



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2016 – 02:17 PM EST

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

The following versions of software and data (see [references ⓘ](#)) 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

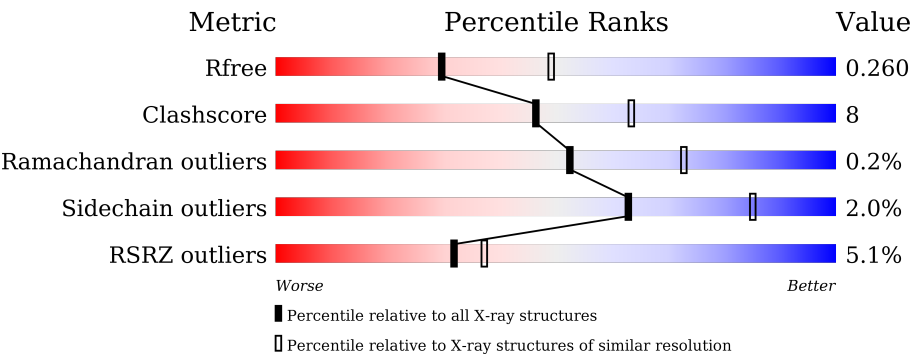
1 Overall quality at a glance i

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 $\leq 5\%$. 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	<div><div>2%</div><div>87%</div><div>13%</div></div>
1	G	569	<div><div>5%</div><div>86%</div><div>13%</div><div>.</div></div>
1	M	569	<div><div>12%</div><div>82%</div><div>17%</div><div>.</div></div>
1	S	569	<div><div>2%</div><div>87%</div><div>12%</div><div>.</div></div>
1	Y	569	<div><div>10%</div><div>87%</div><div>12%</div><div>.</div></div>
1	e	569	<div><div>2%</div><div>98%</div><div>.</div></div>

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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	
5	E	82	
5	K	82	
5	Q	82	
5	W	82	
5	c	82	
5	i	82	
5	o	82	
5	u	82	
6	F	349	
6	L	349	
6	R	349	
6	X	349	
6	d	349	
6	j	349	
6	p	349	
6	v	349	

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			

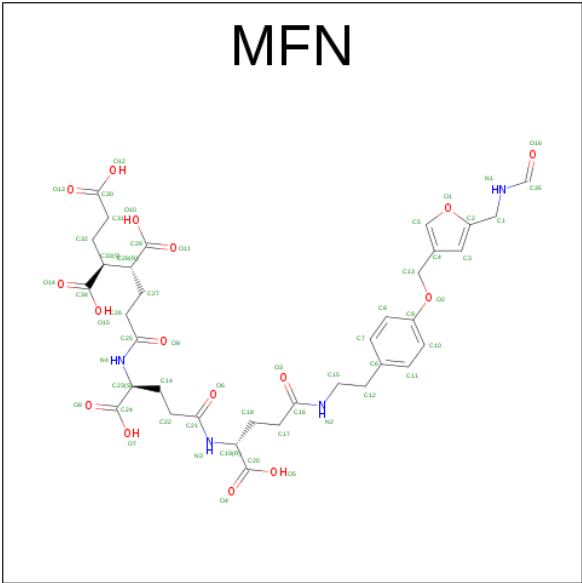
- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdF.

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	0	0
			2	2		
7	q	2	Total	Zn	0	0
			2	2		
7	k	2	Total	Zn	0	0
			2	2		
7	e	2	Total	Zn	0	0
			2	2		
7	A	2	Total	Zn	0	0
			2	2		
7	Y	2	Total	Zn	0	0
			2	2		
7	S	2	Total	Zn	0	0
			2	2		
7	M	2	Total	Zn	0	0
			2	2		

- 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: C₃₅H₄₄N₄O₁₆).



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

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

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

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

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

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

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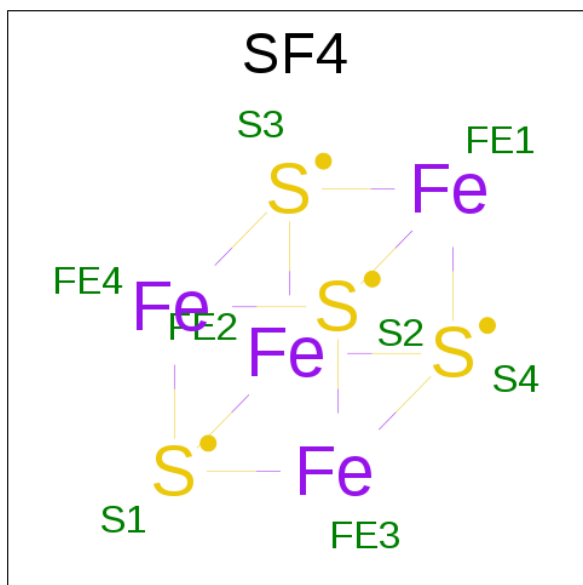
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	N	1	Total K 1 1	0	0
10	X	3	Total K 3 3	0	0
10	o	1	Total K 1 1	0	0
10	S	2	Total K 2 2	0	0
10	p	3	Total K 3 3	0	0
10	k	1	Total K 1 1	0	0
10	E	1	Total K 1 1	0	0
10	A	1	Total K 1 1	0	0
10	R	3	Total K 3 3	0	0
10	M	2	Total K 2 2	0	0
10	j	6	Total K 6 6	0	0
10	e	4	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	0	0
			1	1		
10	Y	1	Total	K	0	0
			1	1		
10	F	4	Total	K	0	0
			4	4		

