wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2016 – 02:17 PM EST

PDB ID	:	5T61
Title	:	TUNGSTEN-CONTAINING FORMYLMETHANOFURAN DEHYDROGENASE FROM METHANOTHERMOBACTER WOLFEII, TRICLINIC FORM AT 2.55 A
Authors	:	Wagner, T.; Ermler, U.; Shima, S.
Deposited on	:	2016-09-01
Resolution	:	2.55 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

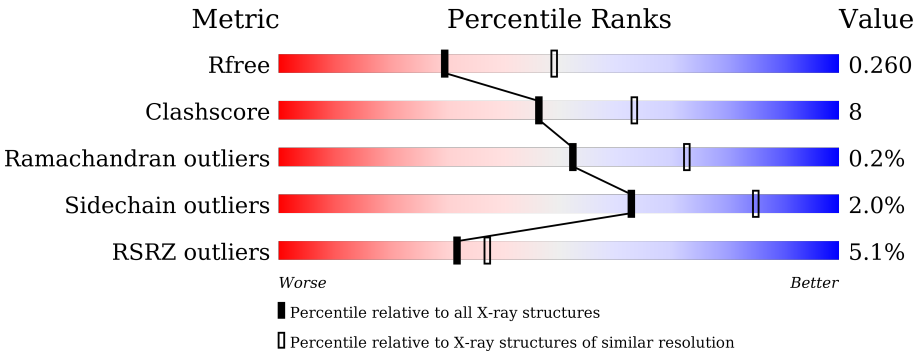
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	569	2% 87% 13%
1	G	569	5% 86% 13%
1	M	569	12% 82% 17%
1	S	569	2% 87% 12%
1	Y	569	10% 87% 12%
1	e	569	2% 98%

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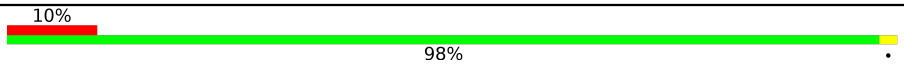
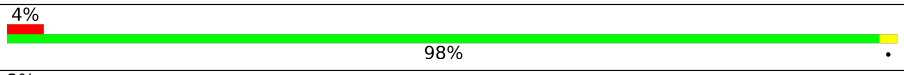
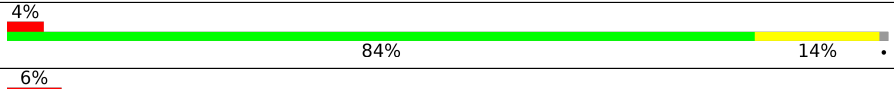
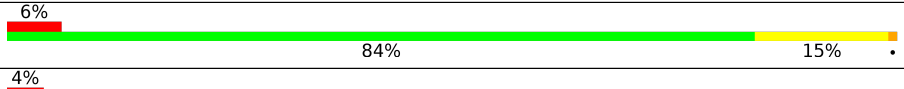
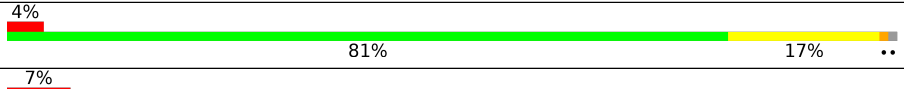
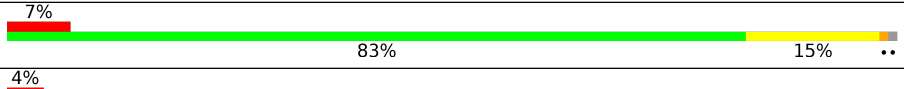
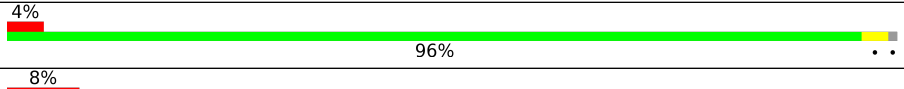
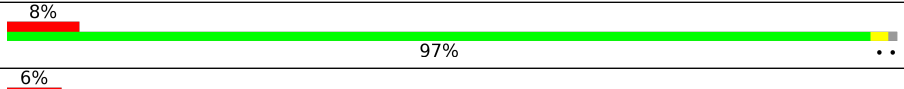
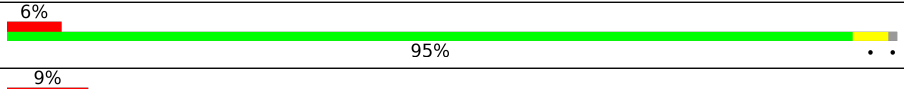
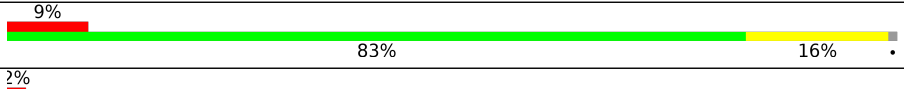
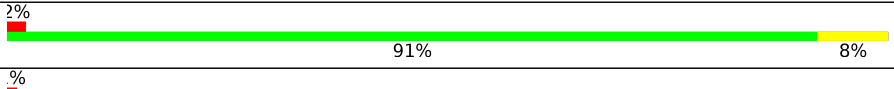
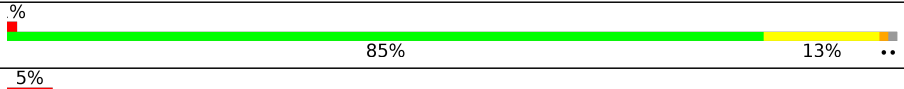
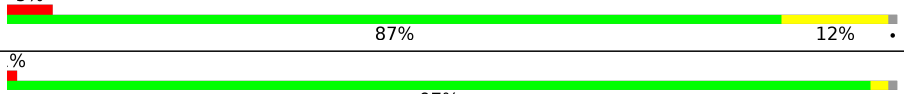
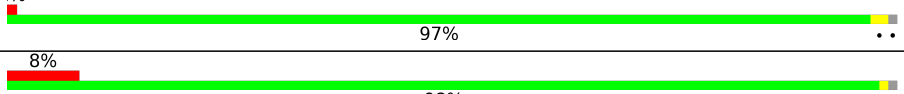
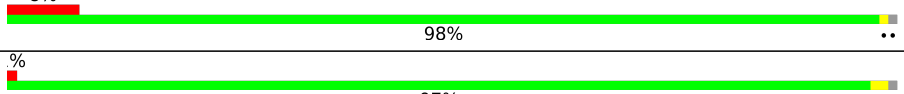
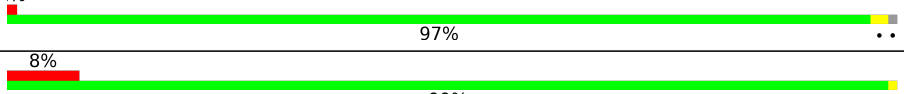
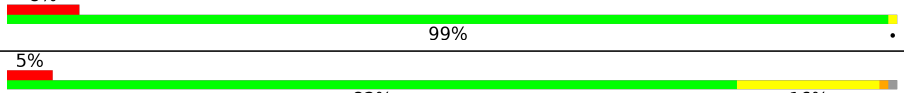
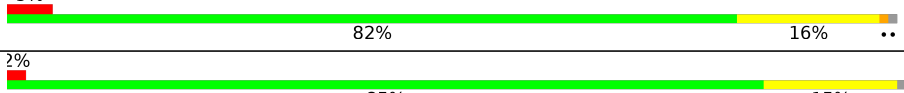
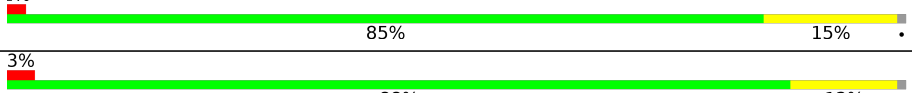
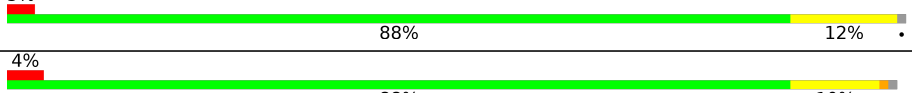
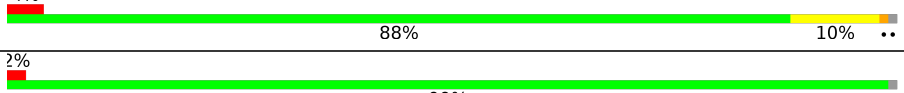
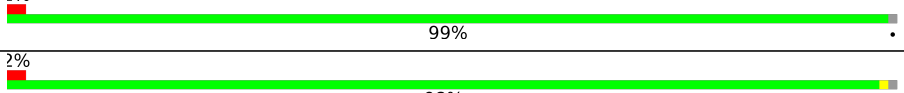
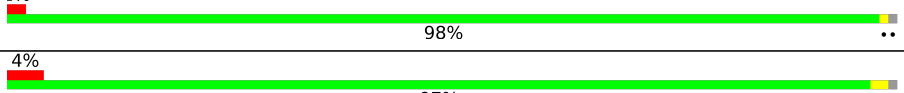
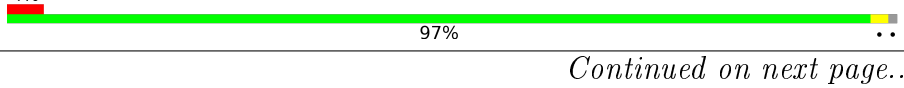
Mol	Chain	Length	Quality of chain
1	k	569	
1	q	569	
2	B	432	
2	H	432	
2	N	432	
2	T	432	
2	Z	432	
2	f	432	
2	l	432	
2	r	432	
3	C	270	
3	I	270	
3	O	270	
3	U	270	
3	a	270	
3	g	270	
3	m	270	
3	s	270	
4	D	130	
4	J	130	
4	P	130	
4	V	130	
4	b	130	
4	h	130	
4	n	130	

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Mol	Chain	Length	Quality of chain
4	t	130	6% 97%
5	E	82	68% 28%
5	K	82	68% 28%
5	Q	82	72% 24%
5	W	82	4% 68% 28%
5	c	82	4% 93% 5%
5	i	82	2% 91% 6%
5	o	82	93% 5%
5	u	82	91% 7%
6	F	349	4% 76% 21%
6	L	349	76% 23%
6	R	349	11% 68% 29%
6	X	349	5% 75% 22%
6	d	349	12% 94%
6	j	349	5% 96%
6	p	349	3% 96%
6	v	349	2% 95%

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
15	MG	B	507	-	-	-	X
15	MG	H	506	-	-	-	X
15	MG	O	301	-	-	-	X
15	MG	T	507	-	-	-	X
15	MG	f	506	-	-	-	X
15	MG	r	507	-	-	-	X
8	MFN	A	603	-	-	-	X
8	MFN	M	603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	MFN	Y	603	-	-	-	X
8	MFN	k	603	-	-	-	X
9	NA	A	604	-	-	-	X
9	NA	G	604	-	-	-	X
9	NA	M	604	-	-	-	X
9	NA	k	604	-	-	-	X
9	NA	q	604	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 114321 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 Tungsten formylmethanofuran dehydrogenase subunit fwdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	G	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	M	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	S	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	Y	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	e	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			
1	k	568	Total	C	N	O	S	0	0	0
			4411	2807	734	848	22			
1	q	569	Total	C	N	O	S	0	0	0
			4419	2812	735	849	23			

- Molecule 2 is a protein called Tungsten formylmethanofuran dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3364	2115	590	629	30			
2	H	427	Total	C	N	O	S	0	0	0
			3352	2109	587	626	30			
2	N	430	Total	C	N	O	S	0	0	0
			3369	2118	591	630	30			
2	T	429	Total	C	N	O	S	0	0	0
			3364	2115	590	629	30			
2	Z	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			
2	f	427	Total	C	N	O	S	0	0	0
			3352	2109	587	626	30			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	l	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			
2	r	428	Total	C	N	O	S	0	0	0
			3357	2112	588	627	30			

- Molecule 3 is a protein called Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	267	Total	C	N	O	S	0	0	0
			1982	1246	334	389	13			
3	I	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			
3	O	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	U	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	a	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	g	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	m	268	Total	C	N	O	S	0	0	0
			1987	1249	335	390	13			
3	s	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			

- Molecule 4 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	J	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	P	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	V	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	b	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	h	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			
4	n	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	129	Total	C	N	O	S	0	0	0
			997	637	162	189	9			

- Molecule 5 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	K	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	Q	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	W	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	c	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	i	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	o	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
5	u	81	Total	C	N	O	S	0	0	0
			581	359	97	116	9			

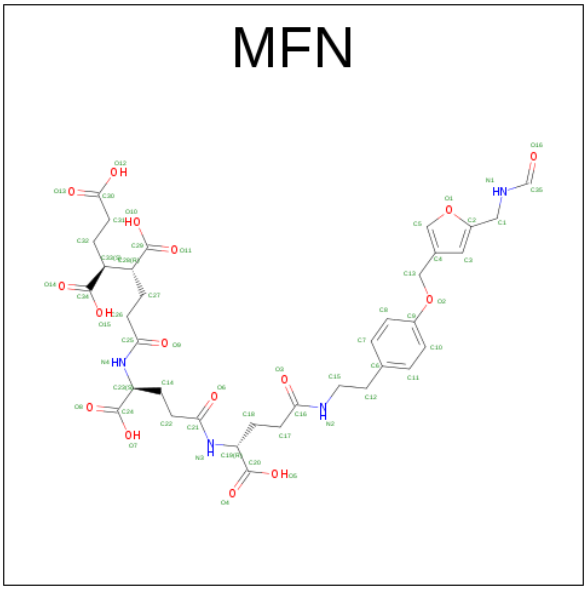
- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	345	Total	C	N	O	S	0	0	0
			2629	1626	438	523	42			
6	L	348	Total	C	N	O	S	0	0	0
			2656	1641	441	532	42			
6	R	341	Total	C	N	O	S	0	0	0
			2602	1611	434	515	42			
6	X	344	Total	C	N	O	S	0	0	0
			2627	1625	437	523	42			
6	d	340	Total	C	N	O	S	0	0	0
			2595	1606	433	514	42			
6	j	344	Total	C	N	O	S	0	0	0
			2625	1624	437	522	42			
6	p	348	Total	C	N	O	S	0	0	0
			2656	1641	441	532	42			
6	v	346	Total	C	N	O	S	0	0	0
			2643	1634	439	528	42			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	2	Total Zn 2 2	0	0
7	q	2	Total Zn 2 2	0	0
7	k	2	Total Zn 2 2	0	0
7	e	2	Total Zn 2 2	0	0
7	A	2	Total Zn 2 2	0	0
7	Y	2	Total Zn 2 2	0	0
7	S	2	Total Zn 2 2	0	0
7	M	2	Total Zn 2 2	0	0

- Molecule 8 is N-[4,5,7-TRICARBOXYHEPTANOYL]-L-GAMMA-GLUTAMYL-N-{2-[4-({5-[(FORMYLAMINO)METHYL]-3-FURYL}METHOXY)PHENYL]ETHYL}-D-GLUTAMINE (three-letter code: MFN) (formula: $C_{35}H_{44}N_4O_{16}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 53 34 4 15	0	0
8	G	1	Total C N O 53 34 4 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C N O 53 34 4 15	0	0
8	S	1	Total C N O 53 34 4 15	0	0
8	Y	1	Total C N O 53 34 4 15	0	0
8	e	1	Total C N O 53 34 4 15	0	0
8	k	1	Total C N O 53 34 4 15	0	0
8	q	1	Total C N O 53 34 4 15	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total Na 1 1	0	0
9	q	1	Total Na 1 1	0	0
9	k	1	Total Na 1 1	0	0
9	e	1	Total Na 1 1	0	0
9	A	1	Total Na 1 1	0	0
9	S	1	Total Na 1 1	0	0
9	M	1	Total Na 1 1	0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	q	2	Total K 2 2	0	0
10	K	1	Total K 1 1	0	0
10	B	1	Total K 1 1	0	0
10	c	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	N	1	Total K 1 1	0	0
10	X	3	Total K 3 3	0	0
10	o	1	Total K 1 1	0	0
10	S	2	Total K 2 2	0	0
10	p	3	Total K 3 3	0	0
10	k	1	Total K 1 1	0	0
10	E	1	Total K 1 1	0	0
10	A	1	Total K 1 1	0	0
10	R	3	Total K 3 3	0	0
10	M	2	Total K 2 2	0	0
10	j	6	Total K 6 6	0	0
10	e	4	Total K 4 4	0	0
10	v	7	Total K 7 7	0	0
10	Z	1	Total K 1 1	0	0
10	r	1	Total K 1 1	0	0
10	L	3	Total K 3 3	0	0
10	G	1	Total K 1 1	0	0
10	Q	1	Total K 1 1	0	0
10	d	2	Total K 2 2	0	0
10	i	1	Total K 1 1	0	0
10	T	1	Total K 1 1	0	0

