	-	expression tag	UNP Q8KTX6
W	572	HIS	-	expression tag	UNP Q8KTX6
W	573	HIS	-	expression tag	UNP Q8KTX6
X	134	ALA	ARG	conflict	UNP Q8KTX6
X	245	ALA	GLU	conflict	UNP Q8KTX6
X	557	LEU	-	expression tag	UNP Q8KTX6
X	558	VAL	-	expression tag	UNP Q8KTX6
X	559	PRO	-	expression tag	UNP Q8KTX6
X	560	ARG	-	expression tag	UNP Q8KTX6

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Chain	Residue	Modelled	Actual	Comment	Reference
X	561	GLY	-	expression tag	UNP Q8KTX6
X	562	SER	-	expression tag	UNP Q8KTX6
X	563	GLY	-	expression tag	UNP Q8KTX6
X	564	GLY	-	expression tag	UNP Q8KTX6
X	565	GLY	-	expression tag	UNP Q8KTX6
X	566	LEU	-	expression tag	UNP Q8KTX6
X	567	GLU	-	expression tag	UNP Q8KTX6
X	568	HIS	-	expression tag	UNP Q8KTX6
X	569	HIS	-	expression tag	UNP Q8KTX6
X	570	HIS	-	expression tag	UNP Q8KTX6
X	571	HIS	-	expression tag	UNP Q8KTX6
X	572	HIS	-	expression tag	UNP Q8KTX6
X	573	HIS	-	expression tag	UNP Q8KTX6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	W	1	Total Mg 1 1	0	0
2	N	1	Total Mg 1 1	0	0
2	X	1	Total Mg 1 1	0	0
2	S	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	V	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	R	1	Total Mg 1 1	0	0
2	M	1	Total Mg 1 1	0	0

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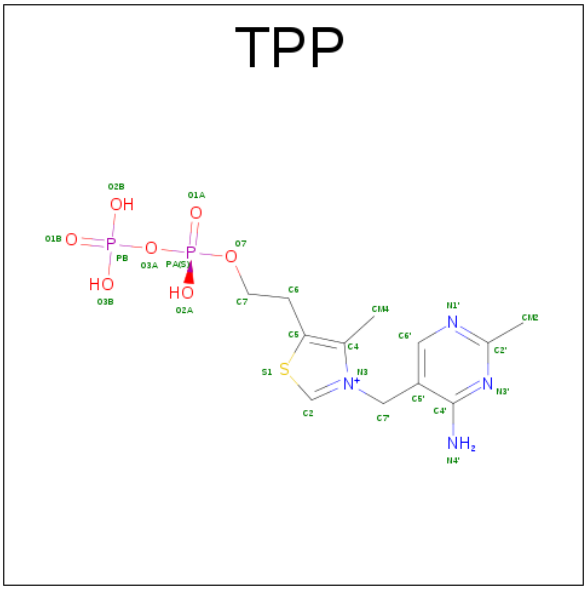
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	U	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	Q	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	T	1	Total Mg 1 1	0	0
2	O	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	G	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	H	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	I	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	J	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	K	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	L	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	M	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	N	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	O	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	P	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	Q	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	R	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	S	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	T	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	U	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	V	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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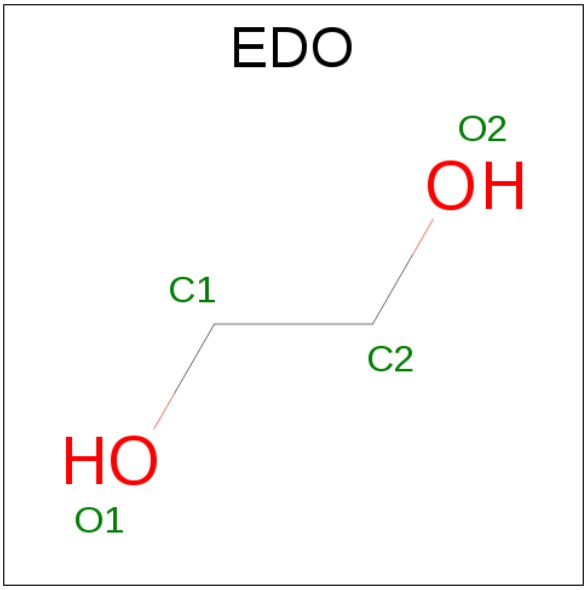
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	W	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	X	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			4	2	2			
4	F	1	Total	C	O		0	0
			4	2	2			
4	I	1	Total	C	O		0	0
			4	2	2			
4	N	1	Total	C	O		0	0
			4	2	2			
4	Q	1	Total	C	O		0	0
			4	2	2			
4	R	1	Total	C	O		0	0
			4	2	2			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	157	Total O 157 157	0	0
5	C	246	Total O 246 246	0	0
5	D	199	Total O 199 199	0	0
5	E	221	Total O 221 221	0	0
5	F	275	Total O 275 275	0	0
5	G	192	Total O 192 192	0	0
5	H	150	Total O 150 150	0	0
5	I	176	Total O 176 176	0	0
5	J	217	Total O 217 217	0	0
5	K	206	Total O 206 206	0	0
5	L	200	Total O 200 200	0	0
5	M	288	Total O 288 288	0	0
5	N	269	Total O 269 269	0	0
5	O	185	Total O 185 185	0	0
5	P	212	Total O 212 212	0	0
5	Q	149	Total O 149 149	0	0
5	R	151	Total O 151 151	0	0
5	S	184	Total O 184 184	0	0
5	T	184	Total O 184 184	0	0
5	U	81	Total O 81 81	0	0
5	V	66	Total O 66 66	0	0

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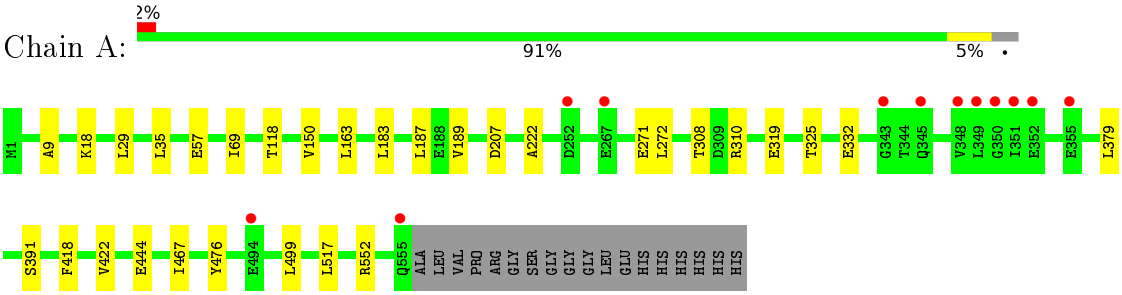
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	W	55	Total O 55 55	0	0
5	X	114	Total O 114 114	0	0

3 Residue-property plots (i)

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

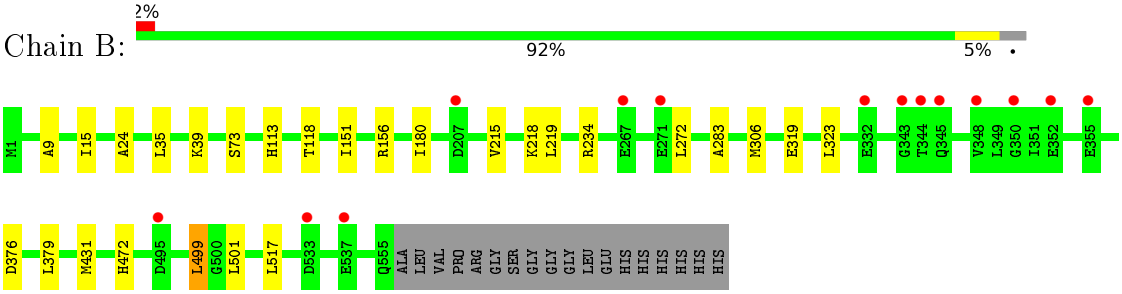
- Molecule 1: Pyruvate decarboxylase

Chain A:



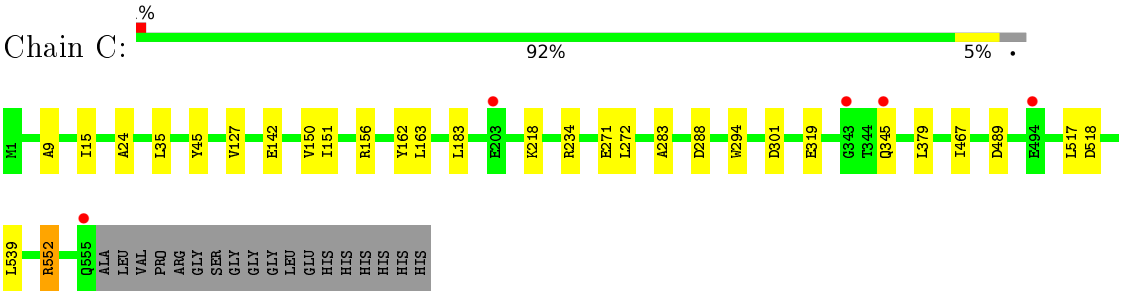
- Molecule 1: Pyruvate decarboxylase

Chain B:



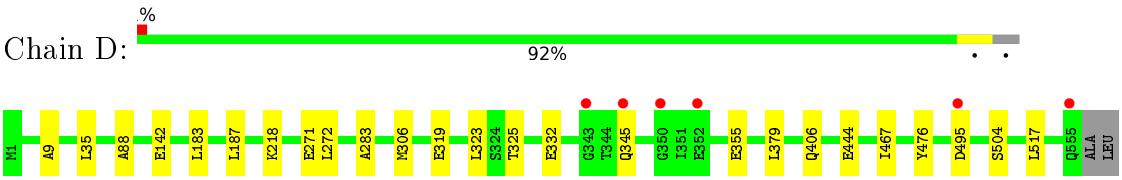
- Molecule 1: Pyruvate decarboxylase

Chain C:



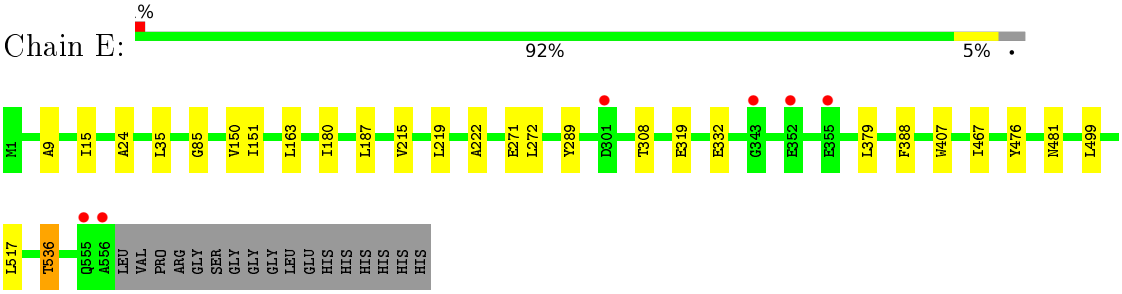
- Molecule 1: Pyruvate decarboxylase

Chain D:



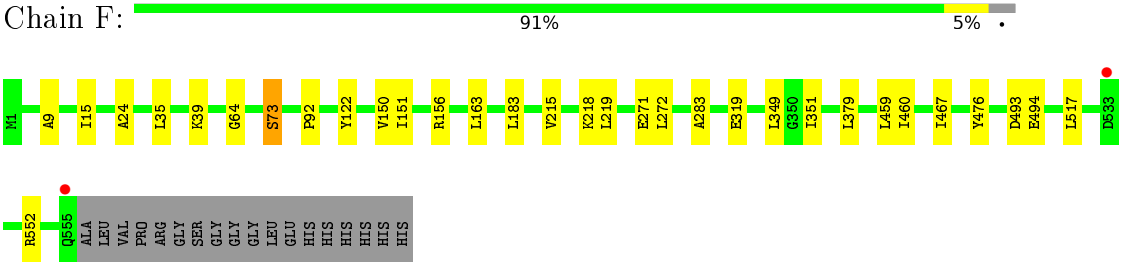
• Molecule 1: Pyruvate decarboxylase

Chain E:



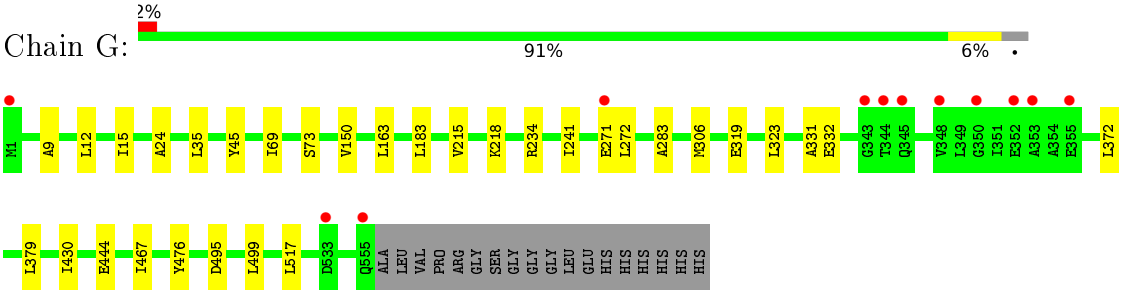
• Molecule 1: Pyruvate decarboxylase

Chain F:



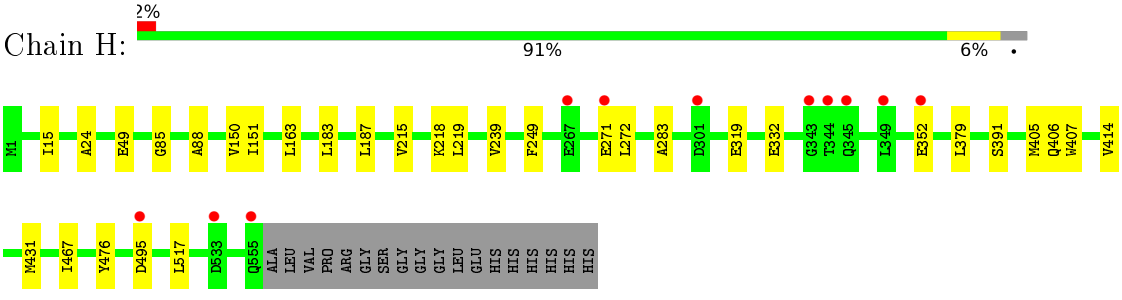
• Molecule 1: Pyruvate decarboxylase

Chain G:



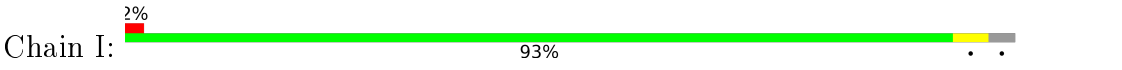
• Molecule 1: Pyruvate decarboxylase

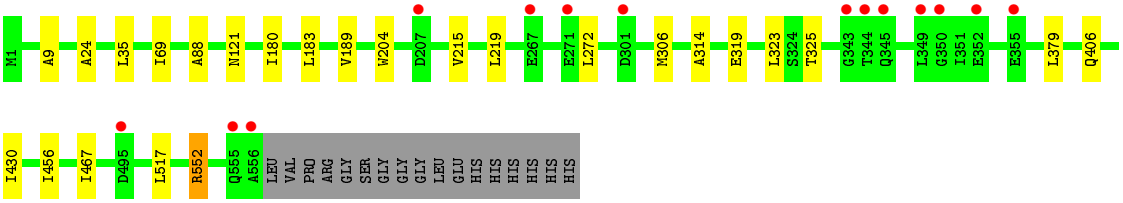
Chain H:



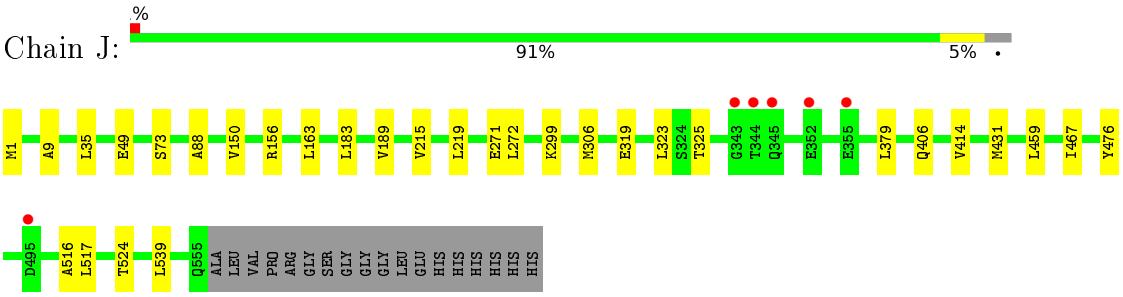
• Molecule 1: Pyruvate decarboxylase

Chain I:

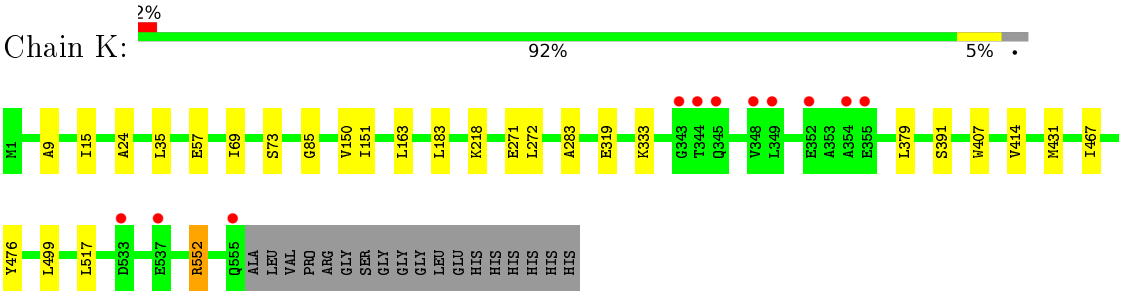




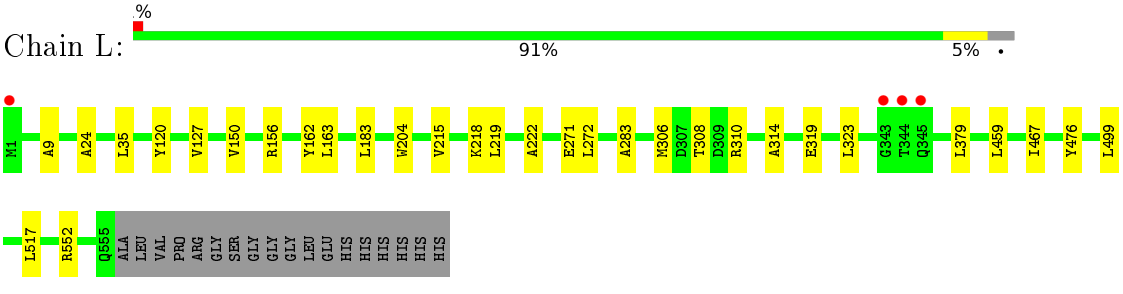
• Molecule 1: Pyruvate decarboxylase



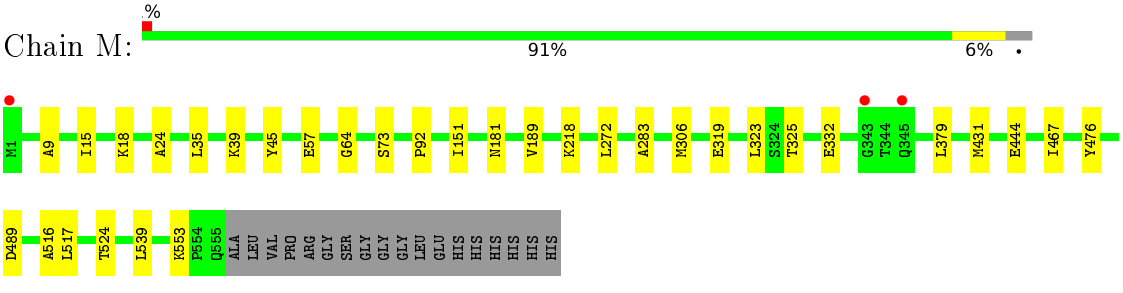
• Molecule 1: Pyruvate decarboxylase



• Molecule 1: Pyruvate decarboxylase

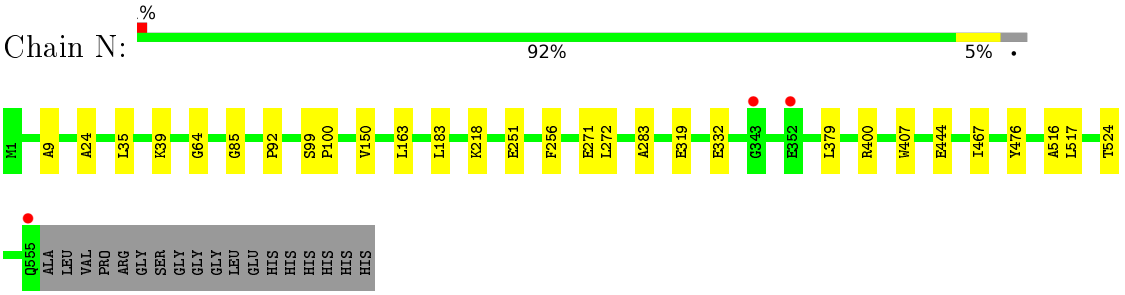


• Molecule 1: Pyruvate decarboxylase



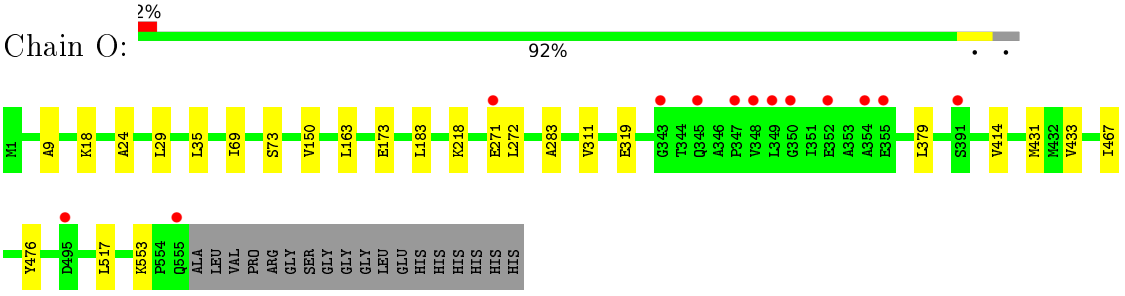
• Molecule 1: Pyruvate decarboxylase

Chain N:



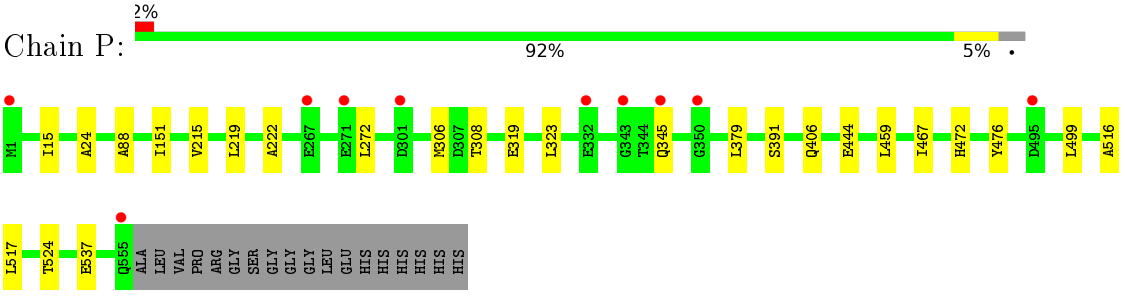
• Molecule 1: Pyruvate decarboxylase

Chain O:



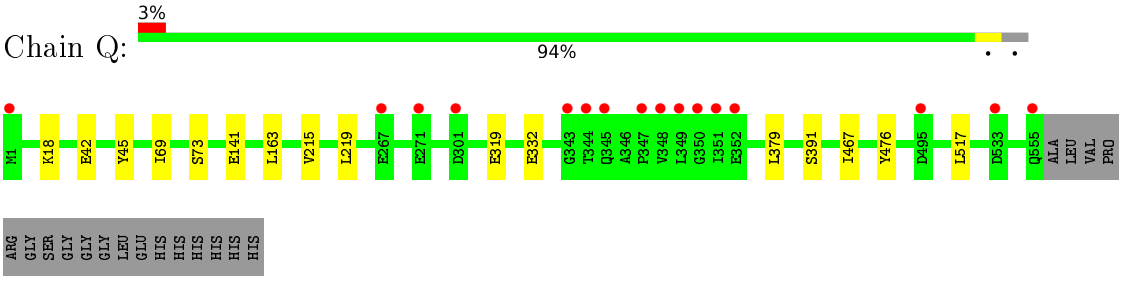
• Molecule 1: Pyruvate decarboxylase

Chain P:



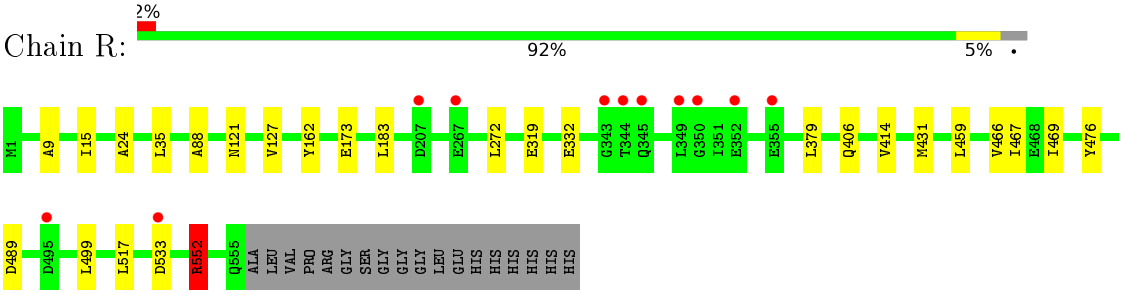
• Molecule 1: Pyruvate decarboxylase

Chain Q:



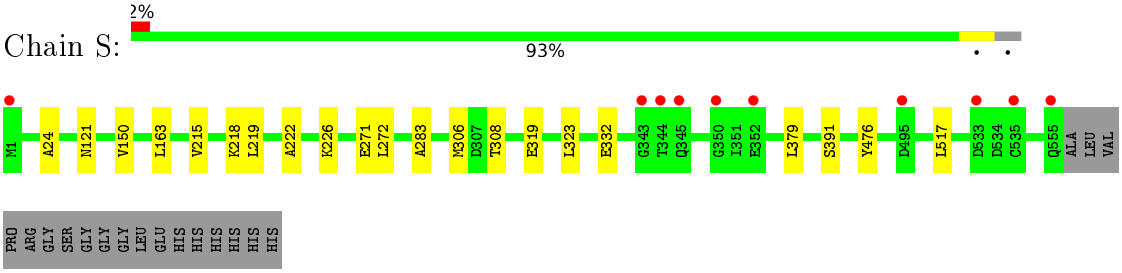
• Molecule 1: Pyruvate decarboxylase

Chain R:



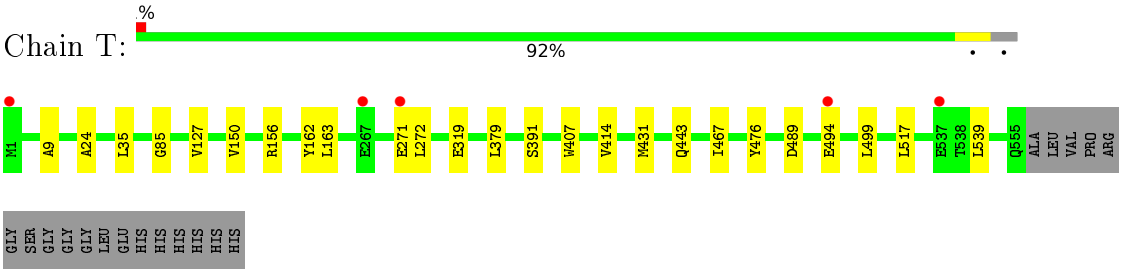
• Molecule 1: Pyruvate decarboxylase

Chain S:



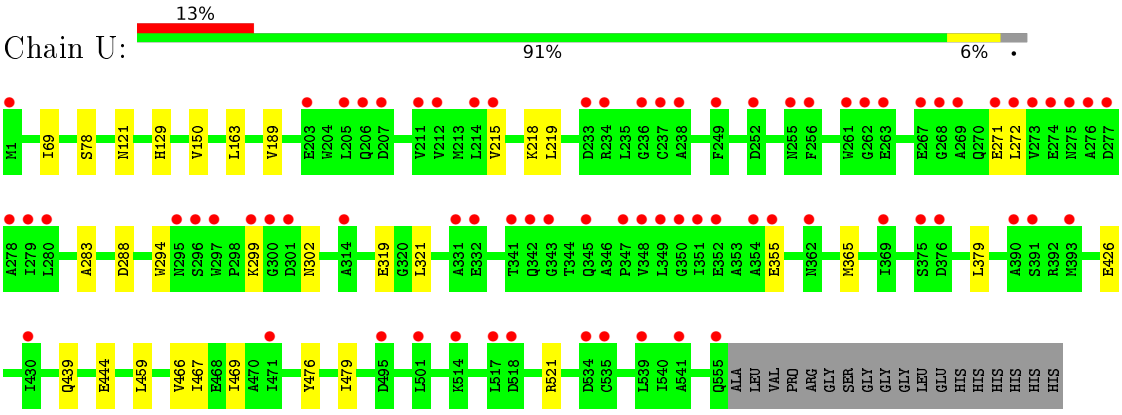
• Molecule 1: Pyruvate decarboxylase

Chain T:



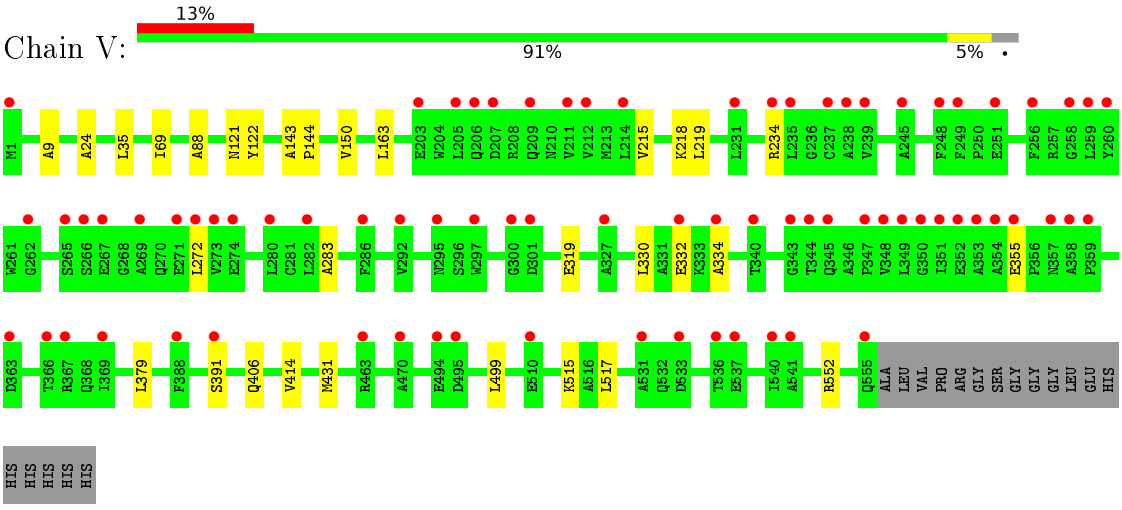
• Molecule 1: Pyruvate decarboxylase

Chain U:



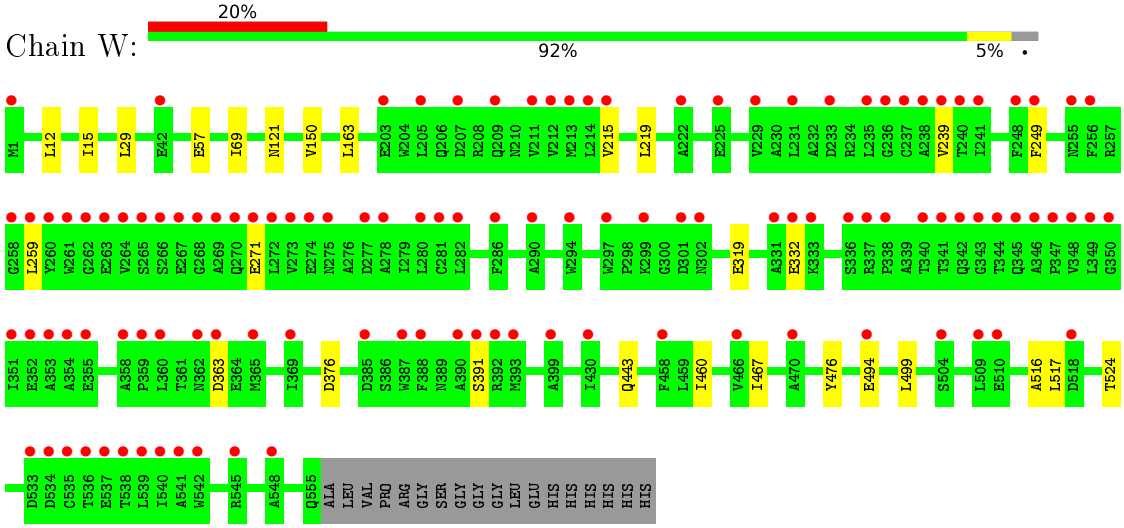
• Molecule 1: Pyruvate decarboxylase

Chain V:



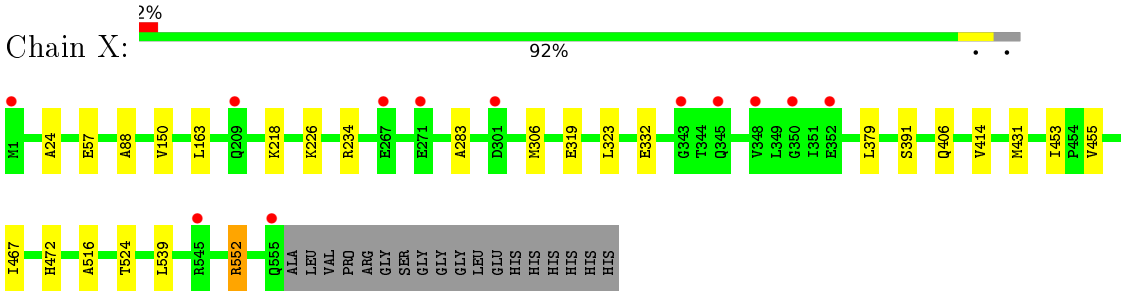
• Molecule 1: Pyruvate decarboxylase

Chain W:



• Molecule 1: Pyruvate decarboxylase

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	204.56Å 177.39Å 244.55Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	75.40 – 2.15 75.47 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (75.40-2.15) 98.8 (75.47-2.15)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.14Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.220 0.191 , 0.222	Depositor DCC
R_{free} test set	42940 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	107004	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.54% 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: MG, EDO, TPP

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	0.43	0/4334	0.65	2/5898 (0.0%)
1	B	0.43	0/4321	0.64	1/5882 (0.0%)
1	C	0.43	0/4344	0.67	3/5911 (0.1%)
1	D	0.44	0/4329	0.66	0/5893
1	E	0.45	0/4327	0.67	0/5888
1	F	0.45	0/4369	0.68	1/5945 (0.0%)
1	G	0.43	0/4350	0.65	0/5921
1	H	0.44	0/4336	0.64	0/5901
1	I	0.42	0/4342	0.67	2/5908 (0.0%)
1	J	0.43	0/4322	0.67	1/5883 (0.0%)
1	K	0.44	0/4350	0.64	0/5920
1	L	0.44	0/4368	0.65	2/5945 (0.0%)
1	M	0.44	0/4346	0.68	0/5916
1	N	0.45	0/4349	0.68	1/5919 (0.0%)
1	O	0.43	0/4313	0.65	0/5870
1	P	0.44	0/4348	0.67	0/5917
1	Q	0.43	0/4330	0.65	0/5894
1	R	0.42	0/4354	0.66	1/5927 (0.0%)
1	S	0.42	0/4305	0.65	0/5860
1	T	0.43	0/4322	0.65	1/5883 (0.0%)
1	U	0.42	0/4323	0.62	0/5884
1	V	0.41	0/4322	0.61	0/5883
1	W	0.43	0/4314	0.61	0/5872
1	X	0.41	0/4312	0.63	0/5870
All	All	0.43	0/104030	0.65	15/141590 (0.0%)

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	T	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	552	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	I	552	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	C	552	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	C	552	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	310	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	156	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	J	156	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	T	156	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	156	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	310	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	N	400	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	R	552	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	L	310	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	L	156	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	F	156	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	494	GLU	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	4250	0	4149	11	0
1	B	4237	0	4138	11	0
1	C	4260	0	4161	16	0
1	D	4245	0	4141	12	0
1	E	4244	0	4141	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4285	0	4179	14	0
1	G	4266	0	4163	14	0
1	H	4252	0	4148	18	0
1	I	4259	0	4151	11	0
1	J	4238	0	4135	13	0
1	K	4266	0	4157	13	0
1	L	4284	0	4176	12	0
1	M	4262	0	4158	15	0
1	N	4265	0	4155	13	0
1	O	4229	0	4129	11	0
1	P	4264	0	4157	11	0
1	Q	4246	0	4143	8	0
1	R	4270	0	4154	12	0
1	S	4221	0	4127	7	0
1	T	4238	0	4135	10	0
1	U	4239	0	4137	13	0
1	V	4238	0	4135	15	0
1	W	4230	0	4132	10	0
1	X	4228	0	4133	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	0	0
3	C	26	0	16	2	0
3	D	26	0	16	2	0
3	E	26	0	16	4	0
3	F	26	0	16	1	0
3	G	26	0	16	3	0
3	H	26	0	16	2	0
3	I	26	0	16	2	0
3	J	26	0	16	2	0
3	K	26	0	16	2	0
3	L	26	0	16	2	0
3	M	26	0	16	2	0
3	N	26	0	16	2	0
3	O	26	0	16	2	0
3	P	26	0	16	2	0
3	Q	26	0	16	2	0
3	R	26	0	16	2	0
3	S	26	0	16	0	0
3	T	26	0	16	1	0
3	U	26	0	16	1	0
3	V	26	0	16	0	0
3	W	26	0	16	1	0
3	X	26	0	16	2	0
4	A	4	0	6	0	0
4	F	4	0	6	2	0
4	I	4	0	6	0	0
4	N	4	0	6	0	0
4	Q	4	0	6	0	0
4	R	4	0	6	0	0
5	A	139	0	0	0	0
5	B	157	0	0	0	0
5	C	246	0	0	2	0
5	D	199	0	0	1	0
5	E	221	0	0	0	0
5	F	275	0	0	0	0
5	G	192	0	0	0	0
5	H	150	0	0	1	0
5	I	176	0	0	0	0
5	J	217	0	0	0	0
5	K	206	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	200	0	0	0	0
5	M	288	0	0	0	0
5	N	269	0	0	0	0
5	O	185	0	0	0	0
5	P	212	0	0	0	0
5	Q	149	0	0	0	0
5	R	151	0	0	1	0
5	S	184	0	0	0	0
5	T	184	0	0	0	0
5	U	81	0	0	0	0
5	V	66	0	0	1	0
5	W	55	0	0	0	0
5	X	114	0	0	1	0
All	All	107004	0	99954	269	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 1.