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

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

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

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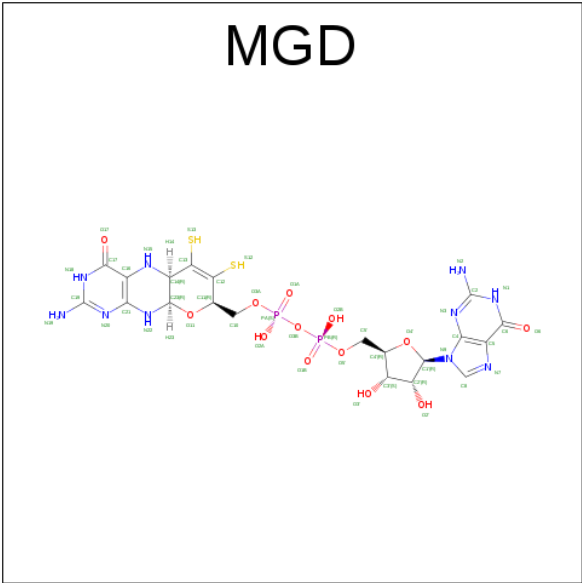
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	o	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	p	1	Total 8	Fe 4	S 4	0	0
11	r	1	Total 8	Fe 4	S 4	0	0
11	u	1	Total 8	Fe 4	S 4	0	0
11	u	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 4	0	0
11	v	1	Total 8	Fe 4	S 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	0	0
			1	1		
12	B	1	Total	W	0	0
			1	1		
12	Z	1	Total	W	0	0
			1	1		
12	T	1	Total	W	0	0
			1	1		
12	N	1	Total	W	0	0
			1	1		
12	r	1	Total	W	0	0
			1	1		
12	l	1	Total	W	0	0
			1	1		
12	f	1	Total	W	0	0
			1	1		

- 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: C₂₀H₂₆N₁₀O₁₃P₂S₂).



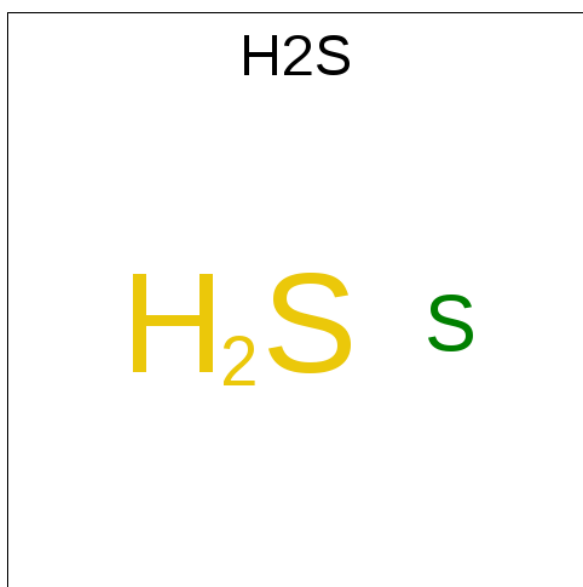
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
13	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

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



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 1	Mg 1	0	0
15	r	1	Total 1	Mg 1	0	0
15	l	1	Total 1	Mg 1	0	0
15	f	1	Total 1	Mg 1	0	0