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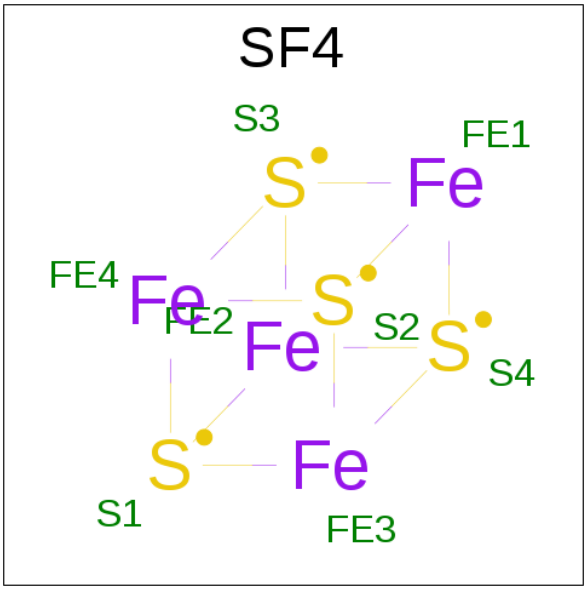
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	u	1	Total K 1 1	0	0
10	Y	1	Total K 1 1	0	0
10	F	4	Total K 4 4	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Fe S 8 4 4	0	0
11	E	1	Total Fe S 8 4 4	0	0
11	E	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0
11	F	1	Total Fe S 8 4 4	0	0
11	H	1	Total Fe S 8 4 4	0	0
11	K	1	Total Fe S 8 4 4	0	0
11	K	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	L	1	Total Fe S 8 4 4	0	0
11	N	1	Total Fe S 8 4 4	0	0
11	Q	1	Total Fe S 8 4 4	0	0
11	Q	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	R	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0
11	R	1	Total Fe S 8 4 4	0	0
11	T	1	Total Fe S 8 4 4	0	0
11	W	1	Total Fe S 8 4 4	0	0
11	W	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	X	1	Total Fe S 8 4 4	0	0
11	Z	1	Total Fe S 8 4 4	0	0
11	c	1	Total Fe S 8 4 4	0	0
11	c	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	d	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0
11	d	1	Total Fe S 8 4 4	0	0
11	f	1	Total Fe S 8 4 4	0	0
11	i	1	Total Fe S 8 4 4	0	0
11	i	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	j	1	Total Fe S 8 4 4	0	0
11	l	1	Total Fe S 8 4 4	0	0
11	o	1	Total Fe S 8 4 4	0	0

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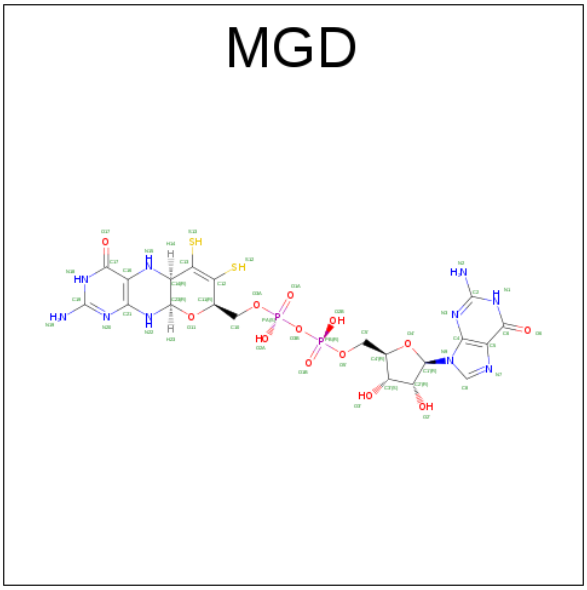
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	o	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	p	1	Total Fe S 8 4 4	0	0
11	r	1	Total Fe S 8 4 4	0	0
11	u	1	Total Fe S 8 4 4	0	0
11	u	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0
11	v	1	Total Fe S 8 4 4	0	0

- Molecule 12 is TUNGSTEN ION (three-letter code: W) (formula: W).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	1	Total W 1 1	0	0
12	B	1	Total W 1 1	0	0
12	Z	1	Total W 1 1	0	0
12	T	1	Total W 1 1	0	0
12	N	1	Total W 1 1	0	0
12	r	1	Total W 1 1	0	0
12	l	1	Total W 1 1	0	0
12	f	1	Total W 1 1	0	0

- Molecule 13 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO -8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O P S 47 20 10 13 2 2	0	0
13	B	1	Total C N O P S 47 20 10 13 2 2	0	0

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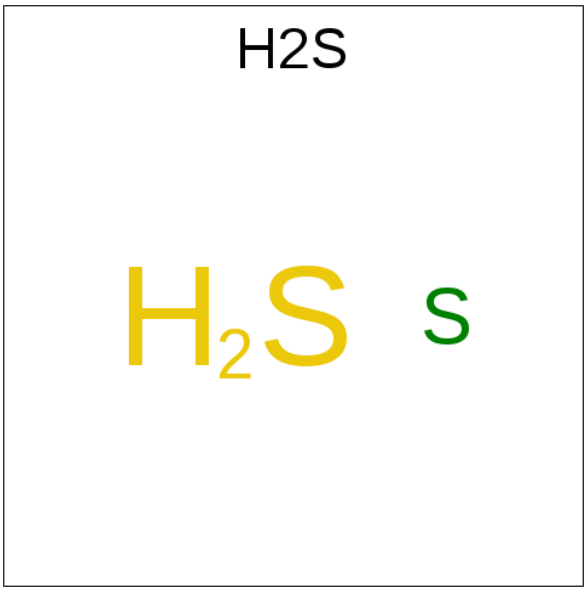
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	H	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	H	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	N	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	N	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	T	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	T	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	Z	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	Z	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	f	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	f	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	l	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	l	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	r	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	r	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 14 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total S 1 1	0	0
14	H	1	Total S 1 1	0	0
14	N	1	Total S 1 1	0	0
14	T	1	Total S 1 1	0	0
14	Z	1	Total S 1 1	0	0
14	f	1	Total S 1 1	0	0
14	l	1	Total S 1 1	0	0
14	r	1	Total S 1 1	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total Mg 1 1	0	0
15	B	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	T	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	O	1	Total Mg 1 1	0	0
15	r	1	Total Mg 1 1	0	0
15	l	1	Total Mg 1 1	0	0
15	f	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	N	1	Total Cl 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	22	Total O 22 22	0	0
17	B	12	Total O 12 12	0	0
17	C	7	Total O 7 7	0	0
17	D	2	Total O 2 2	0	0
17	E	1	Total O 1 1	0	0
17	F	25	Total O 25 25	0	0
17	G	14	Total O 14 14	0	0
17	H	20	Total O 20 20	0	0
17	I	17	Total O 17 17	0	0
17	J	4	Total O 4 4	0	0
17	K	8	Total O 8 8	0	0
17	L	26	Total O 26 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	5	Total O 5 5	0	0
17	N	24	Total O 24 24	0	0
17	O	9	Total O 9 9	0	0
17	P	4	Total O 4 4	0	0
17	Q	2	Total O 2 2	0	0
17	R	6	Total O 6 6	0	0
17	S	59	Total O 59 59	0	0
17	T	29	Total O 29 29	0	0
17	U	10	Total O 10 10	0	0
17	V	9	Total O 9 9	0	0
17	W	3	Total O 3 3	0	0
17	X	19	Total O 19 19	0	0
17	Y	17	Total O 17 17	0	0
17	Z	19	Total O 19 19	0	0
17	a	12	Total O 12 12	0	0
17	b	4	Total O 4 4	0	0
17	c	3	Total O 3 3	0	0
17	d	3	Total O 3 3	0	0
17	e	40	Total O 40 40	0	0
17	f	21	Total O 21 21	0	0
17	g	3	Total O 3 3	0	0

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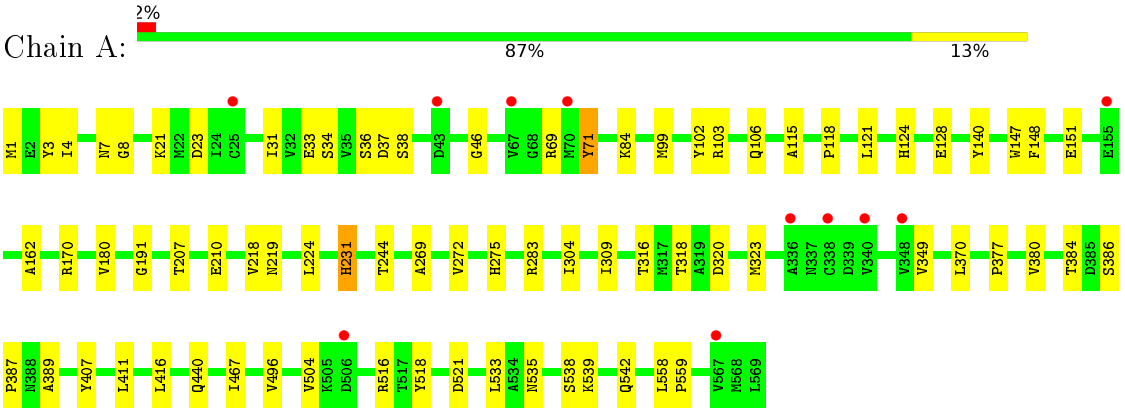
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	h	3	Total O 3 3	0	0
17	i	8	Total O 8 8	0	0
17	j	20	Total O 20 20	0	0
17	k	9	Total O 9 9	0	0
17	l	20	Total O 20 20	0	0
17	m	7	Total O 7 7	0	0
17	n	4	Total O 4 4	0	0
17	o	2	Total O 2 2	0	0
17	p	18	Total O 18 18	0	0
17	q	27	Total O 27 27	0	0
17	r	16	Total O 16 16	0	0
17	s	3	Total O 3 3	0	0
17	t	3	Total O 3 3	0	0
17	u	1	Total O 1 1	0	0
17	v	13	Total O 13 13	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.

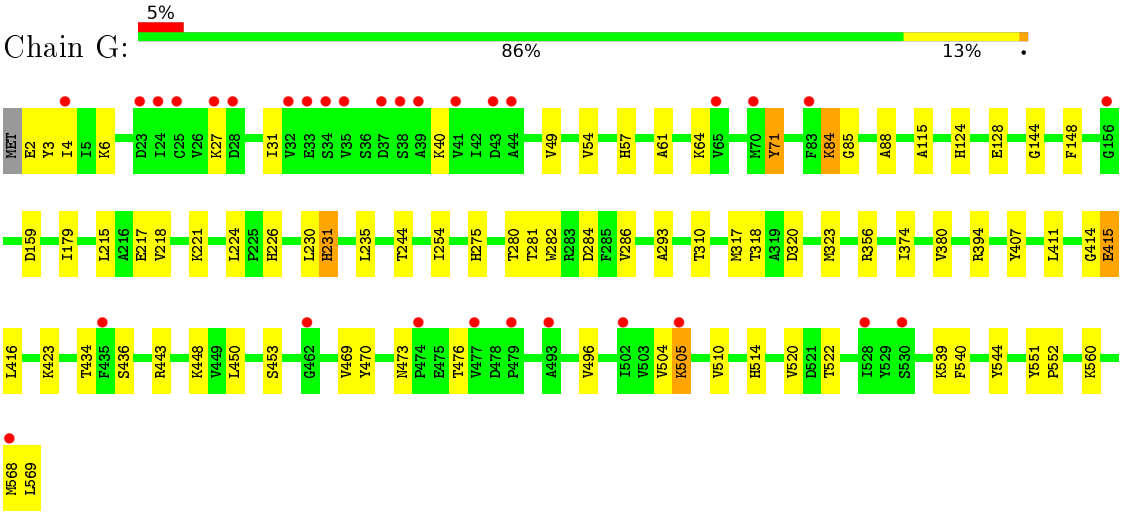
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain A:



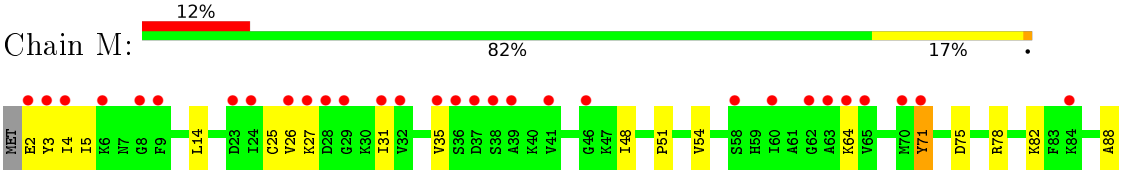
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

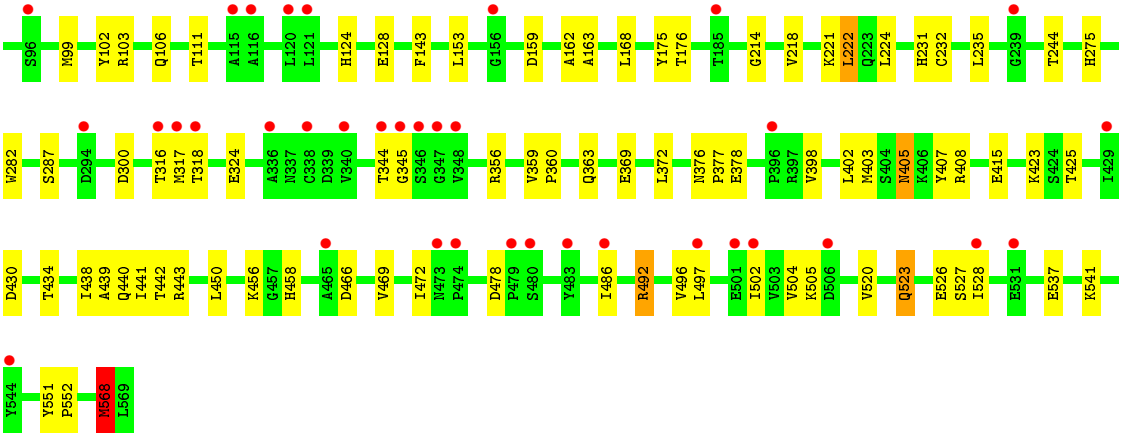
Chain G:



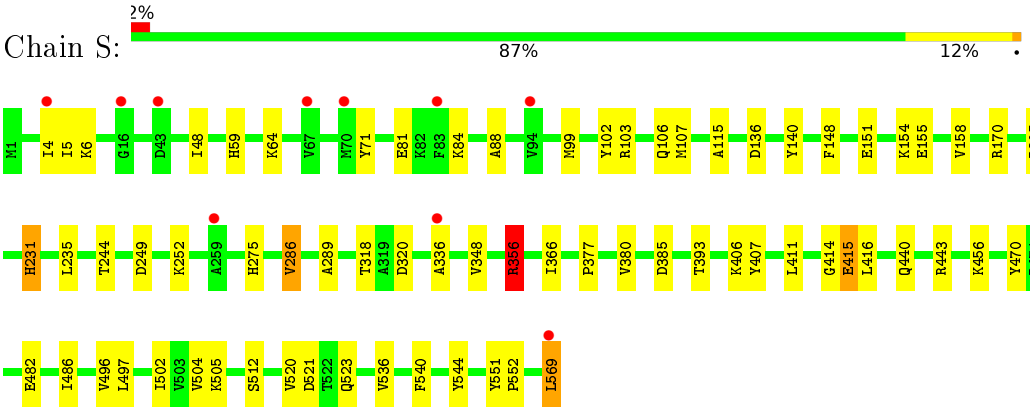
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain M:

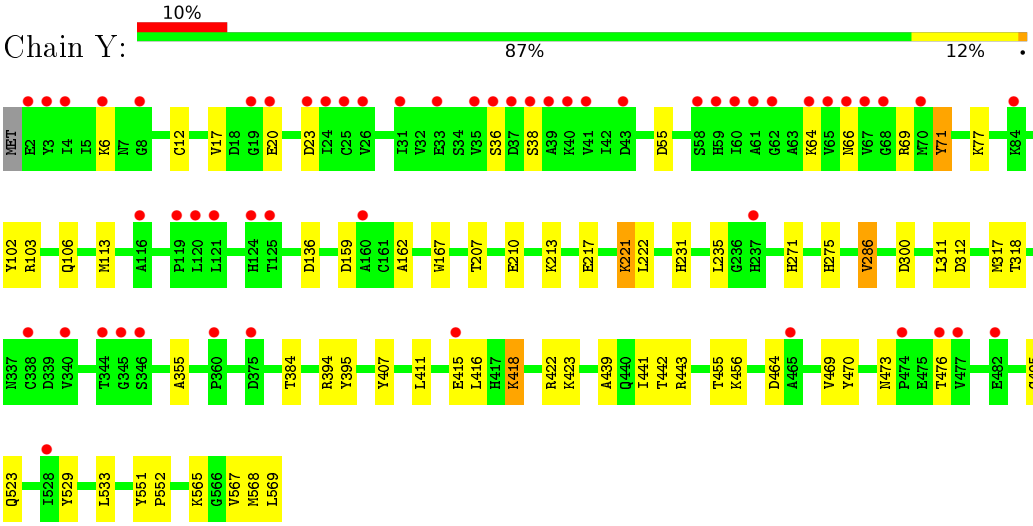




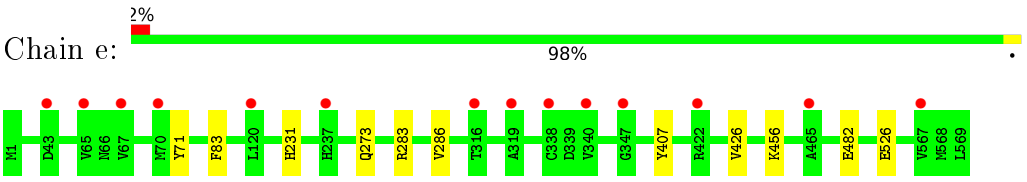
• Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



• Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

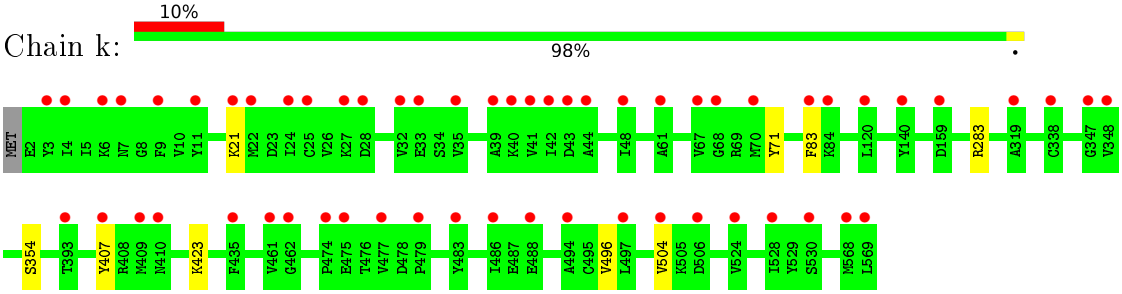


• Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



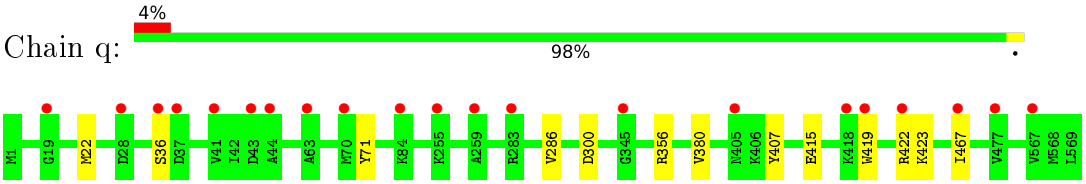
• Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain k:



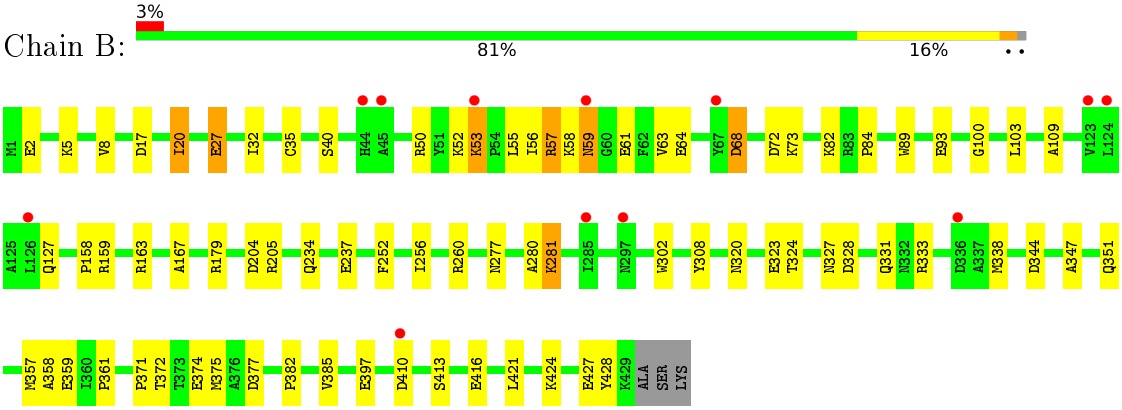
• Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain q:



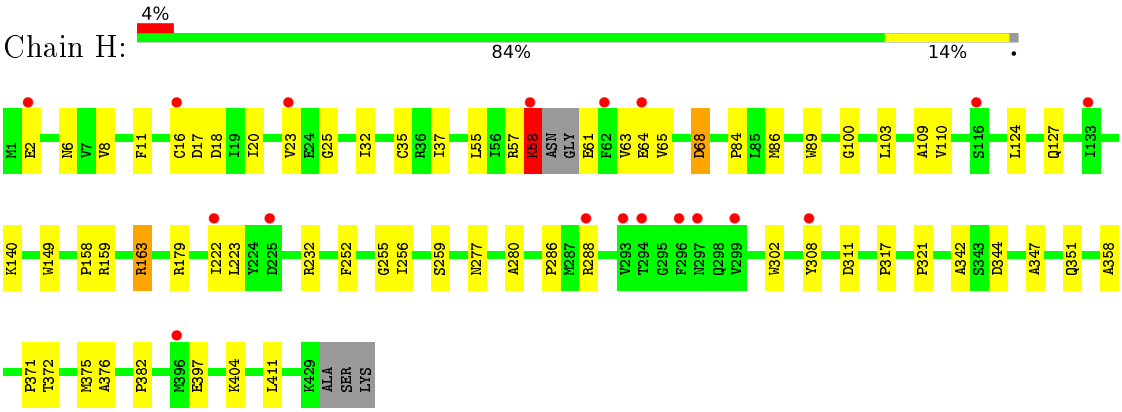
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain B:



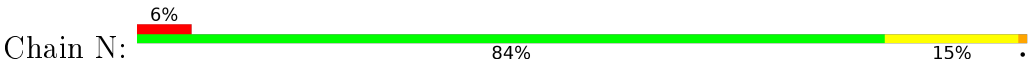
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

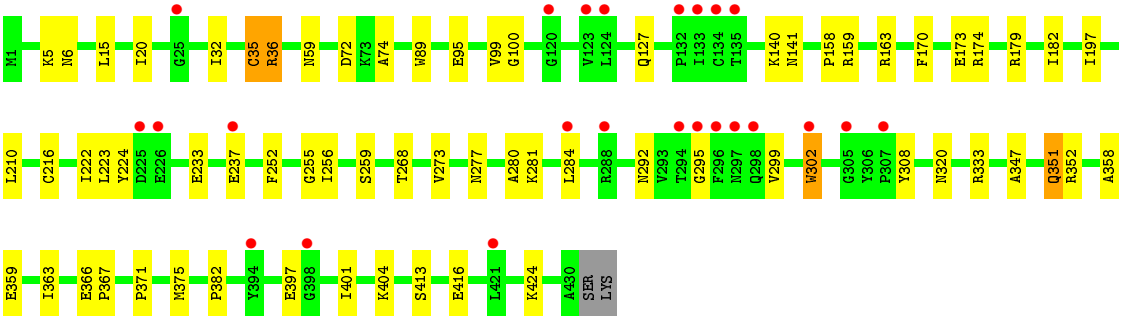
Chain H:



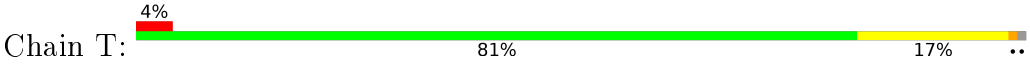
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

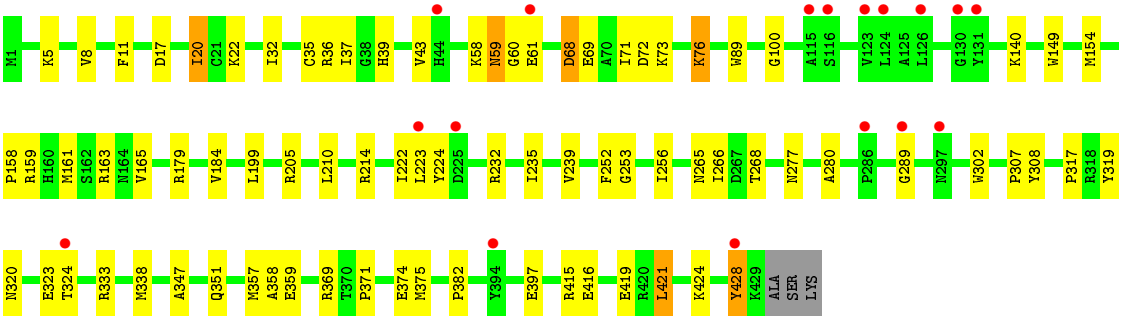
Chain N:



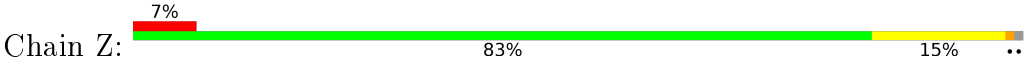


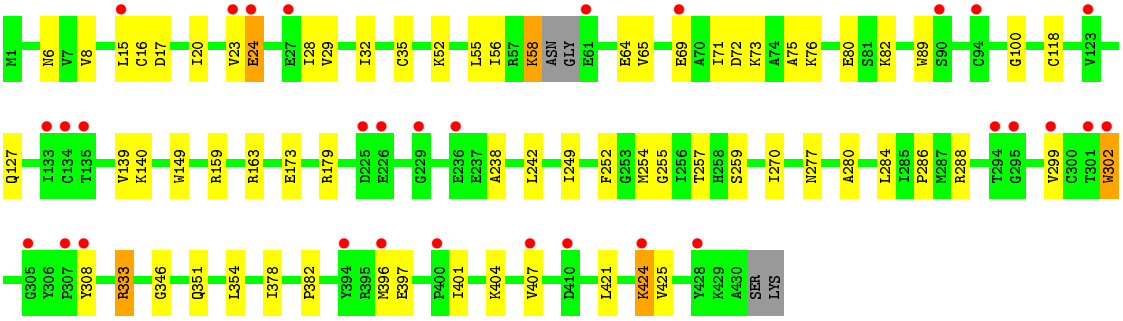
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



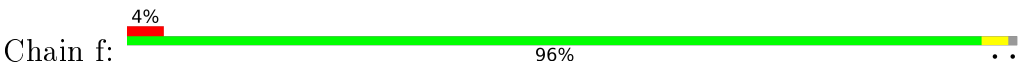


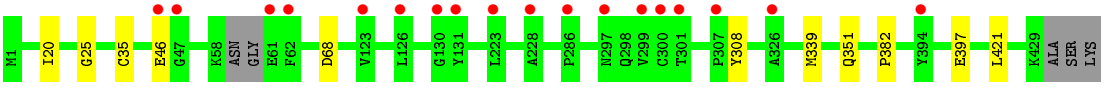
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



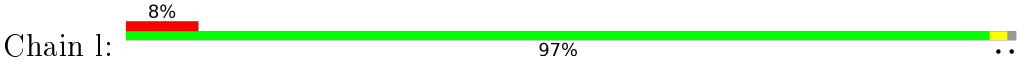


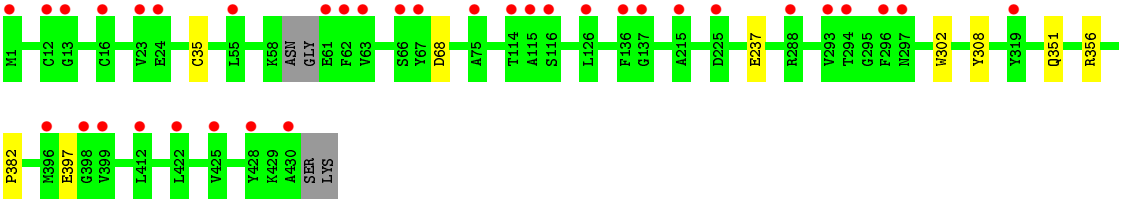
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



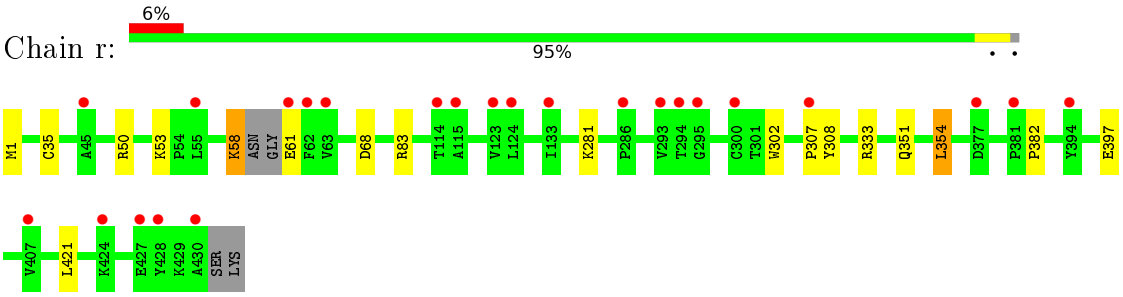


• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

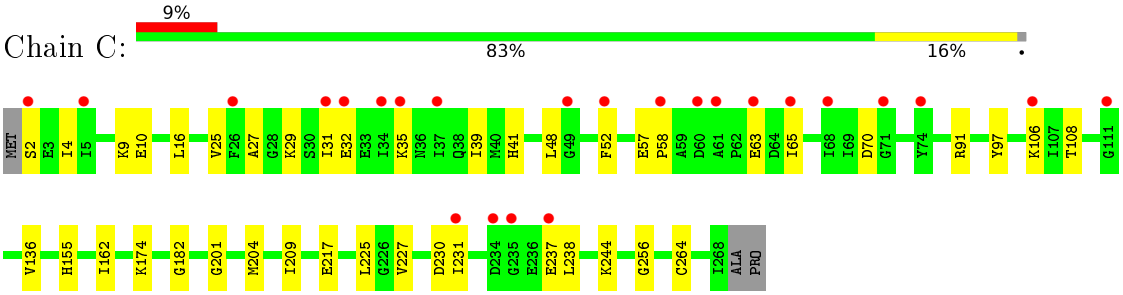




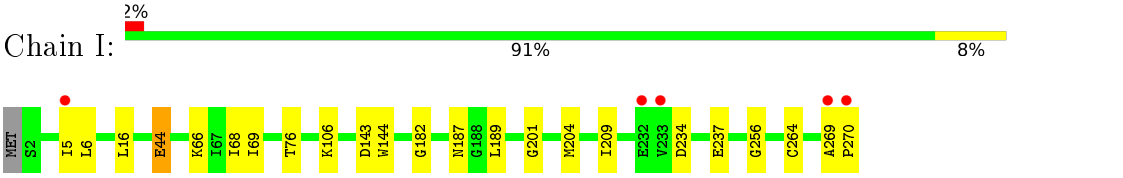
• Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



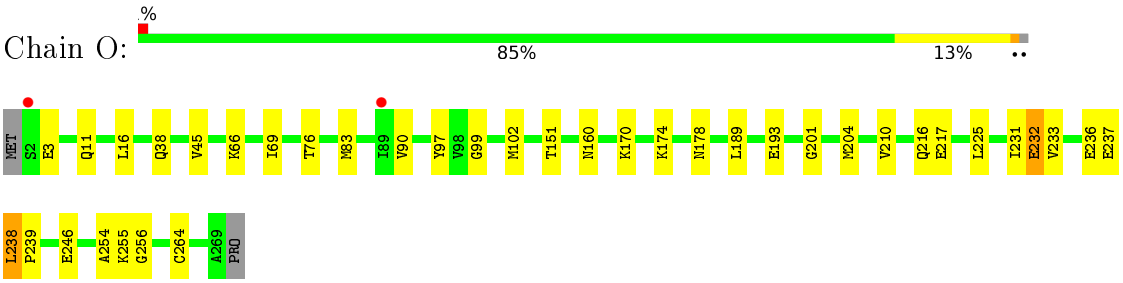
• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