All (269) 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:A:9:ALA:HB2	1:A:35:LEU:HD23	1.70	0.73
1:C:9:ALA:HB2	1:C:35:LEU:HD23	1.72	0.70
1:F:9:ALA:HB2	1:F:35:LEU:HD23	1.77	0.67
1:X:414:VAL:HG22	1:X:431:MET:HE1	1.77	0.66
1:W:215:VAL:HG13	1:W:219:LEU:HD22	1.80	0.64
1:K:467:ILE:HG21	3:K:602:TPP:S1	2.39	0.62
1:U:215:VAL:HG13	1:U:219:LEU:HD22	1.80	0.62
1:H:150:VAL:HG21	1:H:163:LEU:HG	1.82	0.62
3:E:602:TPP:H2	4:F:601:EDO:O2	2.00	0.61
1:J:150:VAL:HG21	1:J:163:LEU:HG	1.81	0.61
1:R:552:ARG:NH1	5:R:701:HOH:O	2.33	0.61
1:V:150:VAL:HG21	1:V:163:LEU:HG	1.83	0.61
1:B:9:ALA:HB2	1:B:35:LEU:HD23	1.82	0.61
1:M:189:VAL:HG11	1:M:325[A]:THR:HG21	1.84	0.59
1:K:150:VAL:HG21	1:K:163:LEU:HG	1.85	0.59
1:E:187:LEU:HD23	1:H:187:LEU:HD23	1.84	0.58
1:T:150:VAL:HG21	1:T:163:LEU:HG	1.85	0.58
1:M:9:ALA:HB2	1:M:35:LEU:HD23	1.84	0.58
1:C:234[B]:ARG:NH2	5:C:702:HOH:O	2.35	0.58
1:N:467:ILE:HG21	3:N:602:TPP:S1	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:414:VAL:HG22	1:T:431:MET:HE1	1.84	0.58
1:N:150:VAL:HG21	1:N:163:LEU:HG	1.85	0.57
1:S:215:VAL:HG13	1:S:219:LEU:HD22	1.87	0.57
1:R:9:ALA:HB2	1:R:35:LEU:HD23	1.88	0.56
1:J:467:ILE:CG2	3:J:602:TPP:S1	2.94	0.56
1:L:9:ALA:HB2	1:L:35:LEU:HD23	1.87	0.56
1:C:552:ARG:NH1	5:C:701:HOH:O	2.29	0.56
1:P:467:ILE:HG21	3:P:602:TPP:S1	2.46	0.56
1:V:215:VAL:HG13	1:V:219:LEU:HD22	1.87	0.56
1:K:9:ALA:HB2	1:K:35:LEU:HD23	1.87	0.56
1:O:150:VAL:HG21	1:O:163:LEU:HG	1.88	0.56
1:C:518:ASP:O	1:M:18:LYS:NZ	2.39	0.55
1:V:234:ARG:NH1	5:V:701:HOH:O	2.25	0.55
1:S:150:VAL:HG21	1:S:163:LEU:HG	1.89	0.55
1:N:9:ALA:HB2	1:N:35:LEU:HD23	1.89	0.54
1:I:9:ALA:HB2	1:I:35:LEU:HD23	1.90	0.54
1:S:24:ALA:HB2	1:T:476:TYR:HB2	1.89	0.54
1:J:9:ALA:HB2	1:J:35:LEU:HD23	1.90	0.54
1:K:467:ILE:CG2	3:K:602:TPP:S1	2.96	0.54
1:N:467:ILE:CG2	3:N:602:TPP:S1	2.96	0.54
1:F:150:VAL:HG21	1:F:163:LEU:HG	1.91	0.53
1:Q:215:VAL:HG13	1:Q:219:LEU:HD22	1.90	0.53
1:U:150:VAL:HG21	1:U:163:LEU:HG	1.89	0.53
1:V:355[A]:GLU:OE1	1:V:355[A]:GLU:N	2.26	0.53
1:A:150:VAL:HG21	1:A:163:LEU:HG	1.91	0.53
1:C:467:ILE:HG21	3:C:602:TPP:S1	2.49	0.53
1:E:9:ALA:HB2	1:E:35:LEU:HD23	1.90	0.53
1:W:150:VAL:HG21	1:W:163:LEU:HG	1.91	0.53
1:H:215:VAL:HG13	1:H:219:LEU:HD22	1.90	0.53
1:C:150:VAL:HG21	1:C:163:LEU:HG	1.89	0.53
1:E:388:PHE:HB3	1:E:536:THR:HG21	1.91	0.53
1:K:552[A]:ARG:NH1	5:K:701:HOH:O	2.42	0.53
1:H:467:ILE:HG21	3:H:602:TPP:S1	2.49	0.52
1:U:439:GLN:NE2	1:U:479:ILE:HD12	2.23	0.52
1:R:414:VAL:HG22	1:R:431:MET:HE1	1.90	0.52
1:R:467:ILE:HG21	3:R:602:TPP:S1	2.50	0.52
1:J:414:VAL:HG22	1:J:431:MET:HE1	1.91	0.52
1:F:15:ILE:HD11	1:F:151:ILE:HG23	1.91	0.52
1:F:73:SER:HG	1:F:122:TYR:HH	1.58	0.52
1:O:414:VAL:HG22	1:O:431:MET:HE1	1.91	0.51
1:U:218:LYS:HB2	1:U:283:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:552:ARG:NH1	5:X:702:HOH:O	2.44	0.51
1:N:218:LYS:HB2	1:N:283:ALA:HB1	1.92	0.51
1:M:467:ILE:HG21	3:M:602:TPP:S1	2.50	0.51
1:E:467:ILE:HG21	3:E:602:TPP:S1	2.51	0.50
1:G:218:LYS:HB2	1:G:283:ALA:HB1	1.93	0.50
1:R:467:ILE:CG2	3:R:602:TPP:S1	3.00	0.50
1:L:306:MET:HB3	1:L:323:LEU:HD13	1.93	0.50
1:F:218:LYS:HB2	1:F:283:ALA:HB1	1.93	0.50
1:M:467:ILE:CG2	3:M:602:TPP:S1	2.99	0.50
1:E:24:ALA:HB2	1:F:476:TYR:HB2	1.93	0.50
1:P:467:ILE:CG2	3:P:602:TPP:S1	2.99	0.50
1:V:88:ALA:HB1	1:V:406:GLN:HG3	1.92	0.50
1:B:15:ILE:HD11	1:B:151:ILE:HG23	1.94	0.50
1:P:215:VAL:HG13	1:P:219:LEU:HD22	1.93	0.50
1:U:69:ILE:N	1:U:69:ILE:HD12	2.26	0.49
1:E:15:ILE:HD11	1:E:151:ILE:HG23	1.93	0.49
1:H:218:LYS:HB2	1:H:283:ALA:HB1	1.94	0.49
1:S:476:TYR:HB2	1:T:24:ALA:HB2	1.95	0.49
1:X:516:ALA:HB2	1:X:524:THR:HG21	1.94	0.49
1:P:15:ILE:HD11	1:P:151:ILE:HG23	1.93	0.49
1:J:467:ILE:HG21	3:J:602:TPP:S1	2.53	0.49
1:B:499:LEU:HD22	1:B:501:LEU:HD21	1.95	0.49
1:A:69:ILE:N	1:A:69:ILE:HD12	2.27	0.49
1:R:489[B]:ASP:OD1	1:R:489[B]:ASP:N	2.45	0.49
1:M:15:ILE:HD11	1:M:151:ILE:HG23	1.95	0.49
1:O:467:ILE:CG2	3:O:602:TPP:S1	3.01	0.49
1:S:218:LYS:HB2	1:S:283:ALA:HB1	1.94	0.48
1:C:24:ALA:HB2	1:D:476:TYR:HB2	1.96	0.48
1:E:289:TYR:OH	4:F:601:EDO:H22	2.14	0.48
1:J:189:VAL:HG11	1:J:325:THR:HG21	1.96	0.48
1:V:218:LYS:HB2	1:V:283:ALA:HB1	1.95	0.48
1:D:467:ILE:HG21	3:D:602:TPP:S1	2.54	0.48
1:I:215:VAL:HG13	1:I:219:LEU:HD22	1.94	0.47
1:L:215:VAL:HG13	1:L:219:LEU:HD22	1.94	0.47
1:C:467:ILE:CG2	3:C:602:TPP:S1	3.02	0.47
1:G:69:ILE:N	1:G:69:ILE:HD12	2.30	0.47
1:H:467:ILE:CG2	3:H:602:TPP:S1	3.02	0.47
1:I:24:ALA:HB2	1:J:476:TYR:HB2	1.95	0.47
1:N:516:ALA:HB2	1:N:524:THR:HG21	1.96	0.47
1:K:218:LYS:HB2	1:K:283:ALA:HB1	1.96	0.47
1:E:222:ALA:HB2	1:E:308:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:9:ALA:HB2	1:T:35:LEU:HD23	1.97	0.47
1:L:218:LYS:HB2	1:L:283:ALA:HB1	1.97	0.46
1:V:69:ILE:N	1:V:69:ILE:HD12	2.31	0.46
1:B:306:MET:HB3	1:B:323:LEU:HD13	1.97	0.46
1:E:215:VAL:HG13	1:E:219:LEU:HD22	1.98	0.46
1:H:85:GLY:HA2	1:H:407:TRP:CG	2.51	0.46
1:D:355[A]:GLU:H	1:D:355[A]:GLU:CD	2.17	0.46
1:G:150:VAL:HG21	1:G:163:LEU:HG	1.98	0.46
1:H:15:ILE:HD11	1:H:151:ILE:HG23	1.96	0.46
1:F:64:GLY:O	1:F:92:PRO:HG2	2.16	0.46
1:C:218:LYS:HB2	1:C:283:ALA:HB1	1.98	0.46
1:G:45:TYR:CE1	1:H:476:TYR:HB3	2.50	0.46
1:V:414:VAL:HG22	1:V:431:MET:HE1	1.98	0.46
1:G:372:LEU:HB3	1:G:430[B]:ILE:HD11	1.97	0.46
1:W:516:ALA:HB2	1:W:524:THR:HG21	1.98	0.46
1:A:222:ALA:HB2	1:A:308:THR:HG22	1.98	0.46
1:E:388:PHE:CB	1:E:536:THR:HG21	2.45	0.46
1:F:349:LEU:HD11	1:F:351:ILE:HD12	1.98	0.46
1:O:431:MET:HE2	1:O:433:VAL:HB	1.97	0.46
1:E:467:ILE:CG2	3:E:602:TPP:S1	3.05	0.45
1:G:24:ALA:HB2	1:H:476:TYR:HB2	1.97	0.45
1:L:467:ILE:CG2	3:L:602:TPP:S1	3.04	0.45
1:R:127:VAL:HG11	1:R:162:TYR:CG	2.51	0.45
1:X:218:LYS:HB2	1:X:283:ALA:HB1	1.97	0.45
1:J:215:VAL:HG13	1:J:219:LEU:HD22	1.99	0.45
1:K:15:ILE:HD11	1:K:151:ILE:HG23	1.98	0.45
1:S:306:MET:HB3	1:S:323:LEU:HD13	1.99	0.45
1:W:69:ILE:N	1:W:69:ILE:HD12	2.31	0.45
1:D:467:ILE:CG2	3:D:602:TPP:S1	3.05	0.45
1:U:466:VAL:HA	1:U:469:ILE:HD12	1.98	0.45
1:V:9:ALA:HB2	1:V:35:LEU:HD23	1.99	0.45
1:G:306:MET:HB3	1:G:323:LEU:HD13	1.99	0.45
1:J:306:MET:HB3	1:J:323:LEU:HD13	1.99	0.45
1:L:150:VAL:HG21	1:L:163:LEU:HG	2.00	0.44
1:O:467:ILE:HG21	3:O:602:TPP:S1	2.57	0.44
1:V:143:ALA:HB3	1:V:144:PRO:HD3	1.99	0.44
1:X:467:ILE:HG21	3:X:602:TPP:S1	2.57	0.44
1:G:467:ILE:HG21	3:G:602:TPP:S1	2.58	0.44
1:M:476:TYR:HB2	1:N:24:ALA:HB2	1.99	0.44
1:V:330:LEU:O	1:V:334:ALA:HB2	2.18	0.44
1:W:29:LEU:HD13	1:X:472:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:467:ILE:CG2	3:G:602:TPP:S1	3.05	0.44
1:C:15:ILE:HG22	1:C:15:ILE:O	2.17	0.44
1:H:88:ALA:HB1	1:H:406:GLN:HG3	2.00	0.44
1:M:306:MET:HB3	1:M:323:LEU:HD13	2.00	0.44
1:U:467:ILE:HG21	3:U:602:TPP:S1	2.57	0.44
1:Q:467:ILE:HG21	3:Q:602:TPP:S1	2.58	0.44
1:R:88:ALA:HB1	1:R:406:GLN:HG3	1.98	0.44
1:X:306:MET:HB3	1:X:323:LEU:HD13	1.98	0.44
1:M:24:ALA:HB2	1:N:476:TYR:HB2	1.99	0.44
1:Q:141[A]:GLU:CD	1:Q:141[A]:GLU:H	2.21	0.44
1:E:85:GLY:HA2	1:E:407:TRP:CG	2.53	0.44
1:Q:476:TYR:HB2	1:R:24:ALA:HB2	1.98	0.44
1:U:288:ASP:HB3	1:U:294:TRP:CZ2	2.53	0.44
1:O:476:TYR:HB2	1:P:24:ALA:HB2	2.00	0.43
1:T:467:ILE:CG2	3:T:602:TPP:S1	3.07	0.43
1:W:12:LEU:HA	1:W:15:ILE:HD12	2.00	0.43
1:W:476:TYR:HB2	1:X:24:ALA:HB2	2.00	0.43
1:E:180:ILE:O	1:E:180:ILE:HD12	2.18	0.43
1:D:325[A]:THR:HG23	5:D:806:HOH:O	2.18	0.43
1:K:69:ILE:HD12	1:K:69:ILE:N	2.33	0.43
1:U:189:VAL:HG13	1:U:321:LEU:HA	2.01	0.43
1:W:239:VAL:HG11	1:W:249:PHE:CE2	2.54	0.43
1:C:467:ILE:HG13	1:C:539:LEU:HD11	1.99	0.43
1:V:414:VAL:HG22	1:V:431:MET:CE	2.49	0.43
1:A:418:PHE:O	1:A:422:VAL:HG23	2.19	0.43
1:D:306:MET:HB3	1:D:323:LEU:HD13	2.01	0.43
1:X:453:ILE:HG22	1:X:455:VAL:HG23	2.00	0.43
1:A:476:TYR:HB2	1:B:24:ALA:HB2	2.01	0.43
1:B:73:SER:HB2	1:B:113:HIS:O	2.19	0.43
1:B:218:LYS:HB2	1:B:283:ALA:HB1	2.01	0.43
1:B:215:VAL:HG13	1:B:219:LEU:HD22	2.00	0.43
1:I:430:ILE:CD1	1:I:456:ILE:HD12	2.49	0.43
1:N:251:GLU:HG3	1:N:256:PHE:CE2	2.54	0.43
1:S:222:ALA:HB2	1:S:308:THR:HG22	1.99	0.43
1:T:127:VAL:HG11	1:T:162:TYR:CG	2.54	0.43
1:A:189:VAL:HG11	1:A:325:THR:HG21	2.01	0.43
1:B:180:ILE:O	1:B:180:ILE:HD12	2.19	0.43
1:G:476:TYR:HB2	1:H:24:ALA:HB2	2.01	0.43
1:P:306:MET:HB3	1:P:323:LEU:HD13	2.00	0.43
1:T:414:VAL:HG22	1:T:431:MET:CE	2.47	0.43
1:V:355[A]:GLU:H	1:V:355[A]:GLU:CD	2.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:VAL:HG13	1:F:219:LEU:HD22	2.01	0.42
1:L:222:ALA:HB2	1:L:308:THR:HG22	2.01	0.42
1:D:88:ALA:HB1	1:D:406:GLN:HG3	2.00	0.42
1:D:9:ALA:HB2	1:D:35:LEU:HD23	2.01	0.42
1:G:9:ALA:HB2	1:G:35:LEU:HD23	2.01	0.42
1:K:476:TYR:HB2	1:L:24:ALA:HB2	2.00	0.42
1:M:218:LYS:HB2	1:M:283:ALA:HB1	2.00	0.42
1:M:64:GLY:O	1:M:92:PRO:HG2	2.19	0.42
1:P:516:ALA:HB2	1:P:524:THR:HG21	2.01	0.42
1:C:288:ASP:HB3	1:C:294:TRP:CZ2	2.55	0.42
1:A:29:LEU:HD13	1:B:472:HIS:HB3	2.00	0.42
1:L:467:ILE:HG21	3:L:602:TPP:S1	2.60	0.42
1:F:15:ILE:HD11	1:F:151:ILE:CG2	2.49	0.42
1:I:189:VAL:HG11	1:I:325[A]:THR:HG21	2.02	0.42
1:K:24:ALA:HB2	1:L:476:TYR:HB2	2.01	0.42
1:R:15:ILE:HG22	1:R:15:ILE:O	2.19	0.42
1:K:414:VAL:HG22	1:K:431:MET:HE1	2.01	0.42
1:N:99:SER:HB2	1:N:100:PRO:CD	2.50	0.42
1:Q:467:ILE:CG2	3:Q:602:TPP:S1	3.07	0.42
1:I:69:ILE:HD12	1:I:69:ILE:N	2.34	0.42
1:O:9:ALA:HB2	1:O:35:LEU:HD23	2.02	0.42
1:W:467:ILE:HG21	3:W:602:TPP:S1	2.59	0.42
1:X:467:ILE:CG2	3:X:602:TPP:S1	3.08	0.42
1:C:15:ILE:HD11	1:C:151:ILE:HG23	2.02	0.42
1:N:85:GLY:HA2	1:N:407:TRP:CG	2.55	0.42
1:P:88:ALA:HB1	1:P:406:GLN:HG3	2.02	0.42
1:X:467:ILE:HG13	1:X:539:LEU:HD11	2.01	0.42
3:I:602:TPP:N1'	1:J:49:GLU:OE2	2.53	0.42
1:O:29:LEU:HD13	1:P:472:HIS:HB3	2.02	0.42
1:W:460:ILE:N	1:W:460:ILE:HD12	2.35	0.42
1:E:467:ILE:HG22	3:E:602:TPP:O3B	2.20	0.41
1:E:481:ASN:ND2	1:F:493:ASP:OD2	2.51	0.41
1:N:64:GLY:O	1:N:92:PRO:HG2	2.20	0.41
1:Q:141[A]:GLU:CD	1:Q:141[A]:GLU:N	2.73	0.41
1:E:476:TYR:HB2	1:F:24:ALA:HB2	2.01	0.41
1:X:88:ALA:HB1	1:X:406:GLN:HG3	2.02	0.41
1:H:239:VAL:HG11	1:H:249:PHE:CE1	2.56	0.41
3:G:602:TPP:N1'	1:H:49:GLU:OE2	2.54	0.41
1:I:180:ILE:HD12	1:I:180:ILE:O	2.20	0.41
1:K:15:ILE:HG22	1:K:15:ILE:O	2.18	0.41
1:D:218:LYS:HB2	1:D:283:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:ILE:HD11	1:M:151:ILE:CG2	2.51	0.41
1:Q:45:TYR:CE1	1:R:476:TYR:HB3	2.56	0.41
1:U:476:TYR:HB2	1:V:24:ALA:HB2	2.03	0.41
1:B:118:THR:HG21	1:D:142:GLU:OE1	2.20	0.41
1:F:467:ILE:CG2	3:F:603:TPP:S1	3.09	0.41
1:M:516:ALA:HB2	1:M:524:THR:HG21	2.02	0.41
1:P:222:ALA:HB2	1:P:308:THR:HG22	2.02	0.41
1:H:405[A]:MET:CE	5:H:839:HOH:O	2.69	0.41
1:H:414:VAL:HG22	1:H:431:MET:HE1	2.02	0.41
1:I:306:MET:HB3	1:I:323:LEU:HD13	2.03	0.41
1:M:467:ILE:HG13	1:M:539:LEU:HD11	2.01	0.41
1:R:466:VAL:HA	1:R:469:ILE:HD12	2.03	0.41
1:E:150:VAL:HG21	1:E:163:LEU:HG	2.02	0.41
1:I:204:TRP:CD1	1:I:314:ALA:HB2	2.55	0.41
1:O:69:ILE:N	1:O:69:ILE:HD12	2.35	0.41
1:H:405[A]:MET:HB3	1:H:405[A]:MET:HE2	1.72	0.41
1:L:204:TRP:CD1	1:L:314:ALA:HB2	2.55	0.41
1:O:24:ALA:HB2	1:P:476:TYR:HB2	2.02	0.41
1:A:187:LEU:HD23	1:D:187:LEU:HD23	2.02	0.41
1:G:234:ARG:HG2	1:G:331:ALA:O	2.21	0.41
1:I:467:ILE:HG21	3:I:602:TPP:S1	2.61	0.41
1:L:127:VAL:HG11	1:L:162:TYR:CG	2.56	0.41
1:U:129:HIS:HB3	1:V:122:TYR:HB2	2.02	0.41
1:A:467:ILE:CG2	3:A:602:TPP:S1	3.09	0.41
1:G:215:VAL:HB	1:G:241:ILE:HG22	2.03	0.41
1:J:88:ALA:HB1	1:J:406:GLN:HG3	2.03	0.41
1:A:118:THR:HG21	1:C:142:GLU:OE1	2.21	0.40
1:T:467:ILE:HG13	1:T:539:LEU:HD11	2.02	0.40
1:U:426[B]:GLU:CD	1:U:426[B]:GLU:H	2.23	0.40
1:C:45:TYR:CE1	1:D:476:TYR:HB3	2.56	0.40
1:F:460:ILE:HD12	1:F:460:ILE:N	2.37	0.40
1:G:12:LEU:HA	1:G:15:ILE:HD12	2.03	0.40
1:H:15:ILE:HD11	1:H:151:ILE:CG2	2.51	0.40
1:O:218:LYS:HB2	1:O:283:ALA:HB1	2.03	0.40
1:U:426[A]:GLU:HA	1:U:426[A]:GLU:OE1	2.20	0.40
1:C:127:VAL:HG11	1:C:162:TYR:CG	2.56	0.40
1:J:516:ALA:HB2	1:J:524:THR:HG21	2.04	0.40
1:T:85:GLY:HA2	1:T:407:TRP:CG	2.56	0.40
1:I:88:ALA:HB1	1:I:406:GLN:HG3	2.04	0.40
1:J:467:ILE:HG13	1:J:539:LEU:HD11	2.04	0.40
1:K:85:GLY:HA2	1:K:407:TRP:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:45:TYR:CE1	1:N:476:TYR:HB3	2.56	0.40
1:Q:69:ILE:N	1:Q:69:ILE:HD12	2.36	0.40
1:X:150:VAL:HG21	1:X:163:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	558/573 (97%)	551 (99%)	7 (1%)	0	100	100
1	B	557/573 (97%)	547 (98%)	10 (2%)	0	100	100
1	C	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	D	558/573 (97%)	548 (98%)	10 (2%)	0	100	100
1	E	557/573 (97%)	550 (99%)	7 (1%)	0	100	100
1	F	562/573 (98%)	552 (98%)	10 (2%)	0	100	100
1	G	560/573 (98%)	552 (99%)	7 (1%)	1 (0%)	52	51
1	H	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	I	559/573 (98%)	549 (98%)	10 (2%)	0	100	100
1	J	557/573 (97%)	546 (98%)	10 (2%)	1 (0%)	52	51
1	K	560/573 (98%)	554 (99%)	5 (1%)	1 (0%)	52	51
1	L	562/573 (98%)	550 (98%)	12 (2%)	0	100	100
1	M	560/573 (98%)	548 (98%)	11 (2%)	1 (0%)	52	51
1	N	560/573 (98%)	554 (99%)	6 (1%)	0	100	100
1	O	556/573 (97%)	546 (98%)	9 (2%)	1 (0%)	52	51
1	P	560/573 (98%)	549 (98%)	11 (2%)	0	100	100
1	Q	558/573 (97%)	547 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	561/573 (98%)	553 (99%)	8 (1%)	0	100	100
1	S	555/573 (97%)	545 (98%)	10 (2%)	0	100	100
1	T	557/573 (97%)	548 (98%)	9 (2%)	0	100	100
1	U	557/573 (97%)	536 (96%)	21 (4%)	0	100	100
1	V	557/573 (97%)	536 (96%)	21 (4%)	0	100	100
1	W	556/573 (97%)	537 (97%)	19 (3%)	0	100	100
1	X	556/573 (97%)	545 (98%)	11 (2%)	0	100	100
All	All	13401/13752 (97%)	13141 (98%)	255 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	73	SER
1	K	73	SER
1	O	73	SER
1	M	73	SER
1	G	73	SER