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

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	22	Total 22	O 22	0	0
17	B	12	Total 12	O 12	0	0
17	C	7	Total 7	O 7	0	0
17	D	2	Total 2	O 2	0	0
17	E	1	Total 1	O 1	0	0
17	F	25	Total 25	O 25	0	0
17	G	14	Total 14	O 14	0	0
17	H	20	Total 20	O 20	0	0
17	I	17	Total 17	O 17	0	0
17	J	4	Total 4	O 4	0	0
17	K	8	Total 8	O 8	0	0
17	L	26	Total 26	O 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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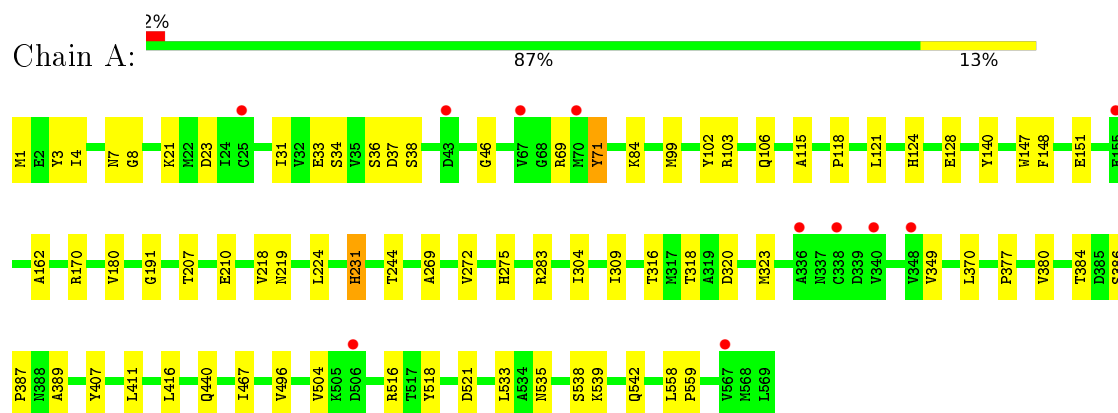
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	h	3	Total 3	O 3	0	0
17	i	8	Total 8	O 8	0	0
17	j	20	Total 20	O 20	0	0
17	k	9	Total 9	O 9	0	0
17	l	20	Total 20	O 20	0	0
17	m	7	Total 7	O 7	0	0
17	n	4	Total 4	O 4	0	0
17	o	2	Total 2	O 2	0	0
17	p	18	Total 18	O 18	0	0
17	q	27	Total 27	O 27	0	0
17	r	16	Total 16	O 16	0	0
17	s	3	Total 3	O 3	0	0
17	t	3	Total 3	O 3	0	0
17	u	1	Total 1	O 1	0	0
17	v	13	Total 13	O 13	0	0

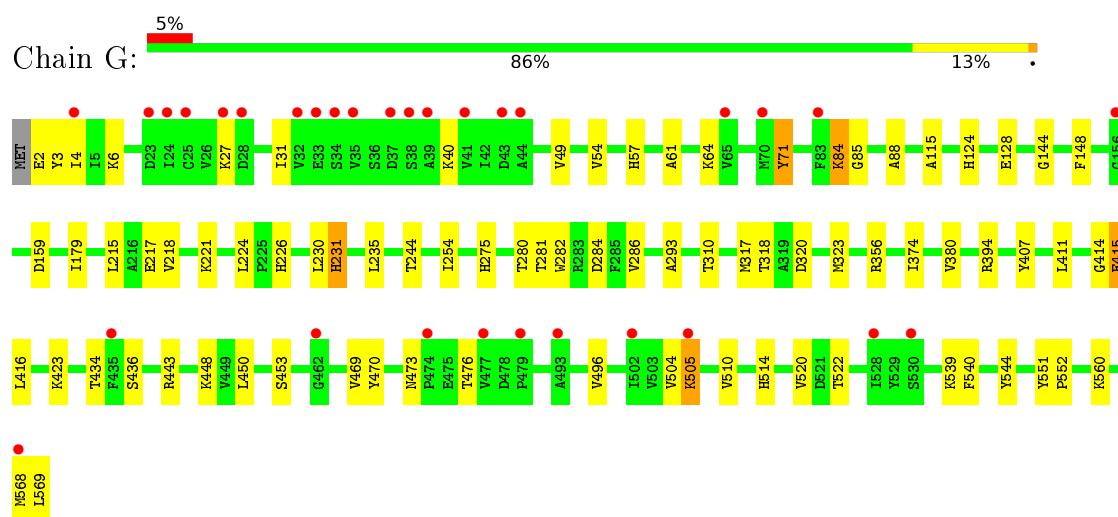
3 Residue-property plots [i](#)

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.

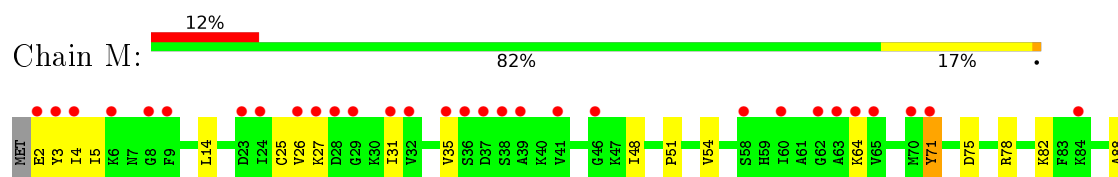
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