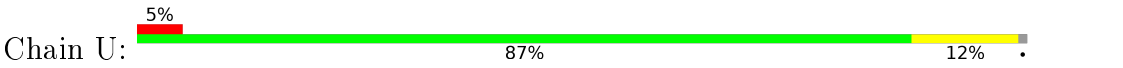
• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

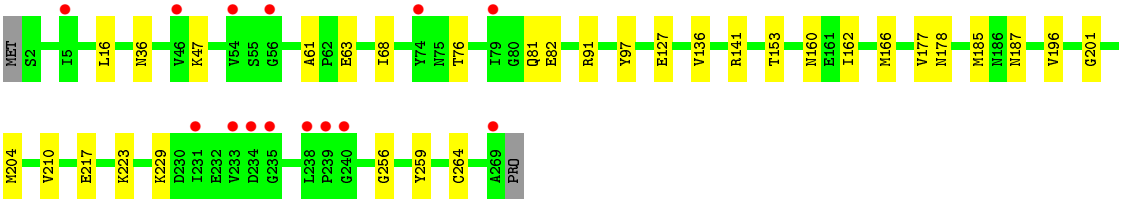


• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

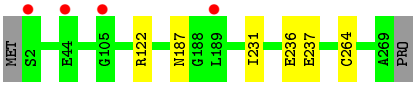


• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

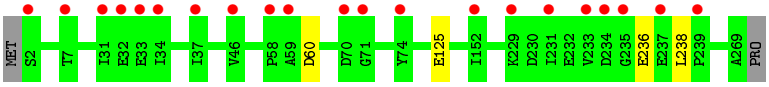




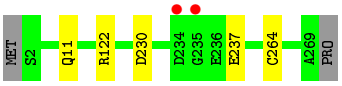
• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



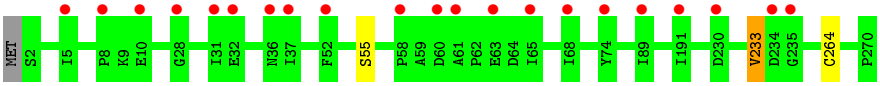
• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



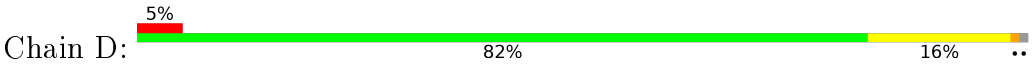
• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

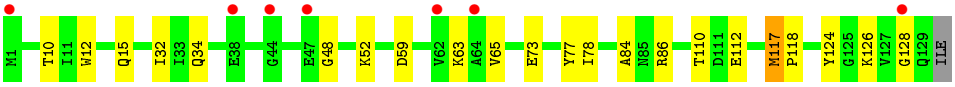


• Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

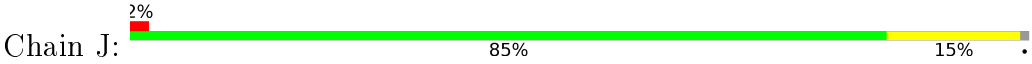


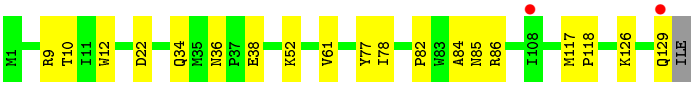
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD





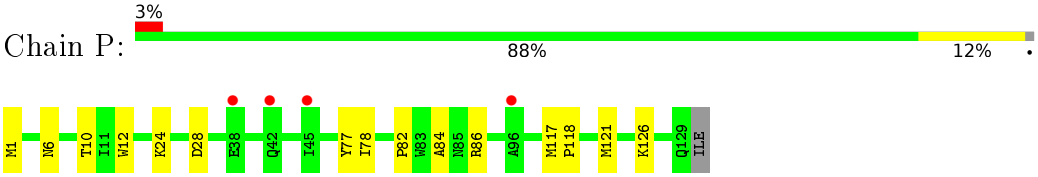
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD





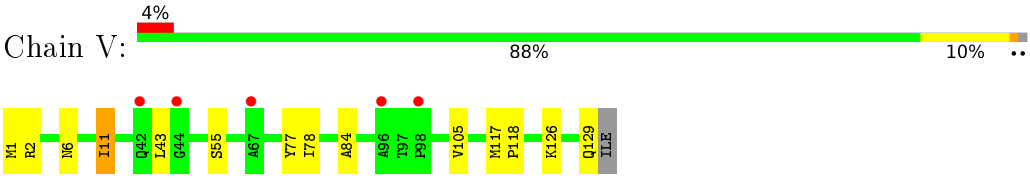
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain P:



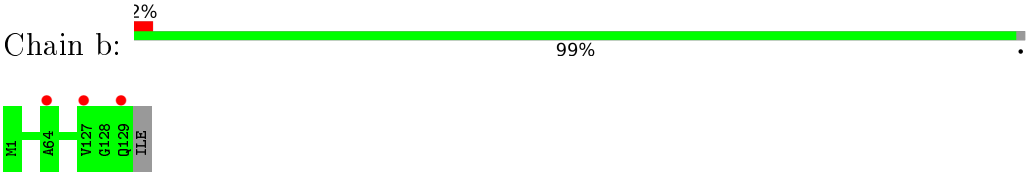
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain V:



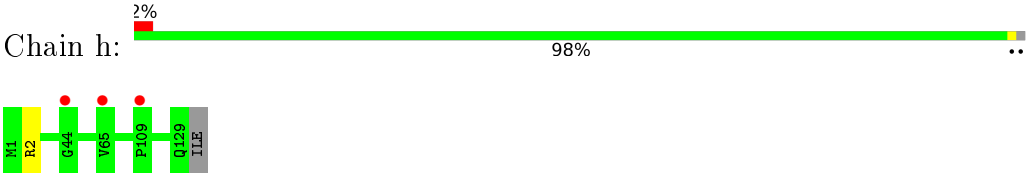
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain b:



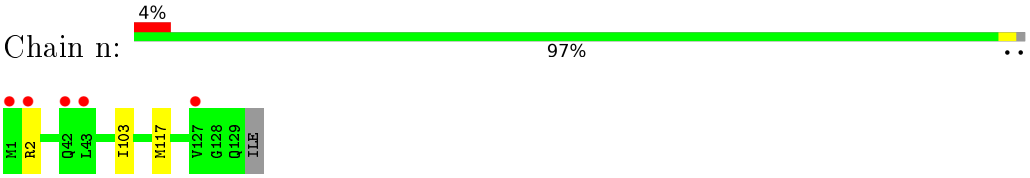
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain h:



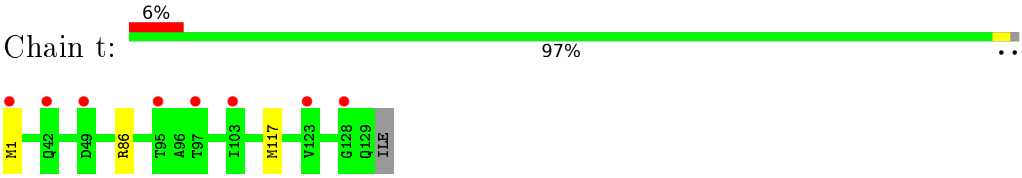
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain n:



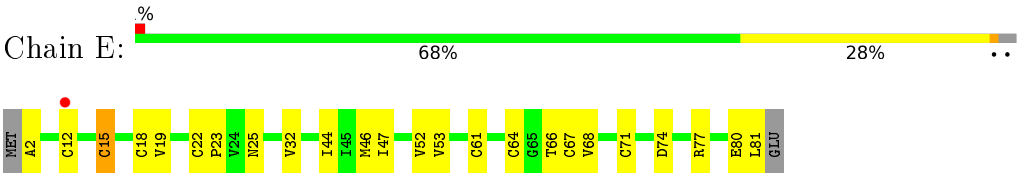
• Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain t:



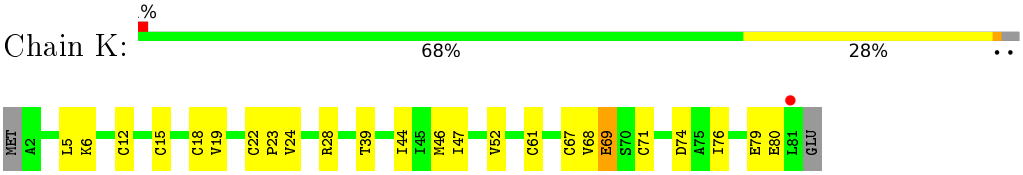
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain E:



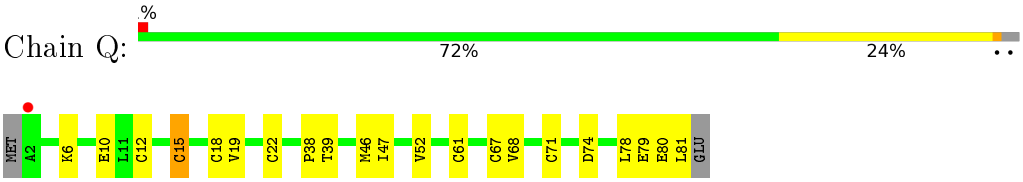
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain K:



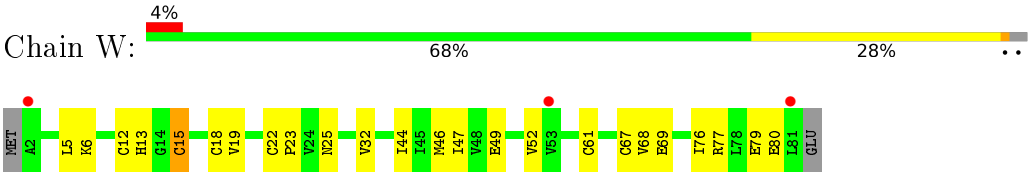
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain Q:



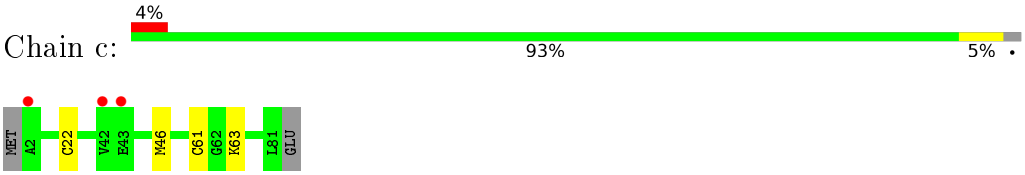
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain W:



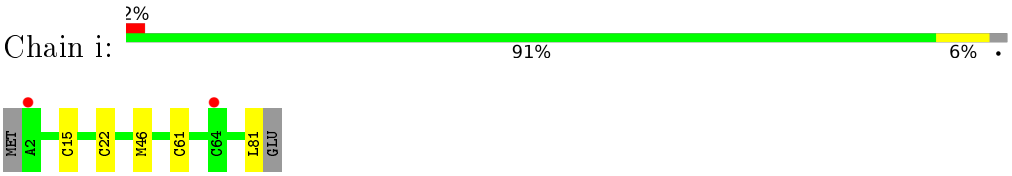
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain c:



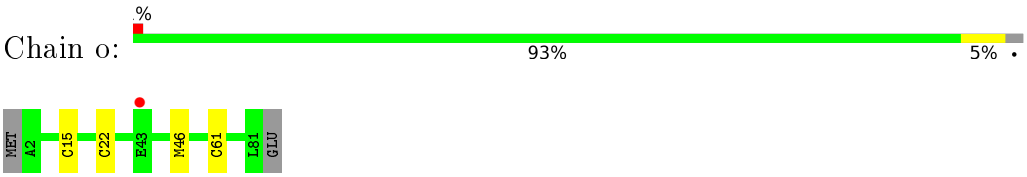
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain i:



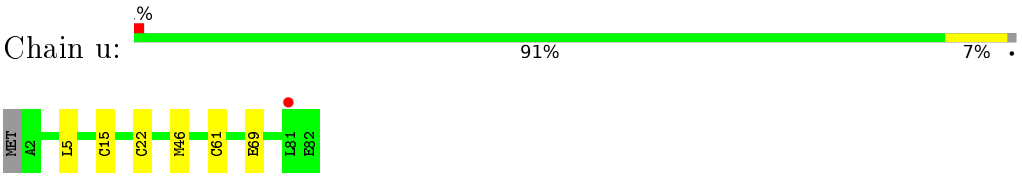
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain o:



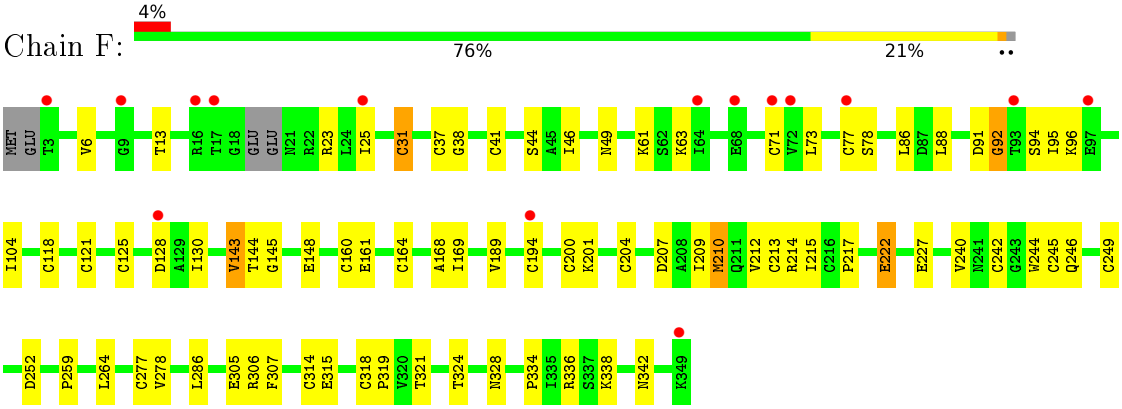
• Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain u:



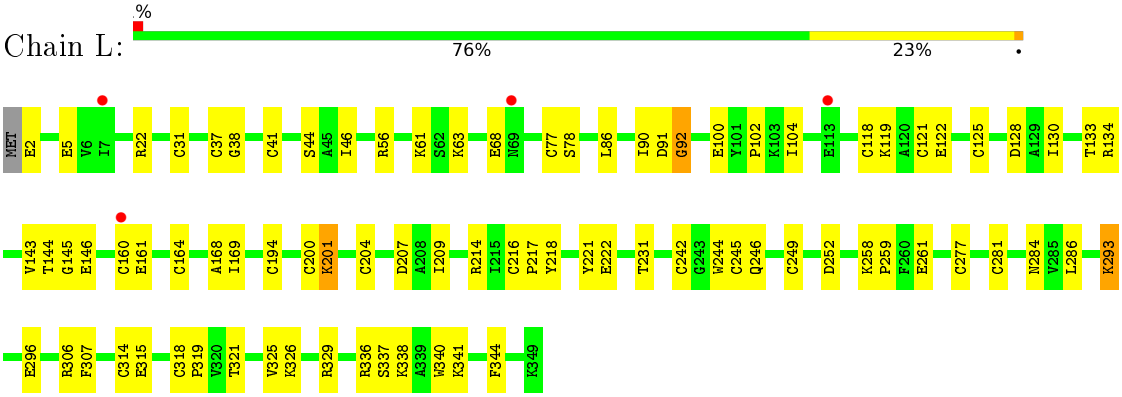
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

Chain F:



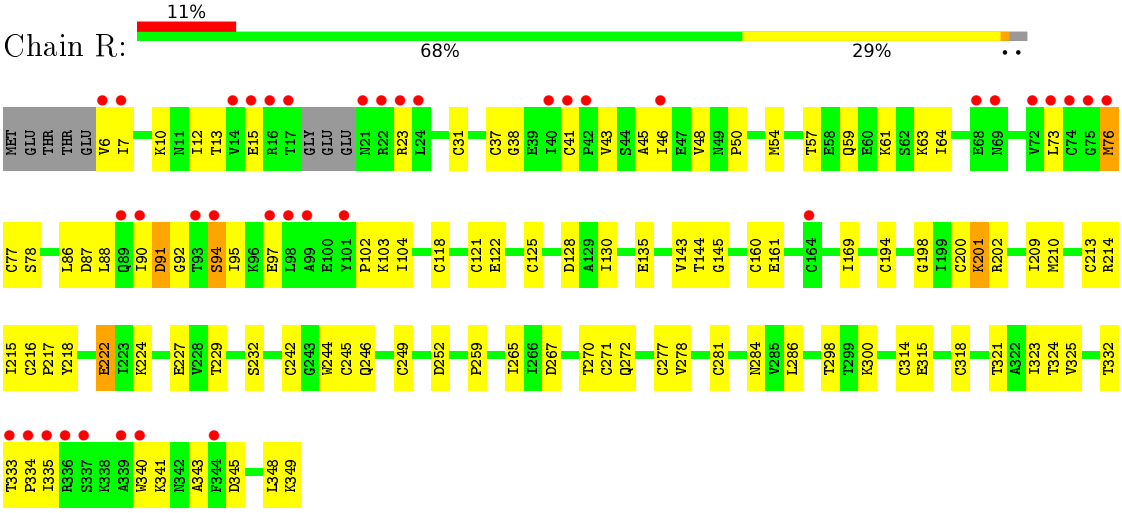
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

Chain L:



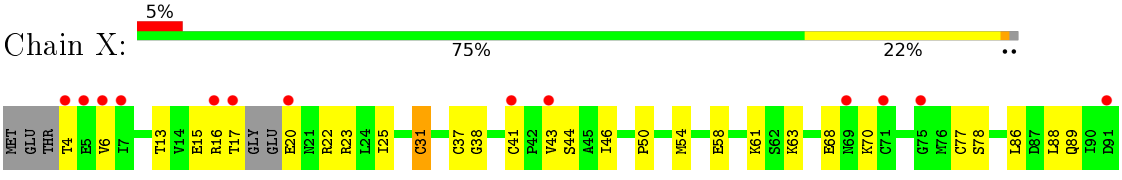
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

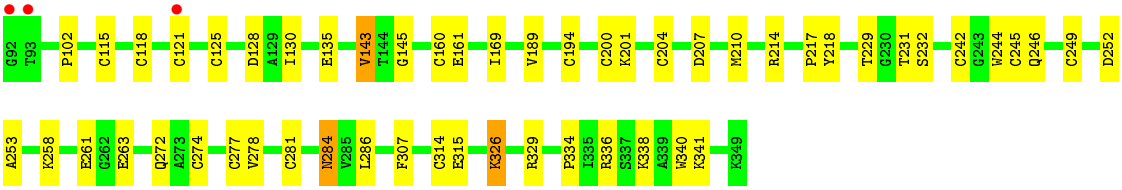
Chain R:



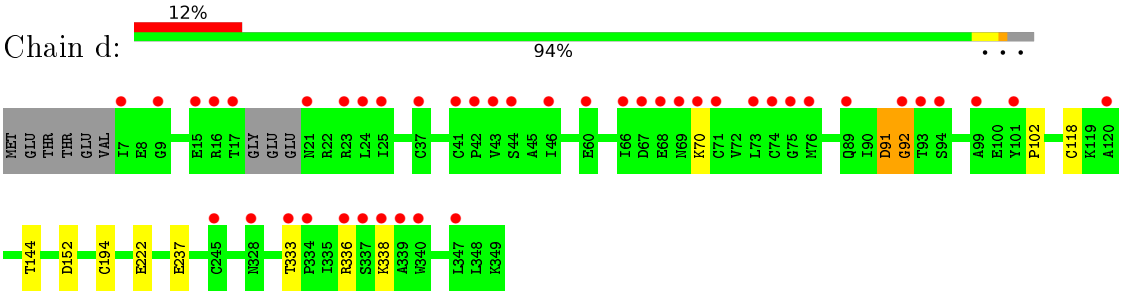
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

Chain X:

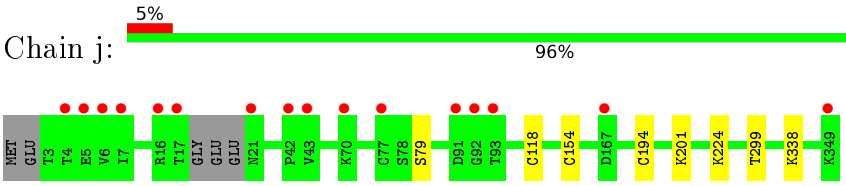




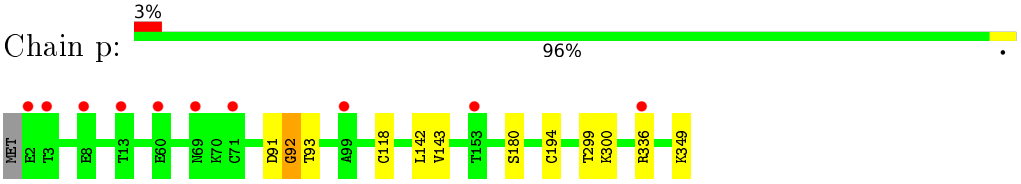
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



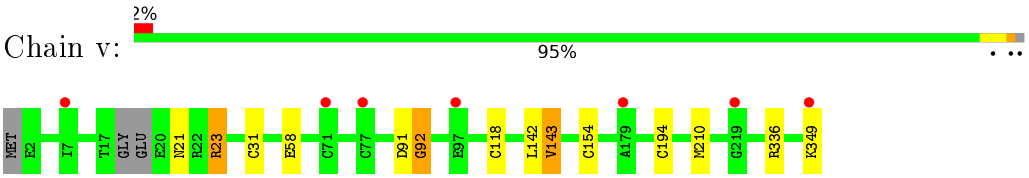
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	174.18Å 173.68Å 183.16Å 89.98° 95.42° 92.14°	Depositor
Resolution (Å)	48.97 – 2.55 48.97 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.97-2.55) 96.7 (48.97-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.259 0.230 , 0.260	Depositor DCC
R_{free} test set	34057 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.118 for -h,k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	114321	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: ZN, MGD, NA, K, CL, MG, H2S, MFN, W, SF4, KCX

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	0.36	3/4523 (0.1%)	0.54	0/6161
1	G	0.32	0/4515	0.54	0/6151
1	M	0.34	0/4515	0.59	4/6151 (0.1%)
1	S	0.35	2/4523 (0.0%)	0.56	3/6161 (0.0%)
1	Y	0.34	0/4515	0.61	5/6151 (0.1%)
1	e	0.33	0/4523	0.54	1/6161 (0.0%)
1	k	0.34	0/4515	0.60	4/6151 (0.1%)
1	q	0.51	9/4523 (0.2%)	0.66	12/6161 (0.2%)
2	B	0.35	1/3434 (0.0%)	0.58	1/4647 (0.0%)
2	H	0.42	2/3421 (0.1%)	0.62	4/4628 (0.1%)
2	N	0.29	0/3439	0.56	1/4654 (0.0%)
2	T	0.35	2/3434 (0.1%)	0.58	4/4647 (0.1%)
2	Z	0.42	5/3426 (0.1%)	0.59	2/4635 (0.0%)
2	f	0.37	2/3421 (0.1%)	0.54	0/4628
2	l	0.33	1/3426 (0.0%)	0.56	2/4635 (0.0%)
2	r	0.50	4/3426 (0.1%)	0.70	10/4635 (0.2%)
3	C	0.36	0/2014	0.64	1/2710 (0.0%)
3	I	0.43	4/2027 (0.2%)	0.57	0/2729
3	O	0.29	0/2019	0.56	1/2717 (0.0%)
3	U	0.30	0/2019	0.58	1/2717 (0.0%)
3	a	0.30	0/2019	0.59	1/2717 (0.0%)
3	g	0.34	0/2019	0.63	2/2717 (0.1%)
3	m	0.31	0/2019	0.59	2/2717 (0.1%)
3	s	0.39	0/2027	0.63	1/2729 (0.0%)
4	D	0.30	0/1016	0.60	0/1379
4	J	0.29	0/1016	0.54	0/1379
4	P	0.27	0/1016	0.56	0/1379
4	V	0.28	0/1016	0.57	0/1379
4	b	0.29	0/1016	0.54	0/1379
4	h	0.30	0/1016	0.59	0/1379
4	n	0.31	0/1016	0.62	1/1379 (0.1%)
4	t	0.37	0/1016	0.71	2/1379 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	E	0.37	0/579	0.53	0/787
5	K	0.43	0/579	0.61	0/787
5	Q	0.32	0/579	0.54	0/787
5	W	0.31	0/579	0.56	0/787
5	c	0.30	0/579	0.57	0/787
5	i	0.33	0/579	0.60	1/787 (0.1%)
5	o	0.34	0/579	0.54	0/787
5	u	0.32	0/588	0.58	0/799
6	F	0.35	1/2667 (0.0%)	0.58	1/3616 (0.0%)
6	L	0.37	1/2695 (0.0%)	0.61	2/3655 (0.1%)
6	R	0.42	3/2640 (0.1%)	0.68	5/3579 (0.1%)
6	X	0.40	2/2665 (0.1%)	0.65	2/3613 (0.1%)
6	d	0.43	2/2633 (0.1%)	0.66	3/3569 (0.1%)
6	j	0.33	0/2663	0.58	0/3611
6	p	0.37	2/2695 (0.1%)	0.59	1/3655 (0.0%)
6	v	0.47	4/2681 (0.1%)	0.65	2/3635 (0.1%)
All	All	0.37	50/113850 (0.0%)	0.59	82/154383 (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	k	0	1
2	T	0	1
2	Z	0	1
6	F	0	1
6	L	0	1
6	R	0	1
6	d	0	1
6	p	0	1
6	v	0	1
All	All	0	9

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	61	GLU	CD-OE1	13.10	1.40	1.25
2	H	61	GLU	CD-OE2	12.01	1.38	1.25
2	r	61	GLU	CD-OE2	11.46	1.38	1.25
1	q	423	LYS	CB-CG	-10.87	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	58	LYS	CD-CE	-9.80	1.26	1.51

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	r	58	LYS	CD-CE-NZ	-19.53	66.79	111.70
2	H	61	GLU	OE1-CD-OE2	12.47	138.26	123.30
2	r	354	LEU	CB-CG-CD1	-12.13	90.38	111.00
1	q	356	ARG	NE-CZ-NH1	-11.58	114.51	120.30
6	v	92	GLY	N-CA-C	11.39	141.59	113.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	91	ASP	Peptide
6	L	91	ASP	Peptide
6	R	91	ASP	Peptide
2	T	58	LYS	Peptide
2	Z	173	GLU	Sidechain

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	4419	0	4272	44	0
1	G	4411	0	4260	54	0
1	M	4411	0	4260	83	0
1	S	4419	0	4270	45	0
1	Y	4411	0	4260	74	0
1	e	4419	0	4271	0	1
1	k	4411	0	4260	0	0
1	q	4419	0	4271	0	0
2	B	3364	0	3307	56	0
2	H	3352	0	3297	40	0
2	N	3369	0	3312	41	0
2	T	3364	0	3307	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	3357	0	3302	45	0
2	f	3352	0	3297	0	0
2	l	3357	0	3302	0	0
2	r	3357	0	3300	0	0
3	C	1982	0	1950	33	0
3	I	1994	0	1962	13	0
3	O	1987	0	1955	29	0
3	U	1987	0	1955	18	0
3	a	1987	0	1955	0	0
3	g	1987	0	1955	0	0
3	m	1987	0	1955	0	0
3	s	1994	0	1962	0	0
4	D	997	0	1021	17	0
4	J	997	0	1022	16	0
4	P	997	0	1022	11	0
4	V	997	0	1022	8	0
4	b	997	0	1022	0	0
4	h	997	0	1022	0	0
4	n	997	0	1022	0	0
4	t	997	0	1022	0	0
5	E	572	0	567	15	0
5	K	572	0	567	14	0
5	Q	572	0	567	13	0
5	W	572	0	567	16	0
5	c	572	0	567	0	0
5	i	572	0	567	0	0
5	o	572	0	567	0	0
5	u	581	0	573	0	0
6	F	2629	0	2588	48	1
6	L	2656	0	2607	54	0
6	R	2602	0	2565	70	0
6	X	2627	0	2584	62	0
6	d	2595	0	2556	0	0
6	j	2625	0	2585	0	0
6	p	2656	0	2607	0	0
6	v	2643	0	2597	0	0
7	A	2	0	0	0	0
7	G	2	0	0	0	0
7	M	2	0	0	0	0
7	S	2	0	0	0	0
7	Y	2	0	0	0	0
7	e	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	k	2	0	0	0	0
7	q	2	0	0	0	0
8	A	53	0	37	1	0
8	G	53	0	37	2	0
8	M	53	0	37	3	0
8	S	53	0	37	3	0
8	Y	53	0	37	5	0
8	e	53	0	37	0	0
8	k	53	0	37	0	0
8	q	53	0	37	0	0
9	A	1	0	0	0	0
9	G	1	0	0	0	0
9	M	1	0	0	0	0
9	S	1	0	0	0	0
9	e	1	0	0	0	0
9	k	1	0	0	0	0
9	q	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
10	F	4	0	0	0	0
10	G	1	0	0	0	0
10	K	1	0	0	0	0
10	L	3	0	0	0	0
10	M	2	0	0	0	0
10	N	1	0	0	0	0
10	Q	1	0	0	0	0
10	R	3	0	0	0	0
10	S	2	0	0	0	0
10	T	1	0	0	0	0
10	X	3	0	0	0	0
10	Y	1	0	0	0	0
10	Z	1	0	0	0	0
10	c	1	0	0	0	0
10	d	2	0	0	0	0
10	e	4	0	0	0	0
10	i	1	0	0	0	0
10	j	6	0	0	0	0
10	k	1	0	0	0	0
10	o	1	0	0	0	0
10	p	3	0	0	0	0
10	q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	r	1	0	0	0	0
10	u	1	0	0	0	0
10	v	7	0	0	0	0
11	B	8	0	0	0	0
11	E	16	0	0	1	0
11	F	72	0	0	0	0
11	H	8	0	0	0	0
11	K	16	0	0	0	0
11	L	64	0	0	0	0
11	N	8	0	0	0	0
11	Q	16	0	0	0	0
11	R	72	0	0	0	0
11	T	8	0	0	0	0
11	W	16	0	0	0	0
11	X	64	0	0	0	0
11	Z	8	0	0	0	0
11	c	16	0	0	0	0
11	d	72	0	0	0	0
11	f	8	0	0	0	0
11	i	16	0	0	0	0
11	j	64	0	0	0	0
11	l	8	0	0	0	0
11	o	16	0	0	0	0
11	p	72	0	0	0	0
11	r	8	0	0	0	0
11	u	16	0	0	0	0
11	v	64	0	0	0	0
12	B	1	0	0	0	0
12	H	1	0	0	0	0
12	N	1	0	0	0	0
12	T	1	0	0	0	0
12	Z	1	0	0	0	0
12	f	1	0	0	0	0
12	l	1	0	0	0	0
12	r	1	0	0	0	0
13	B	94	0	44	1	0
13	H	94	0	44	2	0
13	N	94	0	44	0	0
13	T	94	0	44	1	0
13	Z	94	0	44	1	0
13	f	94	0	44	0	0
13	l	94	0	44	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	r	94	0	44	0	0
14	B	1	0	0	0	0
14	H	1	0	0	0	0
14	N	1	0	0	0	0
14	T	1	0	0	0	0
14	Z	1	0	0	1	0
14	f	1	0	0	0	0
14	l	1	0	0	0	0
14	r	1	0	0	0	0
15	B	1	0	0	0	0
15	H	1	0	0	0	0
15	O	1	0	0	0	0
15	T	1	0	0	0	0
15	Z	1	0	0	0	0
15	f	1	0	0	0	0
15	l	1	0	0	0	0
15	r	1	0	0	0	0
16	N	1	0	0	1	0
17	A	22	0	0	1	0
17	B	12	0	0	0	0
17	C	7	0	0	0	0
17	D	2	0	0	1	0
17	E	1	0	0	0	0
17	F	25	0	0	0	0
17	G	14	0	0	0	0
17	H	20	0	0	0	0
17	I	17	0	0	1	0
17	J	4	0	0	0	0
17	K	8	0	0	1	0
17	L	26	0	0	0	0
17	M	5	0	0	0	0
17	N	24	0	0	0	0
17	O	9	0	0	0	0
17	P	4	0	0	0	0
17	Q	2	0	0	0	0
17	R	6	0	0	0	0
17	S	59	0	0	0	0
17	T	29	0	0	1	0
17	U	10	0	0	0	0
17	V	9	0	0	0	0
17	W	3	0	0	0	0
17	X	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	17	0	0	2	0
17	Z	19	0	0	0	0
17	a	12	0	0	0	0
17	b	4	0	0	0	0
17	c	3	0	0	0	0
17	d	3	0	0	0	0
17	e	40	0	0	0	0
17	f	21	0	0	0	0
17	g	3	0	0	0	0
17	h	3	0	0	0	0
17	i	8	0	0	0	0
17	j	20	0	0	0	0
17	k	9	0	0	0	0
17	l	20	0	0	0	0
17	m	7	0	0	0	0
17	n	4	0	0	0	0
17	o	2	0	0	0	0
17	p	18	0	0	0	0
17	q	27	0	0	0	0
17	r	16	0	0	0	0
17	s	3	0	0	0	0
17	t	3	0	0	0	0
17	u	1	0	0	0	0
17	v	13	0	0	0	0
All	All	114321	0	110251	915	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 8.