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	440/448 (98%)	424 (96%)	16 (4%)	42	40
1	B	439/448 (98%)	430 (98%)	9 (2%)	61	65
1	C	441/448 (98%)	432 (98%)	9 (2%)	63	67
1	D	440/448 (98%)	429 (98%)	11 (2%)	55	58
1	E	439/448 (98%)	431 (98%)	8 (2%)	66	71
1	F	444/448 (99%)	432 (97%)	12 (3%)	52	53
1	G	442/448 (99%)	432 (98%)	10 (2%)	58	62
1	H	441/448 (98%)	429 (97%)	12 (3%)	52	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	441/448 (98%)	433 (98%)	8 (2%)	66 71
1	J	439/448 (98%)	430 (98%)	9 (2%)	61 65
1	K	442/448 (99%)	429 (97%)	13 (3%)	50 49
1	L	444/448 (99%)	433 (98%)	11 (2%)	55 58
1	M	442/448 (99%)	430 (97%)	12 (3%)	52 53
1	N	442/448 (99%)	433 (98%)	9 (2%)	63 67
1	O	438/448 (98%)	428 (98%)	10 (2%)	58 62
1	P	442/448 (99%)	431 (98%)	11 (2%)	55 58
1	Q	440/448 (98%)	429 (98%)	11 (2%)	55 58
1	R	443/448 (99%)	430 (97%)	13 (3%)	50 49
1	S	437/448 (98%)	427 (98%)	10 (2%)	58 62
1	T	439/448 (98%)	429 (98%)	10 (2%)	58 62
1	U	439/448 (98%)	425 (97%)	14 (3%)	46 45
1	V	439/448 (98%)	428 (98%)	11 (2%)	55 58
1	W	438/448 (98%)	424 (97%)	14 (3%)	46 45
1	X	438/448 (98%)	429 (98%)	9 (2%)	61 65
All	All	10569/10752 (98%)	10307 (98%)	262 (2%)	58 58

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	57	GLU
1	A	183	LEU
1	A	207	ASP
1	A	271	GLU
1	A	272	LEU
1	A	319	GLU
1	A	332	GLU
1	A	379	LEU
1	A	391[A]	SER
1	A	391[B]	SER
1	A	444	GLU
1	A	499	LEU
1	A	517	LEU
1	A	552[A]	ARG

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Mol	Chain	Res	Type
1	A	552[B]	ARG
1	B	39	LYS
1	B	234	ARG
1	B	272	LEU
1	B	319	GLU
1	B	376	ASP
1	B	379	LEU
1	B	431	MET
1	B	499	LEU
1	B	517	LEU
1	C	183	LEU
1	C	271	GLU
1	C	272	LEU
1	C	301	ASP
1	C	319	GLU
1	C	345	GLN
1	C	379	LEU
1	C	489	ASP
1	C	517	LEU
1	D	183	LEU
1	D	271	GLU
1	D	272	LEU
1	D	319	GLU
1	D	332	GLU
1	D	345	GLN
1	D	379	LEU
1	D	444	GLU
1	D	495	ASP
1	D	504	SER
1	D	517	LEU
1	E	271	GLU
1	E	272	LEU
1	E	319	GLU
1	E	332	GLU
1	E	379	LEU
1	E	499	LEU
1	E	517	LEU
1	E	536	THR
1	F	39	LYS
1	F	73	SER
1	F	183	LEU
1	F	271	GLU

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Mol	Chain	Res	Type
1	F	272	LEU
1	F	319	GLU
1	F	379	LEU
1	F	459	LEU
1	F	494	GLU
1	F	517	LEU
1	F	552[A]	ARG
1	F	552[B]	ARG
1	G	183	LEU
1	G	271	GLU
1	G	272	LEU
1	G	319	GLU
1	G	332	GLU
1	G	379	LEU
1	G	444	GLU
1	G	495	ASP
1	G	499	LEU
1	G	517	LEU
1	H	183	LEU
1	H	271	GLU
1	H	272	LEU
1	H	319	GLU
1	H	332	GLU
1	H	352	GLU
1	H	379	LEU
1	H	391[A]	SER
1	H	391[B]	SER
1	H	495[A]	ASP
1	H	495[B]	ASP
1	H	517	LEU
1	I	121[A]	ASN
1	I	121[B]	ASN
1	I	183	LEU
1	I	272	LEU
1	I	319	GLU
1	I	379	LEU
1	I	517	LEU
1	I	552	ARG
1	J	1	MET
1	J	183	LEU
1	J	271	GLU
1	J	272	LEU

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Mol	Chain	Res	Type
1	J	299	LYS
1	J	319	GLU
1	J	379	LEU
1	J	459	LEU
1	J	517	LEU
1	K	57	GLU
1	K	183	LEU
1	K	271	GLU
1	K	272	LEU
1	K	319	GLU
1	K	333	LYS
1	K	379	LEU
1	K	391[A]	SER
1	K	391[B]	SER
1	K	499	LEU
1	K	517	LEU
1	K	552[A]	ARG
1	K	552[B]	ARG
1	L	120	TYR
1	L	183	LEU
1	L	271	GLU
1	L	272	LEU
1	L	319	GLU
1	L	379	LEU
1	L	459	LEU
1	L	499	LEU
1	L	517	LEU
1	L	552[A]	ARG
1	L	552[B]	ARG
1	M	39	LYS
1	M	57	GLU
1	M	181	ASN
1	M	272	LEU
1	M	319	GLU
1	M	332	GLU
1	M	379	LEU
1	M	431	MET
1	M	444	GLU
1	M	489	ASP
1	M	517	LEU
1	M	553	LYS
1	N	39	LYS

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Mol	Chain	Res	Type
1	N	183	LEU
1	N	271	GLU
1	N	272	LEU
1	N	319	GLU
1	N	332	GLU
1	N	379	LEU
1	N	444	GLU
1	N	517	LEU
1	O	18	LYS
1	O	173	GLU
1	O	183	LEU
1	O	271	GLU
1	O	272	LEU
1	O	311	VAL
1	O	319	GLU
1	O	379	LEU
1	O	517	LEU
1	O	553	LYS
1	P	272	LEU
1	P	319	GLU
1	P	345	GLN
1	P	379	LEU
1	P	391[A]	SER
1	P	391[B]	SER
1	P	444	GLU
1	P	459	LEU
1	P	499	LEU
1	P	517	LEU
1	P	537	GLU
1	Q	18	LYS
1	Q	42[A]	GLU
1	Q	42[B]	GLU
1	Q	73	SER
1	Q	163	LEU
1	Q	319	GLU
1	Q	332	GLU
1	Q	379	LEU
1	Q	391[A]	SER
1	Q	391[B]	SER
1	Q	517	LEU
1	R	121[A]	ASN
1	R	121[B]	ASN

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Mol	Chain	Res	Type
1	R	173	GLU
1	R	183	LEU
1	R	272	LEU
1	R	319	GLU
1	R	332	GLU
1	R	379	LEU
1	R	459	LEU
1	R	499	LEU
1	R	517	LEU
1	R	533	ASP
1	R	552	ARG
1	S	121	ASN
1	S	226	LYS
1	S	271	GLU
1	S	272	LEU
1	S	319	GLU
1	S	332	GLU
1	S	379	LEU
1	S	391[A]	SER
1	S	391[B]	SER
1	S	517	LEU
1	T	271	GLU
1	T	272	LEU
1	T	319	GLU
1	T	379	LEU
1	T	391[A]	SER
1	T	391[B]	SER
1	T	443	GLN
1	T	489	ASP
1	T	499	LEU
1	T	517	LEU
1	U	78	SER
1	U	121	ASN
1	U	271	GLU
1	U	272	LEU
1	U	299	LYS
1	U	302	ASN
1	U	319	GLU
1	U	355[A]	GLU
1	U	355[B]	GLU
1	U	365	MET
1	U	379	LEU

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Mol	Chain	Res	Type
1	U	444	GLU
1	U	459	LEU
1	U	521	ARG
1	V	121	ASN
1	V	272	LEU
1	V	319	GLU
1	V	332	GLU
1	V	379	LEU
1	V	391[A]	SER
1	V	391[B]	SER
1	V	499	LEU
1	V	515	LYS
1	V	517	LEU
1	V	552	ARG
1	W	57	GLU
1	W	121	ASN
1	W	259	LEU
1	W	271	GLU
1	W	319	GLU
1	W	332	GLU
1	W	363	ASP
1	W	376	ASP
1	W	391[A]	SER
1	W	391[B]	SER
1	W	443	GLN
1	W	494	GLU
1	W	499	LEU
1	W	517	LEU
1	X	57	GLU
1	X	226	LYS
1	X	234	ARG
1	X	319	GLU
1	X	332	GLU
1	X	379	LEU
1	X	391[A]	SER
1	X	391[B]	SER
1	X	552	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	34	GLN