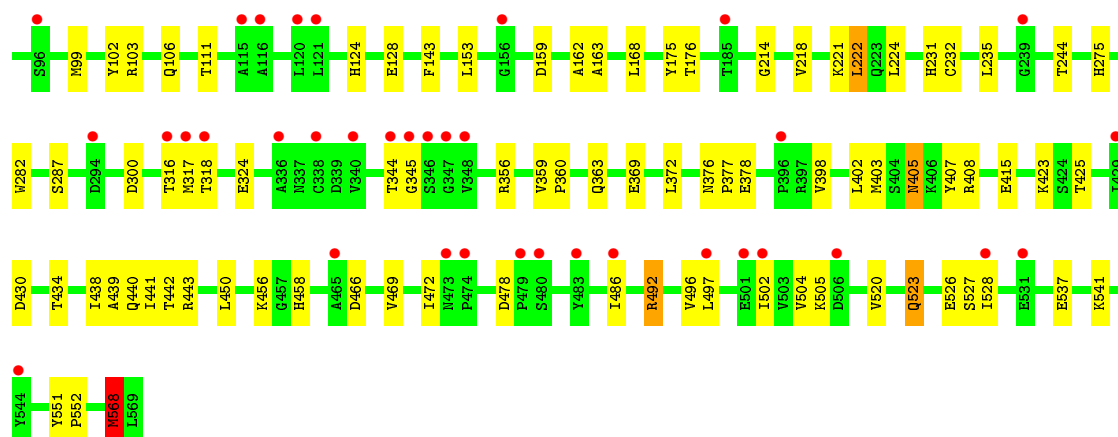


- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

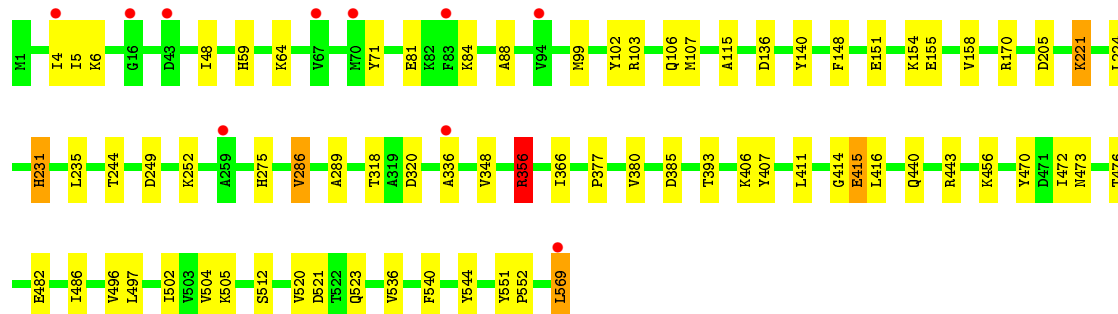
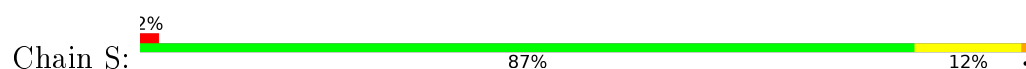


- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

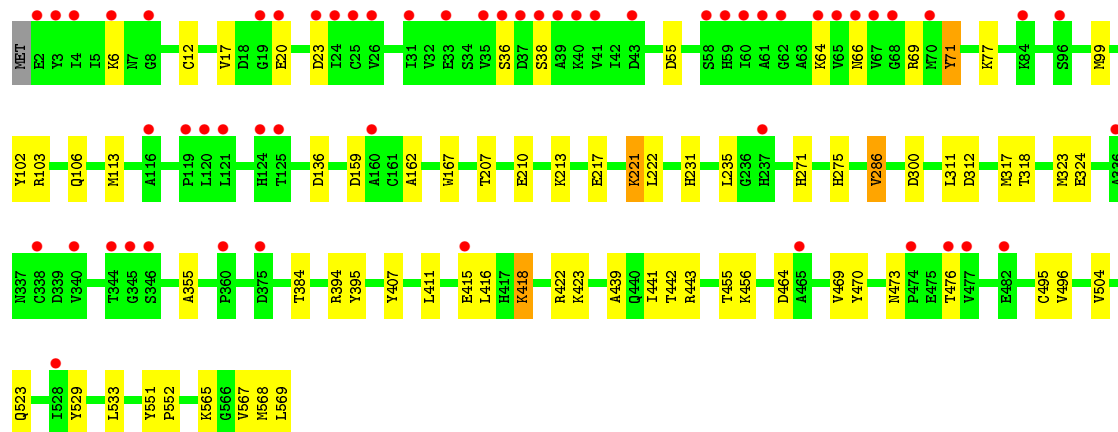
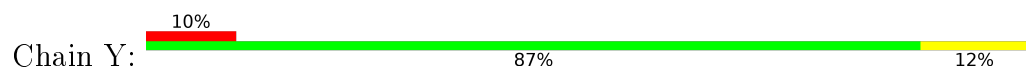




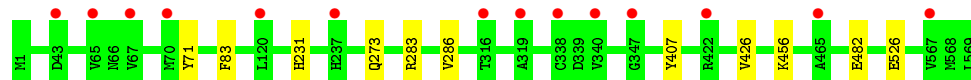
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