The worst 5 of 915 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:Y:418:LYS:NZ	1:Y:422:ARG:NH1	1.72	1.34
1:Y:418:LYS:NZ	1:Y:422:ARG:HH11	0.89	1.33
1:Y:17:VAL:HG23	1:Y:20:GLU:OE1	1.15	1.27
1:M:2:GLU:OE2	1:M:27:LYS:HB2	1.53	1.07
1:G:318:THR:HG22	1:G:320:ASP:H	1.17	1.07

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)
6:F:336:ARG:NH1	1:e:526:GLU:OE1[1_544]	2.01	0.19

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	566/569 (100%)	540 (95%)	25 (4%)	1 (0%)	52	73
1	G	565/569 (99%)	538 (95%)	25 (4%)	2 (0%)	39	60
1	M	565/569 (99%)	542 (96%)	23 (4%)	0	100	100
1	S	566/569 (100%)	540 (95%)	25 (4%)	1 (0%)	52	73
1	Y	565/569 (99%)	539 (95%)	26 (5%)	0	100	100
1	e	566/569 (100%)	542 (96%)	24 (4%)	0	100	100
1	k	565/569 (99%)	540 (96%)	25 (4%)	0	100	100
1	q	566/569 (100%)	542 (96%)	24 (4%)	0	100	100
2	B	427/432 (99%)	407 (95%)	18 (4%)	2 (0%)	34	54
2	H	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	34	54
2	N	428/432 (99%)	413 (96%)	13 (3%)	2 (0%)	34	54
2	T	427/432 (99%)	409 (96%)	14 (3%)	4 (1%)	21	36
2	Z	424/432 (98%)	409 (96%)	14 (3%)	1 (0%)	52	73
2	f	423/432 (98%)	405 (96%)	16 (4%)	2 (0%)	34	54
2	l	424/432 (98%)	408 (96%)	15 (4%)	1 (0%)	52	73
2	r	424/432 (98%)	409 (96%)	13 (3%)	2 (0%)	34	54
3	C	265/270 (98%)	256 (97%)	9 (3%)	0	100	100
3	I	267/270 (99%)	258 (97%)	9 (3%)	0	100	100
3	O	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	U	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	a	266/270 (98%)	257 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	266/270 (98%)	257 (97%)	9 (3%)	0	100	100
3	m	266/270 (98%)	256 (96%)	10 (4%)	0	100	100
3	s	267/270 (99%)	258 (97%)	9 (3%)	0	100	100
4	D	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	J	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	P	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	V	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	b	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	h	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	n	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
4	t	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
5	E	78/82 (95%)	78 (100%)	0	0	100	100
5	K	78/82 (95%)	78 (100%)	0	0	100	100
5	Q	78/82 (95%)	78 (100%)	0	0	100	100
5	W	78/82 (95%)	78 (100%)	0	0	100	100
5	c	78/82 (95%)	78 (100%)	0	0	100	100
5	i	78/82 (95%)	78 (100%)	0	0	100	100
5	o	78/82 (95%)	78 (100%)	0	0	100	100
5	u	79/82 (96%)	79 (100%)	0	0	100	100
6	F	341/349 (98%)	337 (99%)	3 (1%)	1 (0%)	46	66
6	L	346/349 (99%)	340 (98%)	5 (1%)	1 (0%)	46	66
6	R	337/349 (97%)	330 (98%)	7 (2%)	0	100	100
6	X	340/349 (97%)	336 (99%)	4 (1%)	0	100	100
6	d	336/349 (96%)	331 (98%)	3 (1%)	2 (1%)	30	48
6	j	340/349 (97%)	336 (99%)	4 (1%)	0	100	100
6	p	346/349 (99%)	342 (99%)	3 (1%)	1 (0%)	46	66
6	v	342/349 (98%)	337 (98%)	4 (1%)	1 (0%)	46	66
All	All	14422/14656 (98%)	13934 (97%)	462 (3%)	26 (0%)	52	73

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS

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Mol	Chain	Res	Type
6	F	92	GLY
1	G	415	GLU
6	L	92	GLY
1	S	415	GLU

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	470/470 (100%)	466 (99%)	4 (1%)	84 95
1	G	469/470 (100%)	463 (99%)	6 (1%)	76 91
1	M	469/470 (100%)	461 (98%)	8 (2%)	68 88
1	S	470/470 (100%)	461 (98%)	9 (2%)	65 86
1	Y	469/470 (100%)	465 (99%)	4 (1%)	84 95
1	e	470/470 (100%)	461 (98%)	9 (2%)	65 86
1	k	469/470 (100%)	465 (99%)	4 (1%)	84 95
1	q	470/470 (100%)	465 (99%)	5 (1%)	80 93
2	B	359/361 (99%)	346 (96%)	13 (4%)	42 67
2	H	358/361 (99%)	351 (98%)	7 (2%)	63 85
2	N	359/361 (99%)	352 (98%)	7 (2%)	65 86
2	T	359/361 (99%)	351 (98%)	8 (2%)	60 83
2	Z	358/361 (99%)	351 (98%)	7 (2%)	63 85
2	f	358/361 (99%)	350 (98%)	8 (2%)	60 83
2	l	358/361 (99%)	352 (98%)	6 (2%)	68 88
2	r	358/361 (99%)	347 (97%)	11 (3%)	47 73
3	C	202/204 (99%)	200 (99%)	2 (1%)	82 94
3	I	203/204 (100%)	200 (98%)	3 (2%)	72 90
3	O	202/204 (99%)	199 (98%)	3 (2%)	72 90
3	U	202/204 (99%)	199 (98%)	3 (2%)	72 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	a	202/204 (99%)	197 (98%)	5 (2%)	55 80
3	g	202/204 (99%)	200 (99%)	2 (1%)	82 94
3	m	202/204 (99%)	199 (98%)	3 (2%)	72 90
3	s	203/204 (100%)	200 (98%)	3 (2%)	72 90
4	D	110/111 (99%)	109 (99%)	1 (1%)	84 95
4	J	110/111 (99%)	109 (99%)	1 (1%)	84 95
4	P	110/111 (99%)	110 (100%)	0	100 100
4	V	110/111 (99%)	107 (97%)	3 (3%)	52 78
4	b	110/111 (99%)	110 (100%)	0	100 100
4	h	110/111 (99%)	109 (99%)	1 (1%)	84 95
4	n	110/111 (99%)	108 (98%)	2 (2%)	66 87
4	t	110/111 (99%)	109 (99%)	1 (1%)	84 95
5	E	65/67 (97%)	61 (94%)	4 (6%)	23 39
5	K	65/67 (97%)	61 (94%)	4 (6%)	23 39
5	Q	65/67 (97%)	61 (94%)	4 (6%)	23 39
5	W	65/67 (97%)	59 (91%)	6 (9%)	11 20
5	c	65/67 (97%)	61 (94%)	4 (6%)	23 39
5	i	65/67 (97%)	61 (94%)	4 (6%)	23 39
5	o	65/67 (97%)	61 (94%)	4 (6%)	23 39
5	u	66/67 (98%)	60 (91%)	6 (9%)	12 20
6	F	308/312 (99%)	299 (97%)	9 (3%)	50 75
6	L	311/312 (100%)	307 (99%)	4 (1%)	76 91
6	R	305/312 (98%)	298 (98%)	7 (2%)	58 82
6	X	308/312 (99%)	302 (98%)	6 (2%)	65 86
6	d	304/312 (97%)	296 (97%)	8 (3%)	54 79
6	j	308/312 (99%)	300 (97%)	8 (3%)	54 79
6	p	311/312 (100%)	303 (97%)	8 (3%)	54 79
6	v	310/312 (99%)	299 (96%)	11 (4%)	43 68
All	All	12107/12200 (99%)	11861 (98%)	246 (2%)	63 85

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	W	15	CYS
3	a	264	CYS
3	s	264	CYS
5	W	61	CYS
1	Y	407	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	15	ASN
3	a	265	ASN
3	s	81	GLN
1	Y	410	ASN
2	H	297	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	A	178	1,7	6,11,12	0.58	0	7,12,14	1.00	1 (14%)
1	KCX	G	178	1,7	6,11,12	0.58	0	7,12,14	0.96	1 (14%)
1	KCX	M	178	1,7	6,11,12	0.56	0	7,12,14	1.11	1 (14%)
1	KCX	S	178	1,7	6,11,12	0.61	0	7,12,14	1.23	2 (28%)
1	KCX	Y	178	1,7	6,11,12	0.56	0	7,12,14	1.17	1 (14%)
1	KCX	e	178	1,7	6,11,12	0.59	0	7,12,14	0.95	1 (14%)
1	KCX	k	178	1,7	6,11,12	0.55	0	7,12,14	0.98	1 (14%)
1	KCX	q	178	1,7	6,11,12	0.56	0	7,12,14	1.25	2 (28%)

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
1	KCX	A	178	1,7	-	0/6/10/12	0/0/0/0
1	KCX	G	178	1,7	-	0/6/10/12	0/0/0/0
1	KCX	M	178	1,7	-	0/6/10/12	0/0/0/0
1	KCX	S	178	1,7	-	0/6/10/12	0/0/0/0
1	KCX	Y	178	1,7	-	0/6/10/12	0/0/0/0
1	KCX	e	178	1,7	-	0/6/10/12	0/0/0/0
1	KCX	k	178	1,7	-	0/6/10/12	0/0/0/0
1	KCX	q	178	1,7	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	k	178	KCX	O-C-CA	-2.30	119.57	125.72
1	Y	178	KCX	O-C-CA	-2.25	119.68	125.72
1	G	178	KCX	O-C-CA	-2.20	119.83	125.72
1	e	178	KCX	O-C-CA	-2.18	119.86	125.72
1	M	178	KCX	O-C-CA	-2.15	119.96	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 221 ligands modelled in this entry, 8 are modelled with single atom and 97 are monoatomic - leaving 116 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	$\#\|Z\| > 2$
8	MFN	A	603	7	35,54,56	2.20	11 (31%)	41,71,73	1.90	10 (24%)
11	SF4	B	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	B	503	12	41,52,52	1.34	4 (9%)	39,81,81	2.14	10 (25%)
13	MGD	B	504	12	41,52,52	1.40	4 (9%)	39,81,81	2.39	12 (30%)
11	SF4	E	101	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	E	102	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	401	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	402	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	403	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	404	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	405	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	406	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	407	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	408	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	F	409	6	0,12,12	0.00	-	0,24,24	0.00	-
8	MFN	G	603	7	35,54,56	2.09	10 (28%)	41,71,73	1.85	9 (21%)
11	SF4	H	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	H	503	12	41,52,52	1.36	4 (9%)	39,81,81	2.13	10 (25%)
13	MGD	H	504	12	41,52,52	1.34	4 (9%)	39,81,81	2.40	12 (30%)
11	SF4	K	101	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	K	102	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	501	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	502	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	503	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	504	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	505	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	506	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	507	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	L	508	6	0,12,12	0.00	-	0,24,24	0.00	-
8	MFN	M	603	7	35,54,56	2.14	9 (25%)	41,71,73	2.26	15 (36%)
11	SF4	N	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	N	503	12	41,52,52	1.37	4 (9%)	39,81,81	2.11	10 (25%)
13	MGD	N	504	12	41,52,52	1.42	4 (9%)	39,81,81	2.41	12 (30%)
11	SF4	Q	101	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	Q	102	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	401	6	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	SF4	R	402	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	403	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	404	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	405	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	406	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	407	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	408	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	R	409	6	0,12,12	0.00	-	0,24,24	0.00	-
8	MFN	S	603	-	35,54,56	2.18	9 (25%)	41,71,73	1.95	8 (19%)
11	SF4	T	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	T	503	12	41,52,52	1.37	4 (9%)	39,81,81	2.34	9 (23%)
13	MGD	T	504	12	41,52,52	1.38	4 (9%)	39,81,81	2.29	12 (30%)
11	SF4	W	200	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	W	201	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	501	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	502	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	503	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	504	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	505	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	506	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	507	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	X	508	6	0,12,12	0.00	-	0,24,24	0.00	-
8	MFN	Y	603	7	35,54,56	2.12	7 (20%)	41,71,73	1.87	11 (26%)
11	SF4	Z	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	Z	503	12	41,52,52	1.37	4 (9%)	39,81,81	2.14	10 (25%)
13	MGD	Z	504	12	41,52,52	1.40	4 (9%)	39,81,81	2.33	12 (30%)
11	SF4	c	101	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	c	102	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	401	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	402	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	403	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	404	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	405	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	406	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	407	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	408	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	d	409	6	0,12,12	0.00	-	0,24,24	0.00	-
8	MFN	e	603	-	35,54,56	2.13	8 (22%)	41,71,73	1.81	7 (17%)
11	SF4	f	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	f	503	12	41,52,52	1.40	4 (9%)	39,81,81	2.27	9 (23%)
13	MGD	f	504	12	41,52,52	1.40	4 (9%)	39,81,81	2.42	12 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	SF4	i	101	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	i	102	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	501	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	502	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	503	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	504	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	505	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	506	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	507	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	j	508	6	0,12,12	0.00	-	0,24,24	0.00	-
8	MFN	k	603	7	35,54,56	2.17	7 (20%)	41,71,73	2.98	16 (39%)
11	SF4	l	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	l	503	12	41,52,52	1.38	4 (9%)	39,81,81	2.05	9 (23%)
13	MGD	l	504	12	41,52,52	1.35	4 (9%)	39,81,81	2.34	12 (30%)
11	SF4	o	101	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	o	102	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	401	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	402	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	403	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	404	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	405	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	406	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	407	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	408	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	p	409	6	0,12,12	0.00	-	0,24,24	0.00	-
8	MFN	q	603	-	35,54,56	2.15	10 (28%)	41,71,73	1.82	7 (17%)
11	SF4	r	501	2	0,12,12	0.00	-	0,24,24	0.00	-
13	MGD	r	503	12	41,52,52	1.40	4 (9%)	39,81,81	2.20	11 (28%)
13	MGD	r	504	12	41,52,52	1.44	4 (9%)	39,81,81	2.25	12 (30%)
11	SF4	u	101	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	u	102	5	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	501	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	502	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	503	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	504	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	505	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	506	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	507	6	0,12,12	0.00	-	0,24,24	0.00	-
11	SF4	v	508	6	0,12,12	0.00	-	0,24,24	0.00	-