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Mol	Chain	Res	Type
1	M	181	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

Of 54 ligands modelled in this entry, 24 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
3	TPP	A	602	2	20,27,27	1.39	2 (10%)	27,40,40	1.89	8 (29%)
4	EDO	A	603	-	3,3,3	0.58	0	2,2,2	0.25	0
3	TPP	B	602	2	20,27,27	1.47	2 (10%)	27,40,40	1.70	4 (14%)
3	TPP	C	602	2	20,27,27	1.58	2 (10%)	27,40,40	1.60	5 (18%)
3	TPP	D	602	2	20,27,27	1.67	3 (15%)	27,40,40	1.69	7 (25%)
3	TPP	E	602	2	20,27,27	1.84	2 (10%)	27,40,40	1.58	6 (22%)
4	EDO	F	601	-	3,3,3	0.47	0	2,2,2	0.26	0
3	TPP	F	603	2	20,27,27	1.72	2 (10%)	27,40,40	1.65	7 (25%)
3	TPP	G	602	2	20,27,27	1.58	2 (10%)	27,40,40	1.67	5 (18%)
3	TPP	H	602	2	20,27,27	1.66	2 (10%)	27,40,40	1.51	4 (14%)
3	TPP	I	602	2	20,27,27	1.67	2 (10%)	27,40,40	1.81	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	I	603	-	3,3,3	0.51	0	2,2,2	0.23	0
3	TPP	J	602	2	20,27,27	1.70	2 (10%)	27,40,40	1.81	8 (29%)
3	TPP	K	602	2	20,27,27	1.53	2 (10%)	27,40,40	1.62	6 (22%)
3	TPP	L	602	2	20,27,27	1.58	2 (10%)	27,40,40	1.68	5 (18%)
3	TPP	M	602	2	20,27,27	1.86	2 (10%)	27,40,40	1.63	8 (29%)
3	TPP	N	602	2	20,27,27	1.92	3 (15%)	27,40,40	1.68	6 (22%)
4	EDO	N	603	-	3,3,3	0.47	0	2,2,2	0.40	0
3	TPP	O	602	2	20,27,27	1.53	2 (10%)	27,40,40	1.58	4 (14%)
3	TPP	P	602	2	20,27,27	1.60	2 (10%)	27,40,40	1.59	4 (14%)
3	TPP	Q	602	2	20,27,27	1.56	2 (10%)	27,40,40	1.73	5 (18%)
4	EDO	Q	603	-	3,3,3	0.47	0	2,2,2	0.09	0
3	TPP	R	602	2	20,27,27	1.77	2 (10%)	27,40,40	1.72	6 (22%)
4	EDO	R	603	-	3,3,3	0.55	0	2,2,2	0.05	0
3	TPP	S	602	2	20,27,27	1.60	2 (10%)	27,40,40	1.82	6 (22%)
3	TPP	T	602	2	20,27,27	1.69	2 (10%)	27,40,40	1.72	6 (22%)
3	TPP	U	602	2	20,27,27	1.42	2 (10%)	27,40,40	1.96	8 (29%)
3	TPP	V	602	2	20,27,27	1.51	2 (10%)	27,40,40	1.81	7 (25%)
3	TPP	W	602	2	20,27,27	1.44	2 (10%)	27,40,40	1.79	8 (29%)
3	TPP	X	602	2	20,27,27	1.55	2 (10%)	27,40,40	1.87	7 (25%)

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	TPP	A	602	2	-	0/16/17/17	0/2/2/2
4	EDO	A	603	-	-	0/1/1/1	0/0/0/0
3	TPP	B	602	2	-	0/16/17/17	0/2/2/2
3	TPP	C	602	2	-	0/16/17/17	0/2/2/2
3	TPP	D	602	2	-	0/16/17/17	0/2/2/2
3	TPP	E	602	2	-	0/16/17/17	0/2/2/2
4	EDO	F	601	-	-	0/1/1/1	0/0/0/0
3	TPP	F	603	2	-	0/16/17/17	0/2/2/2
3	TPP	G	602	2	-	0/16/17/17	0/2/2/2
3	TPP	H	602	2	-	0/16/17/17	0/2/2/2
3	TPP	I	602	2	-	0/16/17/17	0/2/2/2
4	EDO	I	603	-	-	0/1/1/1	0/0/0/0
3	TPP	J	602	2	-	0/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	K	602	2	-	0/16/17/17	0/2/2/2
3	TPP	L	602	2	-	0/16/17/17	0/2/2/2
3	TPP	M	602	2	-	0/16/17/17	0/2/2/2
3	TPP	N	602	2	-	0/16/17/17	0/2/2/2
4	EDO	N	603	-	-	0/1/1/1	0/0/0/0
3	TPP	O	602	2	-	0/16/17/17	0/2/2/2
3	TPP	P	602	2	-	0/16/17/17	0/2/2/2
3	TPP	Q	602	2	-	0/16/17/17	0/2/2/2
4	EDO	Q	603	-	-	0/1/1/1	0/0/0/0
3	TPP	R	602	2	-	0/16/17/17	0/2/2/2
4	EDO	R	603	-	-	0/1/1/1	0/0/0/0
3	TPP	S	602	2	-	0/16/17/17	0/2/2/2
3	TPP	T	602	2	-	0/16/17/17	0/2/2/2
3	TPP	U	602	2	-	0/16/17/17	0/2/2/2
3	TPP	V	602	2	-	0/16/17/17	0/2/2/2
3	TPP	W	602	2	-	0/16/17/17	0/2/2/2
3	TPP	X	602	2	-	0/16/17/17	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	TPP	C4-N3	-6.95	1.33	1.39
3	N	602	TPP	C4-N3	-6.70	1.33	1.39
3	M	602	TPP	C4-N3	-6.31	1.34	1.39
3	R	602	TPP	C4-N3	-6.11	1.34	1.39
3	H	602	TPP	C4-N3	-6.01	1.34	1.39
3	J	602	TPP	C4-N3	-5.96	1.34	1.39
3	I	602	TPP	C4-N3	-5.88	1.34	1.39
3	P	602	TPP	C4-N3	-5.75	1.34	1.39
3	C	602	TPP	C4-N3	-5.70	1.34	1.39
3	D	602	TPP	C4-N3	-5.69	1.34	1.39
3	F	603	TPP	C4-N3	-5.66	1.34	1.39
3	Q	602	TPP	C4-N3	-5.62	1.34	1.39
3	G	602	TPP	C4-N3	-5.55	1.34	1.39
3	T	602	TPP	C4-N3	-5.54	1.34	1.39
3	L	602	TPP	C4-N3	-5.37	1.35	1.39
3	O	602	TPP	C4-N3	-5.00	1.35	1.39
3	S	602	TPP	C4-N3	-4.99	1.35	1.39
3	B	602	TPP	C4-N3	-4.92	1.35	1.39
3	V	602	TPP	C4-N3	-4.87	1.35	1.39
3	X	602	TPP	C4-N3	-4.83	1.35	1.39
3	K	602	TPP	C4-N3	-4.68	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	602	TPP	C4-N3	-4.59	1.35	1.39
3	W	602	TPP	C4-N3	-4.49	1.35	1.39
3	A	602	TPP	C4-N3	-3.81	1.36	1.39
3	N	602	TPP	PB-O2B	-2.40	1.46	1.54
3	D	602	TPP	PB-O3B	-2.04	1.47	1.54
3	P	602	TPP	C5'-C4'	3.12	1.48	1.42
3	C	602	TPP	C5'-C4'	3.23	1.48	1.42
3	E	602	TPP	C5'-C4'	3.23	1.48	1.42
3	H	602	TPP	C5'-C4'	3.29	1.48	1.42
3	Q	602	TPP	C5'-C4'	3.45	1.48	1.42
3	G	602	TPP	C5'-C4'	3.45	1.48	1.42
3	U	602	TPP	C5'-C4'	3.50	1.48	1.42
3	B	602	TPP	C5'-C4'	3.55	1.48	1.42
3	J	602	TPP	C5'-C4'	3.62	1.49	1.42
3	L	602	TPP	C5'-C4'	3.63	1.49	1.42
3	I	602	TPP	C5'-C4'	3.65	1.49	1.42
3	V	602	TPP	C5'-C4'	3.72	1.49	1.42
3	O	602	TPP	C5'-C4'	3.78	1.49	1.42
3	N	602	TPP	C5'-C4'	3.79	1.49	1.42
3	D	602	TPP	C5'-C4'	3.83	1.49	1.42
3	S	602	TPP	C5'-C4'	3.85	1.49	1.42
3	W	602	TPP	C5'-C4'	3.86	1.49	1.42
3	R	602	TPP	C5'-C4'	3.86	1.49	1.42
3	T	602	TPP	C5'-C4'	3.88	1.49	1.42
3	X	602	TPP	C5'-C4'	3.92	1.49	1.42
3	F	603	TPP	C5'-C4'	3.96	1.49	1.42
3	K	602	TPP	C5'-C4'	3.98	1.49	1.42
3	A	602	TPP	C5'-C4'	4.13	1.49	1.42
3	M	602	TPP	C5'-C4'	4.34	1.50	1.42