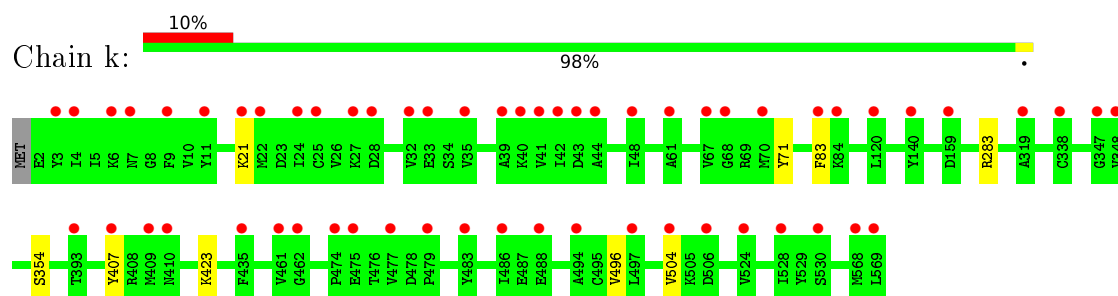
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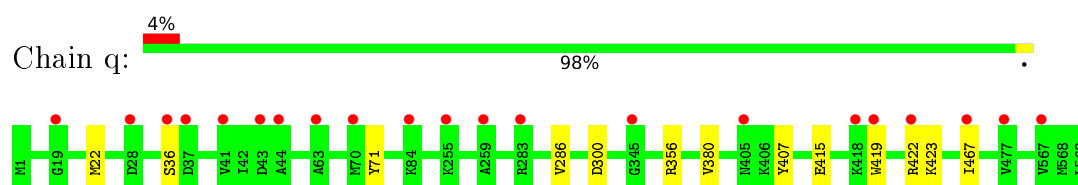
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



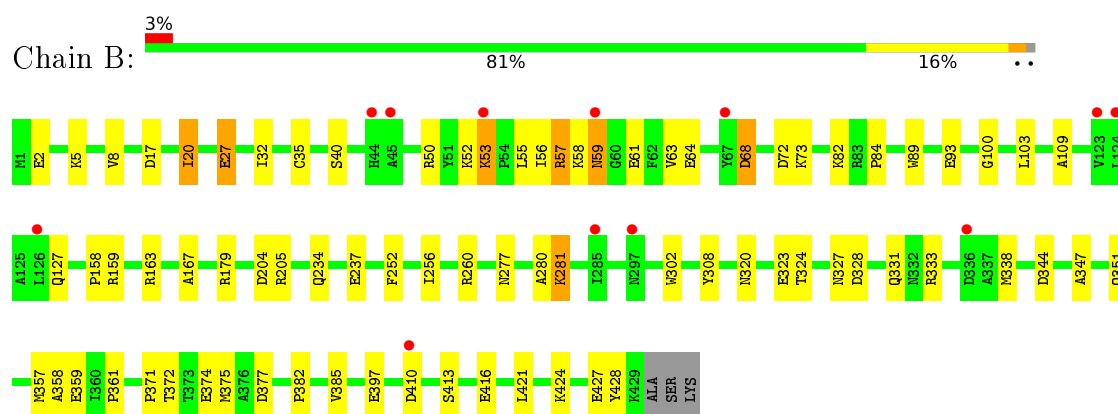
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



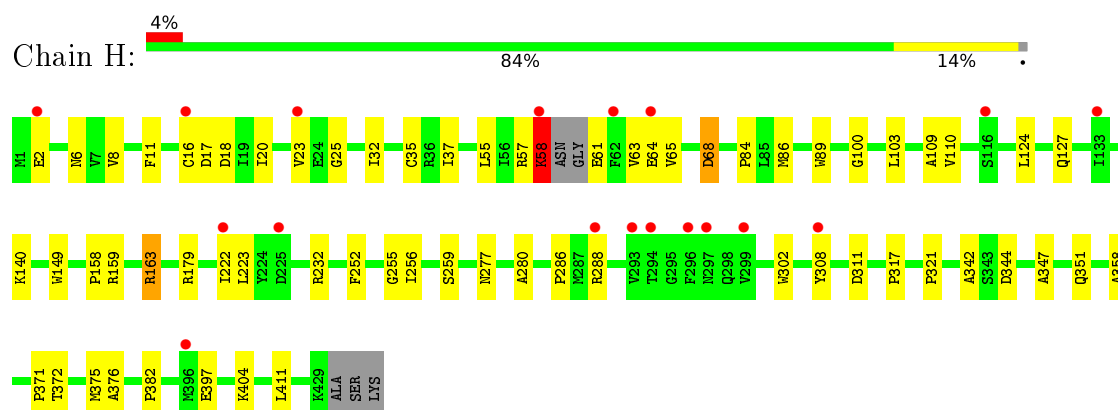
- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA



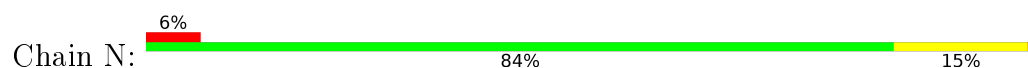
- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