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
8	MFN	A	603	7	-	0/39/61/63	0/1/2/2
11	SF4	B	501	2	-	0/0/48/48	0/6/5/5
13	MGD	B	503	12	-	0/18/66/66	0/6/6/6
13	MGD	B	504	12	-	0/18/66/66	0/6/6/6
11	SF4	E	101	5	-	0/0/48/48	0/6/5/5
11	SF4	E	102	5	-	0/0/48/48	0/6/5/5
11	SF4	F	401	6	-	0/0/48/48	0/6/5/5
11	SF4	F	402	6	-	0/0/48/48	0/6/5/5
11	SF4	F	403	6	-	0/0/48/48	0/6/5/5
11	SF4	F	404	6	-	0/0/48/48	0/6/5/5
11	SF4	F	405	6	-	0/0/48/48	0/6/5/5
11	SF4	F	406	6	-	0/0/48/48	0/6/5/5
11	SF4	F	407	6	-	0/0/48/48	0/6/5/5
11	SF4	F	408	6	-	0/0/48/48	0/6/5/5
11	SF4	F	409	6	-	0/0/48/48	0/6/5/5
8	MFN	G	603	7	-	0/39/61/63	0/1/2/2
11	SF4	H	501	2	-	0/0/48/48	0/6/5/5
13	MGD	H	503	12	-	0/18/66/66	0/6/6/6
13	MGD	H	504	12	-	0/18/66/66	0/6/6/6
11	SF4	K	101	5	-	0/0/48/48	0/6/5/5
11	SF4	K	102	5	-	0/0/48/48	0/6/5/5
11	SF4	L	501	6	-	0/0/48/48	0/6/5/5
11	SF4	L	502	6	-	0/0/48/48	0/6/5/5
11	SF4	L	503	6	-	0/0/48/48	0/6/5/5
11	SF4	L	504	6	-	0/0/48/48	0/6/5/5
11	SF4	L	505	6	-	0/0/48/48	0/6/5/5
11	SF4	L	506	6	-	0/0/48/48	0/6/5/5
11	SF4	L	507	6	-	0/0/48/48	0/6/5/5
11	SF4	L	508	6	-	0/0/48/48	0/6/5/5
8	MFN	M	603	7	-	0/39/61/63	0/1/2/2
11	SF4	N	501	2	-	0/0/48/48	0/6/5/5
13	MGD	N	503	12	-	0/18/66/66	0/6/6/6
13	MGD	N	504	12	-	0/18/66/66	0/6/6/6
11	SF4	Q	101	5	-	0/0/48/48	0/6/5/5
11	SF4	Q	102	5	-	0/0/48/48	0/6/5/5
11	SF4	R	401	6	-	0/0/48/48	0/6/5/5
11	SF4	R	402	6	-	0/0/48/48	0/6/5/5
11	SF4	R	403	6	-	0/0/48/48	0/6/5/5
11	SF4	R	404	6	-	0/0/48/48	0/6/5/5
11	SF4	R	405	6	-	0/0/48/48	0/6/5/5
11	SF4	R	406	6	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	R	407	6	-	0/0/48/48	0/6/5/5
11	SF4	R	408	6	-	0/0/48/48	0/6/5/5
11	SF4	R	409	6	-	0/0/48/48	0/6/5/5
8	MFN	S	603	-	-	0/39/61/63	0/1/2/2
11	SF4	T	501	2	-	0/0/48/48	0/6/5/5
13	MGD	T	503	12	-	0/18/66/66	0/6/6/6
13	MGD	T	504	12	-	0/18/66/66	0/6/6/6
11	SF4	W	200	5	-	0/0/48/48	0/6/5/5
11	SF4	W	201	5	-	0/0/48/48	0/6/5/5
11	SF4	X	501	6	-	0/0/48/48	0/6/5/5
11	SF4	X	502	6	-	0/0/48/48	0/6/5/5
11	SF4	X	503	6	-	0/0/48/48	0/6/5/5
11	SF4	X	504	6	-	0/0/48/48	0/6/5/5
11	SF4	X	505	6	-	0/0/48/48	0/6/5/5
11	SF4	X	506	6	-	0/0/48/48	0/6/5/5
11	SF4	X	507	6	-	0/0/48/48	0/6/5/5
11	SF4	X	508	6	-	0/0/48/48	0/6/5/5
8	MFN	Y	603	7	-	0/39/61/63	0/1/2/2
11	SF4	Z	501	2	-	0/0/48/48	0/6/5/5
13	MGD	Z	503	12	-	0/18/66/66	0/6/6/6
13	MGD	Z	504	12	-	0/18/66/66	0/6/6/6
11	SF4	c	101	5	-	0/0/48/48	0/6/5/5
11	SF4	c	102	5	-	0/0/48/48	0/6/5/5
11	SF4	d	401	6	-	0/0/48/48	0/6/5/5
11	SF4	d	402	6	-	0/0/48/48	0/6/5/5
11	SF4	d	403	6	-	0/0/48/48	0/6/5/5
11	SF4	d	404	6	-	0/0/48/48	0/6/5/5
11	SF4	d	405	6	-	0/0/48/48	0/6/5/5
11	SF4	d	406	6	-	0/0/48/48	0/6/5/5
11	SF4	d	407	6	-	0/0/48/48	0/6/5/5
11	SF4	d	408	6	-	0/0/48/48	0/6/5/5
11	SF4	d	409	6	-	0/0/48/48	0/6/5/5
8	MFN	e	603	-	-	0/39/61/63	0/1/2/2
11	SF4	f	501	2	-	0/0/48/48	0/6/5/5
13	MGD	f	503	12	-	0/18/66/66	0/6/6/6
13	MGD	f	504	12	-	0/18/66/66	0/6/6/6
11	SF4	i	101	5	-	0/0/48/48	0/6/5/5
11	SF4	i	102	5	-	0/0/48/48	0/6/5/5
11	SF4	j	501	6	-	0/0/48/48	0/6/5/5
11	SF4	j	502	6	-	0/0/48/48	0/6/5/5
11	SF4	j	503	6	-	0/0/48/48	0/6/5/5
11	SF4	j	504	6	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	j	505	6	-	0/0/48/48	0/6/5/5
11	SF4	j	506	6	-	0/0/48/48	0/6/5/5
11	SF4	j	507	6	-	0/0/48/48	0/6/5/5
11	SF4	j	508	6	-	0/0/48/48	0/6/5/5
8	MFN	k	603	7	-	0/39/61/63	0/1/2/2
11	SF4	l	501	2	-	0/0/48/48	0/6/5/5
13	MGD	l	503	12	-	0/18/66/66	0/6/6/6
13	MGD	l	504	12	-	0/18/66/66	0/6/6/6
11	SF4	o	101	5	-	0/0/48/48	0/6/5/5
11	SF4	o	102	5	-	0/0/48/48	0/6/5/5
11	SF4	p	401	6	-	0/0/48/48	0/6/5/5
11	SF4	p	402	6	-	0/0/48/48	0/6/5/5
11	SF4	p	403	6	-	0/0/48/48	0/6/5/5
11	SF4	p	404	6	-	0/0/48/48	0/6/5/5
11	SF4	p	405	6	-	0/0/48/48	0/6/5/5
11	SF4	p	406	6	-	0/0/48/48	0/6/5/5
11	SF4	p	407	6	-	0/0/48/48	0/6/5/5
11	SF4	p	408	6	-	0/0/48/48	0/6/5/5
11	SF4	p	409	6	-	0/0/48/48	0/6/5/5
8	MFN	q	603	-	-	0/39/61/63	0/1/2/2
11	SF4	r	501	2	-	0/0/48/48	0/6/5/5
13	MGD	r	503	12	-	0/18/66/66	0/6/6/6
13	MGD	r	504	12	-	0/18/66/66	0/6/6/6
11	SF4	u	101	5	-	0/0/48/48	0/6/5/5
11	SF4	u	102	5	-	0/0/48/48	0/6/5/5
11	SF4	v	501	6	-	0/0/48/48	0/6/5/5
11	SF4	v	502	6	-	0/0/48/48	0/6/5/5
11	SF4	v	503	6	-	0/0/48/48	0/6/5/5
11	SF4	v	504	6	-	0/0/48/48	0/6/5/5
11	SF4	v	505	6	-	0/0/48/48	0/6/5/5
11	SF4	v	506	6	-	0/0/48/48	0/6/5/5
11	SF4	v	507	6	-	0/0/48/48	0/6/5/5
11	SF4	v	508	6	-	0/0/48/48	0/6/5/5

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	k	603	MFN	C23-N4	-5.28	1.39	1.46
8	M	603	MFN	C23-N4	-4.21	1.40	1.46
8	Y	603	MFN	C23-N4	-4.06	1.40	1.46
8	G	603	MFN	C23-N4	-3.40	1.41	1.46
8	q	603	MFN	C23-N4	-3.39	1.41	1.46

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	k	603	MFN	C24-C23-N4	-10.51	91.97	112.93
8	k	603	MFN	C22-C14-C23	-6.47	100.73	113.05
8	A	603	MFN	C8-C9-C10	-5.95	110.67	120.18
8	e	603	MFN	C24-C23-N4	-5.83	101.30	112.93
8	k	603	MFN	C26-C27-C28	-5.82	99.02	113.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	603	MFN	1	0
13	B	503	MGD	1	0
11	E	101	SF4	1	0
8	G	603	MFN	2	0
13	H	503	MGD	2	0
8	M	603	MFN	3	0
8	S	603	MFN	3	0
13	T	504	MGD	1	0
8	Y	603	MFN	5	0
13	Z	504	MGD	1	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	q	1
1	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	356:ARG	C	357:ALA	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	356:ARG	C	357:ALA	N	1.18

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	568/569 (99%)	0.26	11 (1%) 70 74	29, 43, 63, 91	0
1	G	567/569 (99%)	0.44	31 (5%) 29 33	31, 49, 73, 117	0
1	M	567/569 (99%)	0.73	66 (11%) 6 7	34, 55, 81, 113	0
1	S	568/569 (99%)	0.11	10 (1%) 71 76	25, 36, 54, 94	0
1	Y	567/569 (99%)	0.62	57 (10%) 9 10	31, 51, 75, 109	0
1	e	568/569 (99%)	0.14	14 (2%) 61 66	27, 37, 53, 88	0
1	k	567/569 (99%)	0.71	58 (10%) 9 10	33, 56, 80, 102	0
1	q	568/569 (99%)	0.40	21 (3%) 45 51	31, 46, 66, 105	0
2	B	429/432 (99%)	0.47	12 (2%) 56 62	29, 42, 69, 124	0
2	H	427/432 (98%)	0.40	18 (4%) 40 46	26, 38, 61, 87	0
2	N	430/432 (99%)	0.39	24 (5%) 28 33	30, 39, 57, 71	0
2	T	429/432 (99%)	0.45	17 (3%) 42 48	26, 39, 65, 104	0
2	Z	428/432 (99%)	0.53	31 (7%) 18 21	28, 40, 64, 122	0
2	f	427/432 (98%)	0.39	18 (4%) 40 46	25, 39, 61, 109	0
2	l	428/432 (99%)	0.60	35 (8%) 14 16	29, 43, 68, 98	0
2	r	428/432 (99%)	0.57	24 (5%) 28 33	29, 44, 69, 106	0
3	C	267/270 (98%)	0.60	24 (8%) 12 13	35, 53, 78, 108	0
3	I	269/270 (99%)	0.04	5 (1%) 70 74	26, 38, 56, 90	0
3	O	268/270 (99%)	0.02	2 (0%) 89 91	30, 41, 61, 86	0
3	U	268/270 (99%)	0.34	14 (5%) 31 36	28, 46, 70, 110	0
3	a	268/270 (99%)	0.06	4 (1%) 76 80	30, 39, 55, 83	0
3	g	268/270 (99%)	0.46	21 (7%) 16 18	31, 50, 78, 101	0
3	m	268/270 (99%)	0.04	2 (0%) 89 91	28, 41, 62, 93	0
3	s	269/270 (99%)	0.65	21 (7%) 16 18	36, 56, 80, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
4	D	129/130 (99%)	0.49	7 (5%) 29 34	36, 52, 70, 91	0
4	J	129/130 (99%)	0.19	2 (1%) 74 79	31, 41, 56, 66	0
4	P	129/130 (99%)	0.07	4 (3%) 52 58	29, 38, 54, 65	0
4	V	129/130 (99%)	0.27	5 (3%) 43 49	33, 43, 58, 68	0
4	b	129/130 (99%)	0.17	3 (2%) 64 69	33, 41, 56, 83	0
4	h	129/130 (99%)	0.41	3 (2%) 64 69	34, 48, 65, 84	0
4	n	129/130 (99%)	0.22	5 (3%) 43 49	34, 42, 61, 78	0
4	t	129/130 (99%)	0.51	8 (6%) 24 27	37, 51, 70, 83	0
5	E	80/82 (97%)	0.20	1 (1%) 79 83	33, 42, 57, 67	0
5	K	80/82 (97%)	0.18	1 (1%) 79 83	32, 40, 55, 72	0
5	Q	80/82 (97%)	0.24	1 (1%) 79 83	34, 44, 60, 69	0
5	W	80/82 (97%)	0.17	3 (3%) 44 50	31, 39, 52, 68	0
5	c	80/82 (97%)	0.34	3 (3%) 44 50	37, 46, 63, 72	0
5	i	80/82 (97%)	0.08	2 (2%) 61 66	28, 37, 50, 70	0
5	o	80/82 (97%)	0.23	1 (1%) 79 83	34, 43, 57, 71	0
5	u	81/82 (98%)	0.15	1 (1%) 81 84	32, 40, 61, 84	0
6	F	345/349 (98%)	0.32	15 (4%) 39 45	29, 40, 67, 116	0
6	L	348/349 (99%)	0.09	4 (1%) 82 85	28, 38, 60, 83	0
6	R	341/349 (97%)	0.67	38 (11%) 7 8	29, 48, 87, 147	0
6	X	344/349 (98%)	0.32	16 (4%) 35 41	29, 41, 71, 107	0
6	d	340/349 (97%)	0.70	43 (12%) 5 5	28, 49, 96, 130	0
6	j	344/349 (98%)	0.31	16 (4%) 35 41	26, 39, 69, 99	0
6	p	348/349 (99%)	0.15	10 (2%) 55 61	29, 37, 58, 85	0
6	v	346/349 (99%)	0.16	7 (2%) 68 73	27, 38, 63, 87	0
All	All	14540/14656 (99%)	0.38	739 (5%) 32 37	25, 43, 71, 147	0

The worst 5 of 739 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	X	6	VAL	7.5
6	R	14	VAL	7.4
1	k	4	ILE	7.3
6	j	6	VAL	6.7
6	d	336	ARG	6.6

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	KCX	q	178	12/13	0.96	0.15	-	31,35,42,44	0
1	KCX	Y	178	12/13	0.97	0.16	-	36,43,50,51	0
1	KCX	A	178	12/13	0.96	0.17	-	28,35,40,43	0
1	KCX	G	178	12/13	0.94	0.16	-	33,38,40,44	0
1	KCX	e	178	12/13	0.94	0.16	-	21,27,33,35	0
1	KCX	k	178	12/13	0.95	0.20	-	39,45,52,53	0
1	KCX	M	178	12/13	0.95	0.19	-	41,47,48,50	0
1	KCX	S	178	12/13	0.98	0.16	-	25,29,38,39	0