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	602	TPP	C6-C5-S1	-4.96	113.29	120.24
3	I	602	TPP	C6-C5-S1	-4.86	113.44	120.24
3	X	602	TPP	C6-C5-S1	-4.46	114.00	120.24
3	N	602	TPP	C6-C5-S1	-4.35	114.15	120.24
3	B	602	TPP	C6-C5-S1	-4.30	114.22	120.24
3	S	602	TPP	C6-C5-S1	-4.23	114.31	120.24
3	A	602	TPP	C6-C5-S1	-4.10	114.50	120.24
3	V	602	TPP	C6-C5-S1	-4.08	114.53	120.24
3	G	602	TPP	C6-C5-S1	-4.06	114.55	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	602	TPP	C6-C5-S1	-4.03	114.60	120.24
3	R	602	TPP	C6-C5-S1	-4.02	114.62	120.24
3	Q	602	TPP	C6-C5-S1	-4.01	114.62	120.24
3	T	602	TPP	C6-C5-S1	-3.95	114.71	120.24
3	P	602	TPP	C6-C5-S1	-3.72	115.03	120.24
3	J	602	TPP	C6-C5-S1	-3.72	115.04	120.24
3	O	602	TPP	C6-C5-S1	-3.72	115.04	120.24
3	L	602	TPP	C6-C5-S1	-3.69	115.07	120.24
3	M	602	TPP	C6-C5-S1	-3.65	115.13	120.24
3	F	603	TPP	C6-C5-S1	-3.51	115.33	120.24
3	C	602	TPP	C6-C5-S1	-3.38	115.51	120.24
3	A	602	TPP	CM4-C4-C5	-3.33	121.85	128.91
3	D	602	TPP	C6-C5-S1	-3.23	115.72	120.24
3	H	602	TPP	C6-C5-S1	-3.21	115.75	120.24
3	K	602	TPP	C6-C5-S1	-3.01	116.02	120.24
3	D	602	TPP	CM4-C4-C5	-2.98	122.61	128.91
3	J	602	TPP	CM4-C4-C5	-2.95	122.66	128.91
3	C	602	TPP	N1'-C2'-N3'	-2.91	120.04	125.50
3	W	602	TPP	CM4-C4-C5	-2.90	122.76	128.91
3	W	602	TPP	C6-C5-S1	-2.87	116.22	120.24
3	K	602	TPP	N1'-C2'-N3'	-2.74	120.37	125.50
3	X	602	TPP	N1'-C2'-N3'	-2.67	120.48	125.50
3	N	602	TPP	N1'-C2'-N3'	-2.60	120.62	125.50
3	U	602	TPP	N1'-C2'-N3'	-2.60	120.63	125.50
3	R	602	TPP	N1'-C2'-N3'	-2.57	120.68	125.50
3	L	602	TPP	N1'-C2'-N3'	-2.54	120.73	125.50
3	D	602	TPP	N1'-C2'-N3'	-2.54	120.73	125.50
3	H	602	TPP	N1'-C2'-N3'	-2.54	120.74	125.50
3	J	602	TPP	N1'-C2'-N3'	-2.53	120.75	125.50
3	V	602	TPP	N1'-C2'-N3'	-2.52	120.77	125.50
3	P	602	TPP	N1'-C2'-N3'	-2.51	120.78	125.50
3	W	602	TPP	N1'-C2'-N3'	-2.51	120.79	125.50
3	E	602	TPP	N1'-C2'-N3'	-2.50	120.82	125.50
3	M	602	TPP	N1'-C2'-N3'	-2.49	120.82	125.50
3	G	602	TPP	N1'-C2'-N3'	-2.48	120.86	125.50
3	I	602	TPP	N1'-C2'-N3'	-2.47	120.87	125.50
3	T	602	TPP	N1'-C2'-N3'	-2.43	120.93	125.50
3	F	603	TPP	CM4-C4-C5	-2.42	123.79	128.91
3	F	603	TPP	N1'-C2'-N3'	-2.40	120.99	125.50
3	B	602	TPP	N1'-C2'-N3'	-2.36	121.08	125.50
3	Q	602	TPP	N1'-C2'-N3'	-2.33	121.12	125.50
3	S	602	TPP	N1'-C2'-N3'	-2.30	121.18	125.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	602	TPP	C5'-C6'-N1'	-2.27	119.89	123.86
3	F	603	TPP	C5'-C6'-N1'	-2.23	119.96	123.86
3	A	602	TPP	N1'-C2'-N3'	-2.22	121.34	125.50
3	O	602	TPP	N1'-C2'-N3'	-2.21	121.35	125.50
3	I	602	TPP	C5'-C6'-N1'	-2.21	120.00	123.86
3	M	602	TPP	CM4-C4-C5	-2.20	124.25	128.91
3	E	602	TPP	C5'-C6'-N1'	-2.18	120.06	123.86
3	X	602	TPP	CM4-C4-C5	-2.14	124.38	128.91
3	S	602	TPP	CM4-C4-C5	-2.14	124.38	128.91
3	K	602	TPP	CM4-C4-C5	-2.10	124.47	128.91
3	J	602	TPP	C5'-C6'-N1'	-2.10	120.19	123.86
3	D	602	TPP	C5'-C6'-N1'	-2.08	120.23	123.86
3	U	602	TPP	C5'-C6'-N1'	-2.07	120.24	123.86
3	A	602	TPP	C5'-C6'-N1'	-2.07	120.25	123.86
3	T	602	TPP	C5'-C6'-N1'	-2.06	120.25	123.86
3	J	602	TPP	C6-C5-C4	2.00	129.59	127.34
3	Q	602	TPP	O2A-PA-O3A	2.01	113.88	105.27
3	A	602	TPP	CM2-C2'-N1'	2.01	119.53	117.05
3	V	602	TPP	O3B-PB-O2B	2.03	114.91	107.44
3	U	602	TPP	CM2-C2'-N1'	2.09	119.62	117.05
3	M	602	TPP	CM4-C4-N3	2.13	125.04	122.43
3	C	602	TPP	CM2-C2'-N1'	2.13	119.68	117.05
3	N	602	TPP	C6-C5-C4	2.14	129.74	127.34
3	F	603	TPP	CM2-C2'-N1'	2.14	119.69	117.05
3	J	602	TPP	CM2-C2'-N1'	2.15	119.70	117.05
3	W	602	TPP	O3B-PB-O2B	2.16	115.36	107.44
3	E	602	TPP	C6-C5-C4	2.18	129.79	127.34
3	G	602	TPP	CM2-C2'-N1'	2.26	119.83	117.05
3	M	602	TPP	C6-C5-C4	2.28	129.90	127.34
3	U	602	TPP	CM4-C4-N3	2.28	125.23	122.43
3	X	602	TPP	CM4-C4-N3	2.31	125.26	122.43
3	R	602	TPP	O2A-PA-O3A	2.32	115.22	105.27
3	H	602	TPP	O2A-PA-O3A	2.33	115.25	105.27
3	R	602	TPP	O3B-PB-O2B	2.36	116.10	107.44
3	U	602	TPP	O3B-PB-O2B	2.37	116.14	107.44
3	M	602	TPP	O3B-PB-O2B	2.49	116.59	107.44
3	W	602	TPP	CM2-C2'-N1'	2.51	120.15	117.05
3	W	602	TPP	C6-C5-C4	2.52	130.17	127.34
3	C	602	TPP	C6-C5-C4	2.52	130.17	127.34
3	N	602	TPP	O3B-PB-O2B	2.57	116.86	107.44
3	L	602	TPP	CM2-C2'-N1'	2.60	120.26	117.05
3	M	602	TPP	CM2-C2'-N1'	2.61	120.26	117.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	602	TPP	CM2-C2'-N1'	2.71	120.39	117.05
3	D	602	TPP	CM2-C2'-N1'	2.73	120.42	117.05
3	K	602	TPP	CM2-C2'-N1'	2.77	120.46	117.05
3	V	602	TPP	CM2-C2'-N1'	2.81	120.52	117.05
3	N	602	TPP	CM2-C2'-N1'	2.88	120.60	117.05
3	H	602	TPP	C6'-N1'-C2'	2.89	121.42	115.92
3	R	602	TPP	C6-C5-C4	2.90	130.60	127.34
3	I	602	TPP	CM2-C2'-N1'	2.92	120.65	117.05
3	K	602	TPP	C6-C5-C4	2.97	130.68	127.34
3	P	602	TPP	C6-C5-C4	3.02	130.73	127.34
3	T	602	TPP	CM2-C2'-N1'	3.03	120.79	117.05
3	G	602	TPP	C6'-N1'-C2'	3.09	121.79	115.92
3	N	602	TPP	C6'-N1'-C2'	3.10	121.81	115.92
3	S	602	TPP	C6'-N1'-C2'	3.12	121.86	115.92
3	L	602	TPP	C6'-N1'-C2'	3.16	121.92	115.92
3	M	602	TPP	C6'-N1'-C2'	3.17	121.95	115.92
3	G	602	TPP	C6-C5-C4	3.18	130.90	127.34
3	Q	602	TPP	C6'-N1'-C2'	3.25	122.10	115.92
3	B	602	TPP	C6'-N1'-C2'	3.28	122.15	115.92
3	F	603	TPP	CM4-C4-N3	3.29	126.46	122.43
3	O	602	TPP	C6'-N1'-C2'	3.34	122.26	115.92
3	X	602	TPP	C6'-N1'-C2'	3.34	122.27	115.92
3	X	602	TPP	CM2-C2'-N1'	3.35	121.18	117.05
3	D	602	TPP	CM4-C4-N3	3.36	126.55	122.43
3	P	602	TPP	C6'-N1'-C2'	3.39	122.36	115.92
3	I	602	TPP	C6'-N1'-C2'	3.39	122.37	115.92
3	A	602	TPP	C6'-N1'-C2'	3.40	122.38	115.92
3	O	602	TPP	C6-C5-C4	3.41	131.16	127.34
3	W	602	TPP	C6'-N1'-C2'	3.45	122.48	115.92
3	K	602	TPP	C6'-N1'-C2'	3.49	122.55	115.92
3	T	602	TPP	C6'-N1'-C2'	3.51	122.59	115.92
3	R	602	TPP	C6'-N1'-C2'	3.51	122.59	115.92
3	U	602	TPP	C6'-N1'-C2'	3.51	122.60	115.92
3	V	602	TPP	C6'-N1'-C2'	3.52	122.60	115.92
3	J	602	TPP	C6'-N1'-C2'	3.54	122.64	115.92
3	F	603	TPP	C6'-N1'-C2'	3.55	122.67	115.92
3	I	602	TPP	C6-C5-C4	3.60	131.38	127.34
3	E	602	TPP	C6'-N1'-C2'	3.60	122.77	115.92
3	D	602	TPP	C6'-N1'-C2'	3.61	122.79	115.92
3	S	602	TPP	CM2-C2'-N1'	3.63	121.53	117.05
3	X	602	TPP	C6-C5-C4	3.66	131.45	127.34
3	A	602	TPP	C6-C5-C4	3.72	131.52	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	602	TPP	CM4-C4-N3	3.76	127.04	122.43
3	C	602	TPP	C6'-N1'-C2'	3.76	123.07	115.92
3	B	602	TPP	C6-C5-C4	3.78	131.58	127.34
3	S	602	TPP	C6-C5-C4	3.84	131.65	127.34
3	L	602	TPP	C6-C5-C4	3.99	131.81	127.34
3	A	602	TPP	CM4-C4-N3	4.08	127.44	122.43
3	T	602	TPP	C6-C5-C4	4.09	131.93	127.34
3	J	602	TPP	CM4-C4-N3	4.11	127.47	122.43
3	Q	602	TPP	C6-C5-C4	4.14	131.98	127.34
3	V	602	TPP	C6-C5-C4	4.27	132.14	127.34
3	U	602	TPP	C6-C5-C4	4.96	132.90	127.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	TPP	1	0
3	C	602	TPP	2	0
3	D	602	TPP	2	0
3	E	602	TPP	4	0
4	F	601	EDO	2	0
3	F	603	TPP	1	0
3	G	602	TPP	3	0
3	H	602	TPP	2	0
3	I	602	TPP	2	0
3	J	602	TPP	2	0
3	K	602	TPP	2	0
3	L	602	TPP	2	0
3	M	602	TPP	2	0
3	N	602	TPP	2	0
3	O	602	TPP	2	0
3	P	602	TPP	2	0
3	Q	602	TPP	2	0
3	R	602	TPP	2	0
3	T	602	TPP	1	0
3	U	602	TPP	1	0
3	W	602	TPP	1	0
3	X	602	TPP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	555:GLN	C	556:ALA	N	5.35
1	E	555:GLN	C	556:ALA	N	3.78

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	555/573 (96%)	0.16	12 (2%) 65 73	15, 27, 44, 68	0
1	B	555/573 (96%)	0.10	14 (2%) 61 69	12, 25, 44, 66	0
1	C	555/573 (96%)	-0.08	5 (0%) 85 89	10, 19, 36, 57	0
1	D	555/573 (96%)	-0.04	6 (1%) 82 86	12, 21, 37, 58	0
1	E	556/573 (97%)	-0.16	6 (1%) 82 86	11, 20, 35, 76	0
1	F	555/573 (96%)	-0.18	2 (0%) 93 94	9, 17, 31, 55	0
1	G	555/573 (96%)	0.04	12 (2%) 65 73	13, 24, 41, 62	0
1	H	555/573 (96%)	0.11	11 (1%) 68 75	14, 26, 43, 66	0
1	I	556/573 (97%)	0.10	14 (2%) 61 69	12, 23, 44, 88	0
1	J	555/573 (96%)	-0.04	6 (1%) 82 86	12, 21, 38, 66	0
1	K	555/573 (96%)	0.00	11 (1%) 68 75	12, 22, 40, 58	0
1	L	555/573 (96%)	-0.13	4 (0%) 89 91	13, 21, 37, 58	0
1	M	555/573 (96%)	-0.16	3 (0%) 91 93	9, 16, 32, 50	0
1	N	555/573 (96%)	-0.09	3 (0%) 91 93	8, 17, 31, 51	0
1	O	555/573 (96%)	0.06	13 (2%) 64 72	12, 23, 41, 62	0
1	P	555/573 (96%)	-0.06	10 (1%) 71 79	10, 22, 42, 63	0
1	Q	555/573 (96%)	0.11	16 (2%) 55 65	13, 26, 43, 63	0
1	R	555/573 (96%)	0.06	11 (1%) 68 75	13, 25, 44, 74	0
1	S	555/573 (96%)	0.00	10 (1%) 71 79	13, 23, 42, 64	0
1	T	555/573 (96%)	-0.04	5 (0%) 85 89	13, 24, 40, 59	0
1	U	555/573 (96%)	0.85	74 (13%) 4 7	19, 43, 73, 94	0
1	V	555/573 (96%)	0.74	77 (13%) 4 6	21, 41, 68, 98	0
1	W	555/573 (96%)	1.03	115 (20%) 1 2	21, 47, 73, 97	0
1	X	555/573 (96%)	0.13	12 (2%) 65 73	16, 31, 50, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	13322/13752 (96%)	0.10	452 (3%) 49 59	8, 24, 52, 98	0