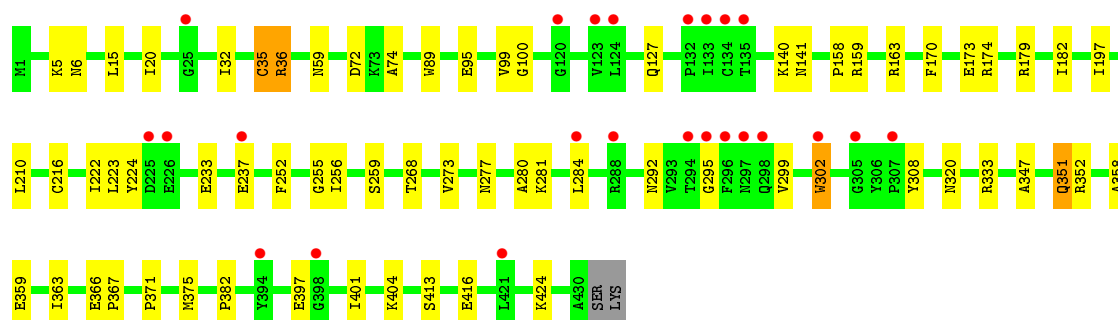


- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

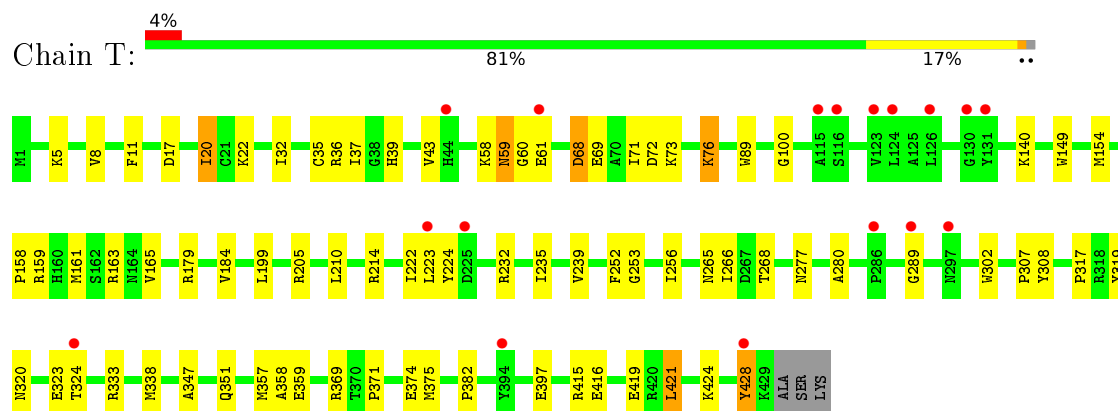


- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

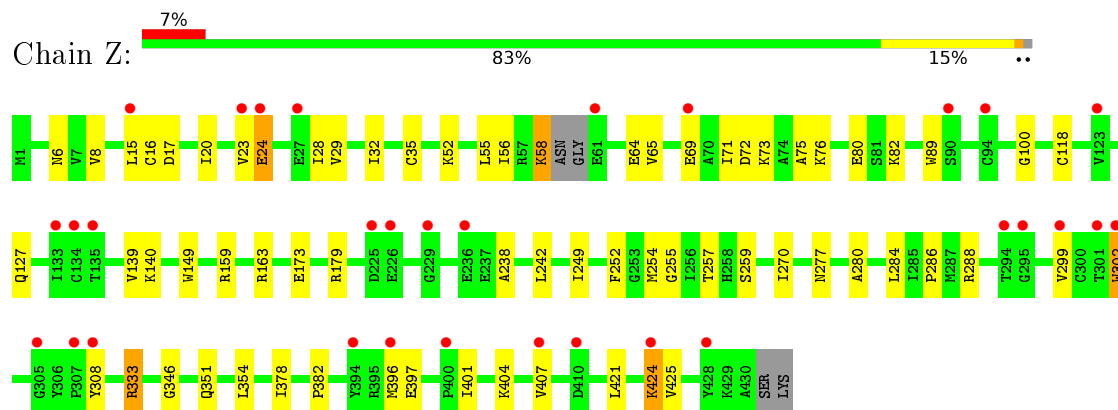




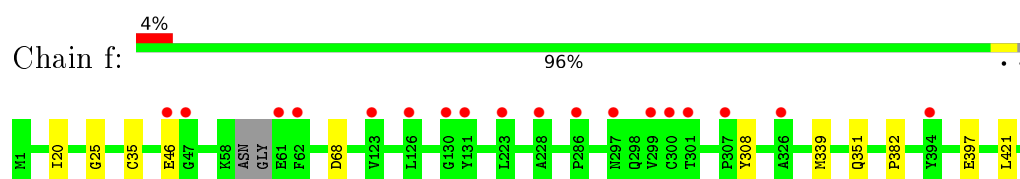
- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