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
9	NA	G	604	1/1	0.87	0.49	14.67	54,54,54,54	0
9	NA	M	604	1/1	0.91	0.61	9.45	56,56,56,56	0
9	NA	q	604	1/1	0.91	0.35	7.67	47,47,47,47	0
9	NA	A	604	1/1	0.90	0.35	7.34	41,41,41,41	0
15	MG	r	507	1/1	0.94	0.41	6.14	34,34,34,34	0
15	MG	B	507	1/1	0.97	0.32	4.79	36,36,36,36	0
15	MG	f	506	1/1	0.98	0.31	4.53	28,28,28,28	0
8	MFN	Y	603	53/55	0.74	0.30	3.80	44,75,101,103	0
15	MG	T	507	1/1	0.98	0.29	3.51	27,27,27,27	0
8	MFN	M	603	53/55	0.57	0.38	3.02	46,85,111,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	NA	k	604	1/1	0.99	0.31	2.46	52,52,52,52	0
15	MG	H	506	1/1	0.98	0.20	2.45	24,24,24,24	0
15	MG	O	301	1/1	0.99	0.24	2.44	31,31,31,31	0
8	MFN	A	603	53/55	0.70	0.28	2.38	40,72,97,107	0
8	MFN	k	603	53/55	0.71	0.29	2.05	51,77,108,110	0
9	NA	e	604	1/1	0.95	0.30	1.81	30,30,30,30	0
15	MG	Z	507	1/1	0.98	0.23	1.77	30,30,30,30	0
8	MFN	q	603	53/55	0.63	0.33	1.75	40,85,115,121	0
8	MFN	G	603	53/55	0.83	0.25	1.53	43,68,86,90	0
15	MG	l	506	1/1	0.98	0.18	1.13	32,32,32,32	0
10	K	Y	604	1/1	0.99	0.31	1.04	38,38,38,38	0
8	MFN	e	603	53/55	0.82	0.25	0.88	35,59,92,101	0
8	MFN	S	603	53/55	0.84	0.22	0.86	30,56,87,89	0
10	K	q	606	1/1	0.98	0.27	0.71	47,47,47,47	0
14	H2S	T	505	1/1	0.99	0.25	0.28	50,50,50,50	0
11	SF4	f	501	8/8	0.96	0.18	0.22	38,41,64,66	0
13	MGD	f	503	47/47	0.97	0.17	0.11	26,37,43,46	0
13	MGD	T	504	47/47	0.95	0.19	0.09	25,37,43,55	0
13	MGD	T	503	47/47	0.97	0.19	0.06	28,38,46,47	0
13	MGD	Z	504	47/47	0.95	0.17	0.03	23,37,43,65	0
13	MGD	Z	503	47/47	0.95	0.17	0.01	29,37,45,56	0
13	MGD	N	504	47/47	0.97	0.15	-0.30	24,32,40,44	0
13	MGD	H	503	47/47	0.98	0.16	-0.30	29,35,41,47	0
13	MGD	B	503	47/47	0.97	0.17	-0.38	34,40,48,51	0
10	K	k	605	1/1	0.99	0.21	-0.45	36,36,36,36	0
13	MGD	l	504	47/47	0.97	0.17	-0.48	25,36,47,50	0
13	MGD	H	504	47/47	0.97	0.17	-0.49	21,32,38,41	0
13	MGD	N	503	47/47	0.98	0.15	-0.52	26,34,43,48	0
11	SF4	N	501	8/8	0.96	0.16	-0.52	30,38,48,55	0
13	MGD	l	503	47/47	0.97	0.15	-0.53	30,37,44,51	0
13	MGD	r	504	47/47	0.96	0.17	-0.55	27,36,45,47	0
10	K	A	605	1/1	0.99	0.17	-0.59	49,49,49,49	0
13	MGD	B	504	47/47	0.97	0.16	-0.61	27,36,42,44	0
10	K	q	605	1/1	0.99	0.16	-0.65	47,47,47,47	0
10	K	G	605	1/1	0.99	0.17	-0.72	62,62,62,62	0
11	SF4	T	501	8/8	0.97	0.15	-0.75	28,39,53,60	0
10	K	r	506	1/1	0.97	0.14	-0.76	57,57,57,57	0
13	MGD	r	503	47/47	0.96	0.17	-0.80	37,46,53,55	0
10	K	F	413	1/1	0.97	0.13	-0.85	40,40,40,40	0
10	K	B	506	1/1	0.97	0.12	-0.86	54,54,54,54	0
10	K	M	605	1/1	0.98	0.21	-0.90	37,37,37,37	0
13	MGD	f	504	47/47	0.97	0.14	-0.94	23,33,38,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	K	j	509	1/1	0.98	0.09	-0.97	37,37,37,37	0
10	K	v	510	1/1	0.96	0.11	-1.03	57,57,57,57	0
10	K	e	606	1/1	0.98	0.17	-1.06	37,37,37,37	0
9	NA	S	604	1/1	0.98	0.15	-1.16	32,32,32,32	0
11	SF4	H	501	8/8	0.96	0.14	-1.23	28,33,40,45	0
11	SF4	r	501	8/8	0.97	0.15	-1.25	31,43,47,51	0
11	SF4	B	501	8/8	0.96	0.13	-1.31	29,38,55,56	0
11	SF4	d	406	8/8	0.97	0.10	-1.32	34,42,54,61	0
11	SF4	Z	501	8/8	0.96	0.12	-1.40	26,36,44,53	0
7	ZN	S	601	1/1	0.99	0.15	-1.45	40,40,40,40	0
10	K	v	512	1/1	0.92	0.11	-1.46	56,56,56,56	0
10	K	j	514	1/1	0.97	0.12	-1.49	48,48,48,48	0
10	K	T	506	1/1	0.95	0.13	-1.51	59,59,59,59	0
11	SF4	p	403	8/8	0.97	0.10	-1.54	20,35,47,51	0
11	SF4	c	102	8/8	0.96	0.11	-1.56	42,53,64,69	0
10	K	M	606	1/1	0.96	0.16	-1.58	55,55,55,55	0
11	SF4	d	405	8/8	0.95	0.09	-1.62	38,43,61,62	0
11	SF4	v	504	8/8	0.98	0.11	-1.62	18,36,41,42	0
10	K	X	511	1/1	0.92	0.10	-1.63	59,59,59,59	0
11	SF4	E	101	8/8	0.97	0.10	-1.64	36,43,51,58	0
11	SF4	X	508	8/8	0.97	0.08	-1.75	26,29,41,46	0
11	SF4	R	402	8/8	0.97	0.11	-1.77	28,41,51,59	0
11	SF4	o	102	8/8	0.97	0.09	-1.77	31,38,49,51	0
11	SF4	L	508	8/8	0.97	0.09	-1.78	27,34,46,52	0
7	ZN	e	601	1/1	0.99	0.12	-1.81	38,38,38,38	0
11	SF4	L	502	8/8	0.97	0.10	-1.81	27,40,50,52	0
11	SF4	R	407	8/8	0.96	0.09	-1.85	23,35,43,46	0
11	SF4	u	102	8/8	0.98	0.11	-1.85	26,34,43,46	0
11	SF4	W	200	8/8	0.97	0.10	-1.88	32,40,47,54	0
11	SF4	X	506	8/8	0.97	0.09	-1.89	22,31,42,42	0
10	K	p	411	1/1	0.95	0.09	-1.90	57,57,57,57	0
10	K	S	605	1/1	0.98	0.17	-1.90	32,32,32,32	0
10	K	F	411	1/1	0.94	0.07	-1.90	38,38,38,38	0
7	ZN	e	602	1/1	0.99	0.11	-1.92	34,34,34,34	0
11	SF4	v	505	8/8	0.97	0.09	-1.93	33,39,51,51	0
11	SF4	p	402	8/8	0.97	0.11	-1.94	28,37,44,57	0
10	K	e	607	1/1	0.97	0.06	-1.97	51,51,51,51	0
11	SF4	F	408	8/8	0.96	0.09	-1.99	26,33,40,49	0
10	K	R	411	1/1	0.94	0.07	-2.03	59,59,59,59	0
11	SF4	v	508	8/8	0.97	0.07	-2.04	27,41,48,52	0
7	ZN	M	601	1/1	0.98	0.13	-2.05	51,51,51,51	0
11	SF4	j	504	8/8	0.97	0.10	-2.07	25,37,42,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	SF4	X	501	8/8	0.97	0.09	-2.08	34,41,58,62	0
11	SF4	Q	102	8/8	0.97	0.10	-2.10	32,45,54,63	0
11	SF4	d	408	8/8	0.96	0.09	-2.11	20,34,50,59	0
11	SF4	j	508	8/8	0.98	0.08	-2.12	22,36,40,59	0
10	K	N	507	1/1	0.97	0.09	-2.14	55,55,55,55	0
11	SF4	F	404	8/8	0.98	0.07	-2.14	22,35,44,57	0
11	SF4	F	401	8/8	0.96	0.10	-2.14	26,38,46,46	0
11	SF4	E	102	8/8	0.97	0.11	-2.18	33,37,52,61	0
11	SF4	i	101	8/8	0.95	0.10	-2.18	26,34,41,47	0
7	ZN	Y	602	1/1	0.99	0.09	-2.19	47,47,47,47	0
11	SF4	l	501	8/8	0.94	0.15	-2.20	30,37,53,53	0
10	K	X	510	1/1	0.95	0.08	-2.20	52,52,52,52	0
11	SF4	F	403	8/8	0.97	0.08	-2.22	41,48,60,66	0
7	ZN	A	601	1/1	0.99	0.13	-2.28	40,40,40,40	0
11	SF4	p	406	8/8	0.96	0.08	-2.30	24,37,43,44	0
11	SF4	R	406	8/8	0.97	0.07	-2.32	33,36,50,59	0
11	SF4	p	404	8/8	0.97	0.09	-2.34	20,30,41,42	0
10	K	X	509	1/1	0.98	0.10	-2.36	42,42,42,42	0
11	SF4	K	101	8/8	0.98	0.10	-2.37	25,34,43,52	0
11	SF4	X	503	8/8	0.98	0.10	-2.40	28,33,40,61	0
11	SF4	d	402	8/8	0.97	0.11	-2.41	37,48,56,66	0
11	SF4	X	507	8/8	0.96	0.09	-2.43	30,31,40,48	0
10	K	e	605	1/1	0.98	0.12	-2.43	34,34,34,34	0
11	SF4	o	101	8/8	0.97	0.10	-2.43	27,35,45,55	0
10	K	F	410	1/1	0.98	0.09	-2.47	53,53,53,53	0
10	K	R	412	1/1	0.89	0.07	-2.48	61,61,61,61	0
10	K	Z	506	1/1	0.90	0.11	-2.49	63,63,63,63	0
10	K	R	410	1/1	0.99	0.04	-2.50	40,40,40,40	0
7	ZN	Y	601	1/1	0.99	0.08	-2.50	45,45,45,45	0
11	SF4	p	401	8/8	0.97	0.08	-2.51	24,34,47,52	0
11	SF4	j	507	8/8	0.97	0.09	-2.55	16,26,43,45	0
11	SF4	p	405	8/8	0.98	0.08	-2.56	17,21,36,39	0
11	SF4	L	504	8/8	0.98	0.11	-2.58	25,31,39,41	0
11	SF4	W	201	8/8	0.97	0.07	-2.59	21,33,41,47	0
7	ZN	k	601	1/1	0.99	0.13	-2.59	46,46,46,46	0
7	ZN	A	602	1/1	0.99	0.12	-2.63	41,41,41,41	0
11	SF4	R	408	8/8	0.98	0.06	-2.64	21,28,40,41	0
11	SF4	L	503	8/8	0.97	0.08	-2.66	24,34,46,47	0
7	ZN	k	602	1/1	0.99	0.13	-2.68	44,44,44,44	0
11	SF4	p	407	8/8	0.97	0.07	-2.69	25,32,44,51	0
11	SF4	j	502	8/8	0.96	0.08	-2.70	18,31,50,53	0
11	SF4	L	507	8/8	0.98	0.08	-2.70	21,27,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	ZN	q	602	1/1	0.99	0.12	-2.70	39,39,39,39	0
11	SF4	X	502	8/8	0.97	0.08	-2.72	22,36,39,53	0
11	SF4	u	101	8/8	0.97	0.10	-2.74	25,39,46,61	0
11	SF4	F	406	8/8	0.97	0.06	-2.75	20,35,46,49	0
11	SF4	i	102	8/8	0.95	0.09	-2.76	20,31,41,52	0
11	SF4	j	503	8/8	0.97	0.08	-2.76	33,38,44,49	0
7	ZN	S	602	1/1	0.99	0.13	-2.80	32,32,32,32	0
11	SF4	F	407	8/8	0.96	0.08	-2.82	29,31,44,53	0
11	SF4	F	402	8/8	0.97	0.10	-2.84	18,36,46,49	0
11	SF4	d	403	8/8	0.96	0.05	-2.88	60,74,85,92	0
11	SF4	F	409	8/8	0.96	0.08	-2.89	18,29,38,39	0
11	SF4	p	408	8/8	0.98	0.09	-2.90	21,34,40,44	0
11	SF4	X	504	8/8	0.93	0.08	-2.91	25,30,48,57	0
11	SF4	j	501	8/8	0.96	0.08	-2.93	27,38,44,57	0
10	K	v	514	1/1	0.94	0.10	-2.94	42,42,42,42	0
11	SF4	j	506	8/8	0.97	0.07	-2.95	25,30,42,43	0
11	SF4	R	404	8/8	0.96	0.08	-2.97	48,54,65,78	0
11	SF4	c	101	8/8	0.96	0.09	-2.99	39,45,51,66	0
11	SF4	R	401	8/8	0.96	0.08	-3.02	31,47,53,59	0
11	SF4	v	501	8/8	0.98	0.07	-3.04	20,33,44,46	0
11	SF4	d	401	8/8	0.96	0.09	-3.07	34,50,53,59	0
7	ZN	G	602	1/1	0.99	0.12	-3.12	40,40,40,40	0
11	SF4	d	404	8/8	0.94	0.07	-3.15	44,57,65,69	0
10	K	p	412	1/1	0.94	0.08	-3.16	53,53,53,53	0
11	SF4	F	405	8/8	0.96	0.08	-3.18	29,37,49,56	0
11	SF4	v	503	8/8	0.97	0.09	-3.20	27,31,39,44	0
10	K	L	510	1/1	0.98	0.04	-3.24	52,52,52,52	0
10	K	S	606	1/1	0.98	0.09	-3.29	46,46,46,46	0
11	SF4	R	405	8/8	0.97	0.07	-3.35	32,44,55,65	0
11	SF4	R	409	8/8	0.97	0.09	-3.35	31,35,47,50	0
11	SF4	v	506	8/8	0.98	0.08	-3.43	19,27,43,47	0
11	SF4	L	501	8/8	0.97	0.05	-3.49	21,34,47,49	0
11	SF4	p	409	8/8	0.96	0.07	-3.50	28,41,43,45	0
10	K	j	513	1/1	0.96	0.05	-3.56	53,53,53,53	0
11	SF4	K	102	8/8	0.97	0.08	-3.58	27,41,47,60	0
11	SF4	d	409	8/8	0.97	0.06	-3.61	24,29,38,60	0
11	SF4	j	505	8/8	0.96	0.06	-3.65	33,47,54,55	0
11	SF4	X	505	8/8	0.96	0.06	-3.77	33,46,57,60	0
10	K	j	511	1/1	0.99	0.05	-3.78	35,35,35,35	0
10	K	j	510	1/1	0.97	0.05	-3.79	49,49,49,49	0
11	SF4	L	505	8/8	0.98	0.07	-3.95	22,32,41,49	0
11	SF4	R	403	8/8	0.96	0.06	-4.00	67,74,83,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	SF4	Q	101	8/8	0.97	0.07	-4.04	23,36,48,49	0
7	ZN	G	601	1/1	1.00	0.11	-4.11	41,41,41,41	0
7	ZN	M	602	1/1	0.99	0.07	-4.37	46,46,46,46	0
10	K	L	509	1/1	0.96	0.08	-4.52	43,43,43,43	0
10	K	d	410	1/1	0.98	0.06	-4.52	47,47,47,47	0
11	SF4	v	502	8/8	0.97	0.07	-4.73	15,26,36,42	0
7	ZN	q	601	1/1	0.99	0.09	-4.77	39,39,39,39	0
11	SF4	L	506	8/8	0.98	0.07	-5.13	15,26,33,44	0
10	K	v	511	1/1	0.96	0.09	-5.25	53,53,53,53	0
11	SF4	d	407	8/8	0.98	0.08	-6.43	34,42,53,55	0
11	SF4	v	507	8/8	0.96	0.07	-7.13	21,33,45,47	0
14	H2S	B	505	1/1	1.00	0.11	-7.73	44,44,44,44	0
10	K	v	509	1/1	0.94	0.07	-10.65	58,58,58,58	0
12	W	T	502	1/1	1.00	0.18	-	49,49,49,49	0
10	K	j	512	1/1	0.99	0.05	-	58,58,58,58	0
10	K	i	103	1/1	0.99	0.08	-	36,36,36,36	0
14	H2S	N	505	1/1	0.99	0.25	-	50,50,50,50	0
10	K	K	103	1/1	0.95	0.08	-	48,48,48,48	0
10	K	o	103	1/1	0.96	0.09	-	42,42,42,42	0
10	K	e	608	1/1	0.90	0.10	-	68,68,68,68	0
14	H2S	l	505	1/1	0.99	0.29	-	66,66,66,66	0
12	W	r	502	1/1	1.00	0.14	-	48,48,48,48	0
10	K	Q	103	1/1	0.97	0.10	-	53,53,53,53	0
14	H2S	f	505	1/1	1.00	0.16	-	38,38,38,38	0
10	K	L	511	1/1	0.87	0.16	-	80,80,80,80	0
12	W	B	502	1/1	1.00	0.13	-	43,43,43,43	0
10	K	c	103	1/1	0.95	0.05	-	57,57,57,57	0
14	H2S	r	505	1/1	0.99	0.18	-	52,52,52,52	0
10	K	E	103	1/1	0.98	0.06	-	43,43,43,43	0
10	K	u	103	1/1	0.98	0.16	-	53,53,53,53	0
10	K	v	515	1/1	0.80	0.10	-	78,78,78,78	0
12	W	N	502	1/1	1.00	0.12	-	34,34,34,34	0
12	W	H	502	1/1	1.00	0.14	-	37,37,37,37	0
12	W	Z	502	1/1	0.99	0.21	-	63,63,63,63	0
16	CL	N	506	1/1	0.83	0.12	-	62,62,62,62	0
12	W	f	502	1/1	1.00	0.20	-	52,52,52,52	0
14	H2S	H	505	1/1	1.00	0.17	-	41,41,41,41	0
10	K	p	410	1/1	0.96	0.12	-	63,63,63,63	0
10	K	d	411	1/1	0.96	0.09	-	60,60,60,60	0
12	W	l	502	1/1	1.00	0.17	-	48,48,48,48	0
10	K	v	513	1/1	0.94	0.09	-	59,59,59,59	0
14	H2S	Z	505	1/1	0.99	0.20	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	K	F	412	1/1	0.96	0.05	-	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.