All (452) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	556	ALA	12.2
1	E	556	ALA	6.7
1	U	343	GLY	6.3
1	W	348	VAL	5.6
1	V	349	LEU	5.5
1	W	1	MET	5.4
1	W	353	ALA	5.4
1	W	354	ALA	5.4
1	W	351	ILE	5.3
1	U	267	GLU	5.2
1	W	267	GLU	5.2
1	I	344	THR	5.2
1	W	391[A]	SER	5.0
1	V	354	ALA	5.0
1	W	346	ALA	5.0
1	U	349	LEU	5.0
1	W	233	ASP	4.9
1	W	347	PRO	4.8
1	W	273	VAL	4.8
1	W	352	GLU	4.8
1	W	280	LEU	4.7
1	W	342	GLN	4.7
1	W	211	VAL	4.7
1	W	541	ALA	4.6
1	W	249	PHE	4.6
1	V	351	ILE	4.5
1	W	344	THR	4.4
1	U	555	GLN	4.4
1	A	351	ILE	4.4
1	V	350	GLY	4.4
1	O	354	ALA	4.3
1	Q	350	GLY	4.3
1	W	338	PRO	4.3
1	W	355[A]	GLU	4.3
1	H	343	GLY	4.2
1	I	352	GLU	4.2
1	U	296	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	V	345	GLN	4.2
1	W	539	LEU	4.1
1	W	268	GLY	4.1
1	W	265	SER	4.1
1	V	555	GLN	4.1
1	W	349	LEU	4.0
1	W	269	ALA	4.0
1	R	349	LEU	4.0
1	V	352	GLU	3.9
1	U	205	LEU	3.9
1	W	205	LEU	3.9
1	U	278	ALA	3.9
1	E	343	GLY	3.9
1	W	301	ASP	3.9
1	W	470	ALA	3.8
1	W	350	GLY	3.8
1	U	517	LEU	3.8
1	W	538	THR	3.8
1	V	347	PRO	3.8
1	B	343	GLY	3.8
1	U	271	GLU	3.7
1	W	392	ARG	3.7
1	A	350	GLY	3.7
1	V	344	THR	3.7
1	L	343	GLY	3.7
1	W	262	GLY	3.7
1	K	352	GLU	3.7
1	U	352	GLU	3.7
1	W	343	GLY	3.6
1	W	278	ALA	3.6
1	V	301	ASP	3.6
1	Q	348	VAL	3.6
1	U	268	GLY	3.6
1	W	259	LEU	3.6
1	W	302	ASN	3.6
1	W	369	ILE	3.6
1	S	343	GLY	3.5
1	U	236	GLY	3.5
1	V	359	PRO	3.5
1	U	300	GLY	3.5
1	R	343	GLY	3.5
1	W	345	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	V	214	LEU	3.5
1	W	282	LEU	3.4
1	X	555	GLN	3.4
1	O	352	GLU	3.4
1	N	343	GLY	3.4
1	V	358	ALA	3.4
1	B	348	VAL	3.4
1	A	343	GLY	3.4
1	V	1	MET	3.4
1	U	275	ASN	3.4
1	X	345	GLN	3.4
1	W	272	LEU	3.3
1	W	341	THR	3.3
1	A	352	GLU	3.3
1	W	260	TYR	3.3
1	U	256	PHE	3.3
1	D	555	GLN	3.3
1	V	353	ALA	3.3
1	H	555	GLN	3.3
1	X	348	VAL	3.3
1	T	1	MET	3.2
1	O	349	LEU	3.2
1	I	207	ASP	3.2
1	U	277	ASP	3.2
1	D	345	GLN	3.2
1	K	343	GLY	3.2
1	V	280	LEU	3.2
1	W	388	PHE	3.2
1	U	269	ALA	3.2
1	V	237	CYS	3.2
1	V	332	GLU	3.2
1	C	345	GLN	3.2
1	U	535	CYS	3.2
1	A	345	GLN	3.2
1	U	348	VAL	3.2
1	W	237	CYS	3.1
1	W	332	GLU	3.1
1	W	358	ALA	3.1
1	F	555	GLN	3.1
1	Q	345	GLN	3.1
1	W	256	PHE	3.1
1	U	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	V	205	LEU	3.1
1	U	391[A]	SER	3.1
1	W	261	TRP	3.1
1	B	355[A]	GLU	3.1
1	S	344	THR	3.1
1	V	340	THR	3.1
1	K	537[A]	GLU	3.1
1	V	355[A]	GLU	3.1
1	W	240	THR	3.0
1	V	269	ALA	3.0
1	X	350	GLY	3.0
1	W	271	GLU	3.0
1	U	350	GLY	3.0
1	U	252	ASP	3.0
1	U	276	ALA	3.0
1	U	471	ILE	3.0
1	W	212	VAL	3.0
1	U	332	GLU	3.0
1	A	355[A]	GLU	3.0
1	W	542	TRP	3.0
1	N	555	GLN	3.0
1	Q	343	GLY	3.0
1	U	539	LEU	3.0
1	O	345	GLN	3.0
1	J	345	GLN	2.9
1	E	352	GLU	2.9
1	G	343	GLY	2.9
1	K	348	VAL	2.9
1	Q	344	THR	2.9
1	B	345	GLN	2.9
1	M	345	GLN	2.9
1	O	555	GLN	2.9
1	W	290	ALA	2.9
1	P	495	ASP	2.9
1	U	369	ILE	2.9
1	H	345	GLN	2.9
1	U	341	THR	2.9
1	U	212	VAL	2.9
1	R	352	GLU	2.9
1	V	206	GLN	2.9
1	W	225	GLU	2.9
1	W	537	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	R	355[A]	GLU	2.9
1	S	350	GLY	2.9
1	U	345	GLN	2.9
1	W	297	TRP	2.9
1	K	533	ASP	2.9
1	Q	495	ASP	2.9
1	Q	349	LEU	2.9
1	I	350	GLY	2.8
1	J	343	GLY	2.8
1	J	352	GLU	2.8
1	V	348	VAL	2.8
1	W	258	GLY	2.8
1	W	235	LEU	2.8
1	V	495	ASP	2.8
1	W	264	VAL	2.8
1	V	470	ALA	2.8
1	V	388	PHE	2.8
1	J	355[A]	GLU	2.8
1	O	350	GLY	2.8
1	V	369	ILE	2.8
1	D	352	GLU	2.8
1	U	211	VAL	2.8
1	V	533	ASP	2.8
1	R	345	GLN	2.8
1	A	349	LEU	2.8
1	W	266	SER	2.8
1	W	255	ASN	2.7
1	W	337	ARG	2.7
1	N	352	GLU	2.7
1	V	209	GLN	2.7
1	V	271	GLU	2.7
1	G	344	THR	2.7
1	W	387	TRP	2.7
1	W	518	ASP	2.7
1	H	267	GLU	2.7
1	A	555	GLN	2.7
1	W	277	ASP	2.7
1	U	249	PHE	2.7
1	V	256	PHE	2.7
1	J	344	THR	2.7
1	V	212	VAL	2.7
1	X	267	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	344	THR	2.7
1	C	555	GLN	2.7
1	Q	351	ILE	2.7
1	Q	1	MET	2.7
1	M	343	GLY	2.6
1	A	267	GLU	2.6
1	V	203	GLU	2.6
1	V	235	LEU	2.6
1	K	345	GLN	2.6
1	B	352	GLU	2.6
1	U	203	GLU	2.6
1	K	344	THR	2.6
1	W	393	MET	2.6
1	V	231	LEU	2.6
1	W	545	ARG	2.6
1	U	273	VAL	2.6
1	V	297	TRP	2.6
1	U	541	ALA	2.6
1	U	233	ASP	2.6
1	B	350	GLY	2.6
1	C	343	GLY	2.6
1	W	294	TRP	2.6
1	V	391[A]	SER	2.6
1	U	237	CYS	2.6
1	D	343	GLY	2.6
1	K	349	LEU	2.6
1	W	509	LEU	2.6
1	G	271	GLU	2.6
1	P	555	GLN	2.6
1	V	367	ARG	2.6
1	U	375	SER	2.6
1	V	327	ALA	2.6
1	D	495	ASP	2.5
1	E	555	GLN	2.6
1	K	555	GLN	2.6
1	Q	533	ASP	2.5
1	U	495	ASP	2.5
1	V	259	LEU	2.6
1	W	215	VAL	2.5
1	W	213	MET	2.5
1	V	267	GLU	2.5
1	U	514	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	349	LEU	2.5
1	G	355[A]	GLU	2.5
1	U	295	ASN	2.5
1	V	282	LEU	2.5
1	O	343	GLY	2.5
1	A	348	VAL	2.5
1	H	344	THR	2.5
1	V	207	ASP	2.5
1	W	340	THR	2.5
1	P	332	GLU	2.5
1	S	555	GLN	2.5
1	W	275	ASN	2.5
1	U	301	ASP	2.5
1	W	238	ALA	2.5
1	G	348	VAL	2.5
1	Q	347	PRO	2.5
1	U	355[A]	GLU	2.5
1	E	301	ASP	2.5
1	H	301	ASP	2.5
1	R	350	GLY	2.5
1	V	258	GLY	2.5
1	W	236	GLY	2.5
1	W	533	ASP	2.5
1	R	344	THR	2.5
1	U	299	LYS	2.5
1	X	1	MET	2.5
1	U	206	GLN	2.5
1	X	301	ASP	2.5
1	T	494	GLU	2.5
1	O	355	GLU	2.4
1	X	343	GLY	2.4
1	V	260	TYR	2.4
1	U	347	PRO	2.4
1	W	286	PHE	2.4
1	O	348	VAL	2.4
1	V	239	VAL	2.4
1	W	270	GLN	2.4
1	H	271	GLU	2.4
1	U	314	ALA	2.4
1	B	533	ASP	2.4
1	U	342	GLN	2.4
1	S	533	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	255	ASN	2.4
1	U	331	ALA	2.4
1	U	393	MET	2.4
1	G	350	GLY	2.4
1	U	272	LEU	2.4
1	S	345	GLN	2.4
1	W	385	ASP	2.4
1	V	245	ALA	2.4
1	G	352	GLU	2.4
1	V	272	LEU	2.4
1	W	360	LEU	2.4
1	J	495	ASP	2.4
1	V	363	ASP	2.4
1	O	391[A]	SER	2.4
1	W	333	LYS	2.4
1	P	350	GLY	2.4
1	I	301	ASP	2.4
1	Q	301	ASP	2.4
1	T	271	GLU	2.3
1	X	271	GLU	2.3
1	L	345	GLN	2.3
1	W	359	PRO	2.3
1	V	541	ALA	2.3
1	V	300	GLY	2.3
1	B	495	ASP	2.3
1	W	534	ASP	2.3
1	K	355[A]	GLU	2.3
1	I	555	GLN	2.3
1	U	234	ARG	2.3
1	V	249	PHE	2.3
1	W	281	CYS	2.3
1	V	262	GLY	2.3
1	B	267	GLU	2.3
1	V	531	ALA	2.3
1	W	241	ILE	2.3
1	V	343	GLY	2.3
1	Q	555	GLN	2.3
1	V	494	GLU	2.3
1	V	537	GLU	2.3
1	V	266	SER	2.3
1	L	1	MET	2.3
1	V	211	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	273	VAL	2.3
1	W	229	VAL	2.3
1	I	495	ASP	2.3
1	V	540	ILE	2.3
1	I	267	GLU	2.3
1	V	286	PHE	2.3
1	W	363	ASP	2.3
1	T	267	GLU	2.3
1	V	510	GLU	2.3
1	S	1	MET	2.2
1	I	345	GLN	2.2
1	W	203	GLU	2.2
1	W	336	SER	2.2
1	U	390	ALA	2.2
1	W	214	LEU	2.2
1	V	234	ARG	2.2
1	I	343	GLY	2.2
1	U	376	ASP	2.2
1	V	251	GLU	2.2
1	W	430	ILE	2.2
1	P	345	GLN	2.2
1	U	354	ALA	2.2
1	W	504	SER	2.2
1	A	494	GLU	2.2
1	M	1	MET	2.2
1	V	334	ALA	2.2
1	V	536	THR	2.2
1	W	535	CYS	2.2
1	W	263	GLU	2.2
1	W	239	VAL	2.2
1	W	331	ALA	2.2
1	C	203	GLU	2.2
1	E	355[A]	GLU	2.2
1	P	271	GLU	2.2
1	W	494	GLU	2.2
1	B	207	ASP	2.2
1	U	534	ASP	2.2
1	W	231	LEU	2.2
1	V	357	ASN	2.2
1	W	362	ASN	2.2
1	W	274	GLU	2.2
1	H	495[A]	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	W	207	ASP	2.2
1	O	347	PRO	2.2
1	X	545	ARG	2.2
1	U	351	ILE	2.1
1	U	297	TRP	2.1
1	B	332	GLU	2.1
1	I	271	GLU	2.1
1	R	495	ASP	2.1
1	R	533	ASP	2.1
1	V	463	ARG	2.1
1	W	548	ALA	2.1
1	Q	267	GLU	2.1
1	W	510	GLU	2.1
1	A	252	ASP	2.1
1	D	350	GLY	2.1
1	G	345	GLN	2.1
1	U	262	GLY	2.1
1	W	209	GLN	2.1
1	B	344	THR	2.1
1	C	494	GLU	2.1
1	S	352	GLU	2.1
1	W	42[A]	GLU	2.1
1	W	390	ALA	2.1
1	U	362	ASN	2.1
1	F	533	ASP	2.1
1	U	279	ILE	2.1
1	U	280	LEU	2.1
1	G	555	GLN	2.1
1	U	263	GLU	2.1
1	U	261	TRP	2.1
1	V	366	THR	2.1
1	S	495	ASP	2.1
1	V	274	GLU	2.1
1	U	501	LEU	2.1
1	V	265	SER	2.1
1	G	1	MET	2.1
1	G	353	ALA	2.1
1	V	238	ALA	2.1
1	W	458	PHE	2.1
1	O	495	ASP	2.1
1	U	518	ASP	2.1
1	H	533	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	207	ASP	2.1
1	W	466	VAL	2.1
1	X	352	GLU	2.1
1	K	354	ALA	2.1
1	V	248	PHE	2.1
1	I	355	GLU	2.0
1	U	274	GLU	2.0
1	G	533	ASP	2.0
1	P	301	ASP	2.0
1	U	207	ASP	2.0
1	U	430	ILE	2.0
1	W	540	ILE	2.0
1	W	365	MET	2.0
1	V	292	VAL	2.0
1	W	222	ALA	2.0
1	W	399	ALA	2.0
1	W	536	THR	2.0
1	W	248	PHE	2.0
1	B	271	GLU	2.0
1	P	343	GLY	2.0
1	T	537	GLU	2.0
1	W	299	LYS	2.0
1	P	1	MET	2.0
1	S	535	CYS	2.0
1	U	214	LEU	2.0
1	U	238	ALA	2.0
1	H	352	GLU	2.0
1	Q	271	GLU	2.0
1	R	267	GLU	2.0
1	V	295	ASN	2.0
1	X	209	GLN	2.0
1	B	537	GLU	2.0
1	O	271	GLU	2.0
1	P	267	GLU	2.0
1	Q	352	GLU	2.0
1	H	349	LEU	2.0
1	U	215	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	EDO	A	603	4/4	0.78	0.36	17.97	42,42,43,44	0
4	EDO	Q	603	4/4	0.73	0.42	9.26	57,59,60,60	0
4	EDO	R	603	4/4	0.73	0.33	5.27	53,55,55,57	0
4	EDO	F	601	4/4	0.88	0.27	5.18	50,50,51,51	0
4	EDO	I	603	4/4	0.75	0.30	4.86	56,58,58,58	0
4	EDO	N	603	4/4	0.67	0.26	4.16	48,51,52,54	0
3	TPP	D	602	26/26	0.94	0.14	1.15	15,17,22,25	0
3	TPP	B	602	26/26	0.94	0.14	1.11	21,27,32,36	0
3	TPP	C	602	26/26	0.96	0.14	0.91	14,16,20,23	0
3	TPP	Q	602	26/26	0.94	0.13	0.85	17,22,27,30	0
3	TPP	A	602	26/26	0.94	0.14	0.81	19,23,31,36	0
3	TPP	F	603	26/26	0.95	0.13	0.75	13,16,20,24	0
3	TPP	T	602	26/26	0.95	0.13	0.72	19,23,28,34	0
3	TPP	H	602	26/26	0.95	0.14	0.66	19,23,27,30	0
3	TPP	K	602	26/26	0.93	0.13	0.66	19,21,29,34	0
3	TPP	O	602	26/26	0.95	0.13	0.62	18,19,25,27	0
3	TPP	E	602	26/26	0.96	0.12	0.52	13,15,21,23	0
3	TPP	L	602	26/26	0.94	0.13	0.50	17,20,24,27	0
3	TPP	M	602	26/26	0.96	0.13	0.50	13,15,19,22	0
3	TPP	W	602	26/26	0.90	0.17	0.48	34,39,50,53	0
3	TPP	N	602	26/26	0.95	0.12	0.44	12,14,19,24	0
3	TPP	G	602	26/26	0.95	0.12	0.44	18,23,27,29	0
3	TPP	I	602	26/26	0.95	0.12	0.40	16,19,25,29	0
3	TPP	P	602	26/26	0.95	0.13	0.39	16,22,26,29	0
3	TPP	R	602	26/26	0.95	0.12	0.35	17,22,27,32	0
3	TPP	J	602	26/26	0.96	0.12	0.31	16,18,22,25	0
3	TPP	S	602	26/26	0.95	0.12	0.18	18,20,26,30	0
2	MG	C	601	1/1	0.97	0.12	0.03	13,13,13,13	0
3	TPP	U	602	26/26	0.92	0.14	0.01	27,36,42,46	0
3	TPP	X	602	26/26	0.94	0.12	-0.01	23,27,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	TPP	V	602	26/26	0.93	0.12	-0.16	27,38,41,45	0
2	MG	R	601	1/1	0.92	0.09	-0.53	25,25,25,25	0
2	MG	H	601	1/1	0.94	0.09	-0.72	19,19,19,19	0
2	MG	I	601	1/1	0.95	0.08	-0.79	19,19,19,19	0
2	MG	G	601	1/1	0.96	0.08	-1.17	21,21,21,21	0
2	MG	M	601	1/1	0.97	0.08	-1.21	13,13,13,13	0
2	MG	S	601	1/1	0.93	0.06	-1.38	23,23,23,23	0
2	MG	L	601	1/1	0.97	0.07	-1.41	24,24,24,24	0
2	MG	K	601	1/1	0.87	0.05	-1.45	23,23,23,23	0
2	MG	P	601	1/1	0.91	0.07	-1.47	21,21,21,21	0
2	MG	V	601	1/1	0.94	0.05	-1.50	34,34,34,34	0
2	MG	A	601	1/1	0.93	0.06	-1.58	25,25,25,25	0
2	MG	F	602	1/1	0.99	0.05	-1.61	15,15,15,15	0
2	MG	T	601	1/1	0.97	0.05	-1.67	19,19,19,19	0
2	MG	X	601	1/1	0.96	0.07	-1.69	32,32,32,32	0
2	MG	E	601	1/1	0.98	0.06	-1.88	14,14,14,14	0
2	MG	B	601	1/1	0.92	0.04	-2.13	25,25,25,25	0
2	MG	O	601	1/1	0.99	0.02	-2.15	17,17,17,17	0
2	MG	N	601	1/1	0.99	0.05	-2.21	11,11,11,11	0
2	MG	U	601	1/1	0.94	0.06	-2.28	31,31,31,31	0
2	MG	W	601	1/1	0.88	0.05	-2.32	37,37,37,37	0
2	MG	D	601	1/1	0.95	0.04	-2.35	22,22,22,22	0
2	MG	Q	601	1/1	0.98	0.04	-2.64	22,22,22,22	0
2	MG	J	601	1/1	0.97	0.03	-2.96	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.