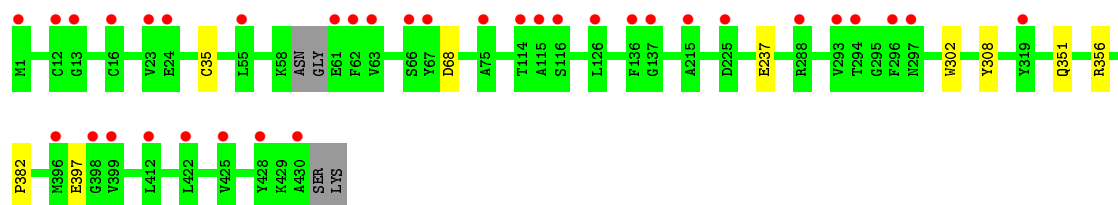


- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

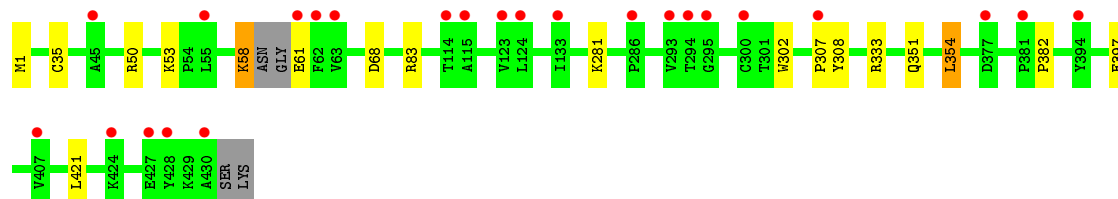


- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

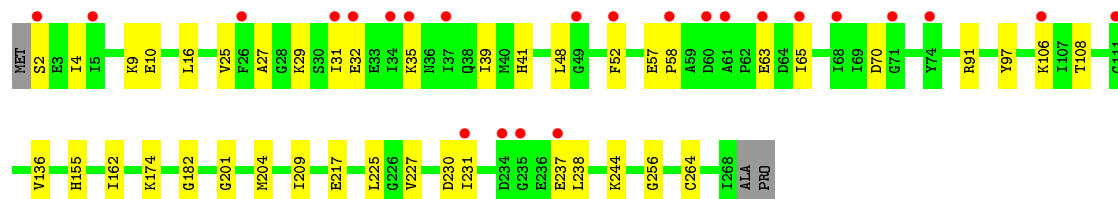
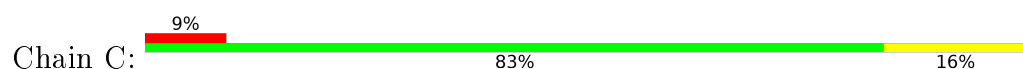




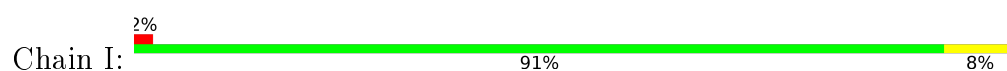
- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B



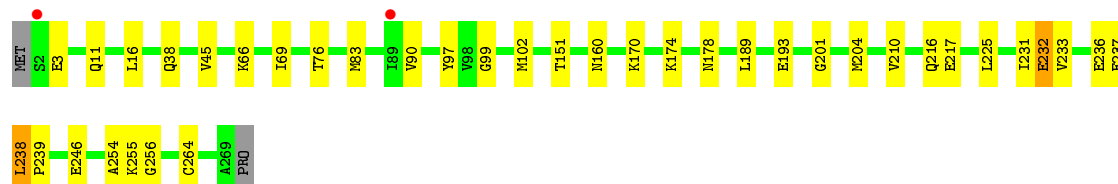
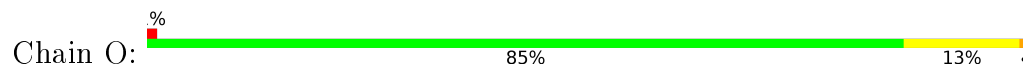
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



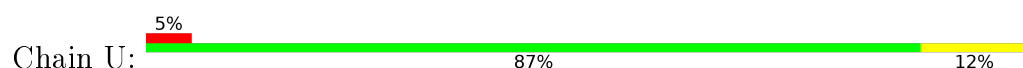
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

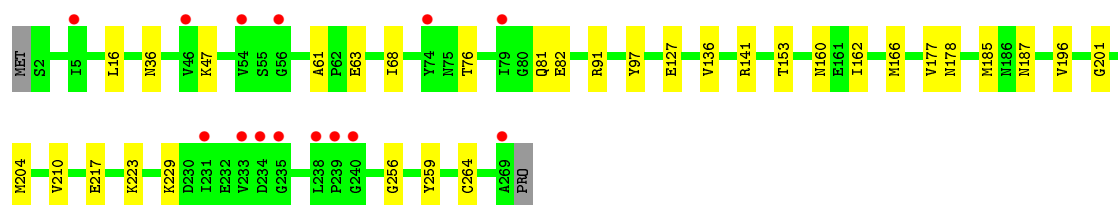


- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

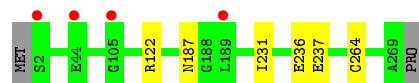


- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

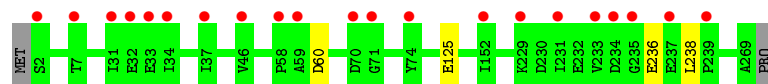




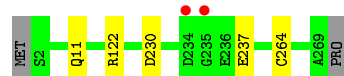
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



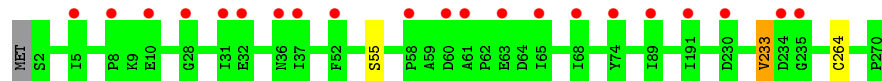
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



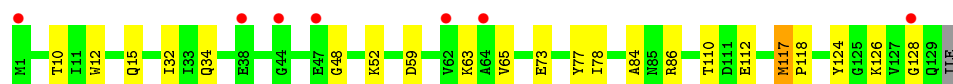
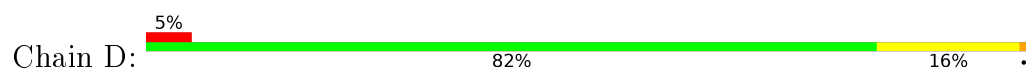
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



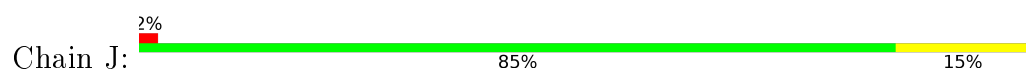
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C




- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

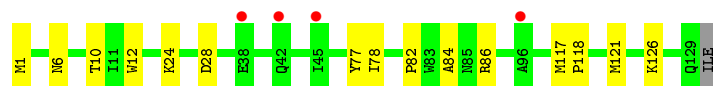


- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD




- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain P: 



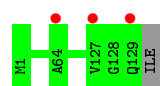
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain V: 



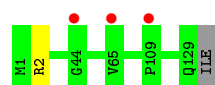
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain b: 



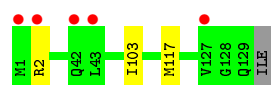
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain h: 



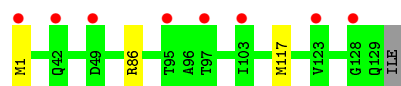
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

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:  68% 28% ..



- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain Q:  72% 24% ..



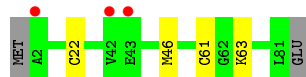
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain W:  68% 28% ..




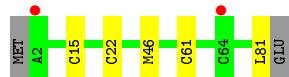
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain c:  93% 5% .

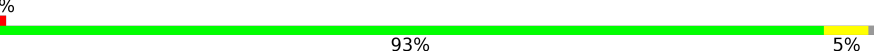


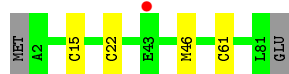
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain i:  91% 6% .

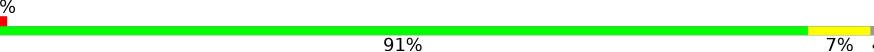


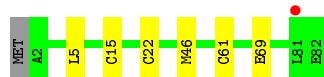
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain o:  93% 5% .

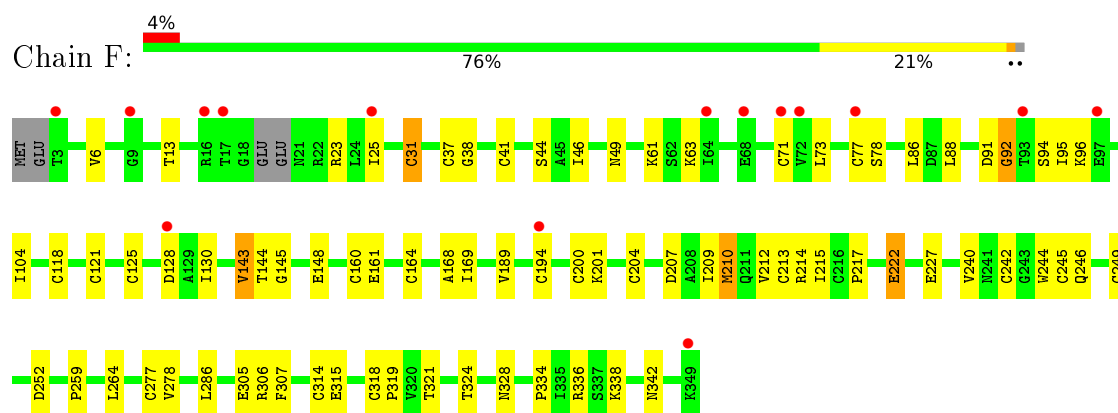


- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdG

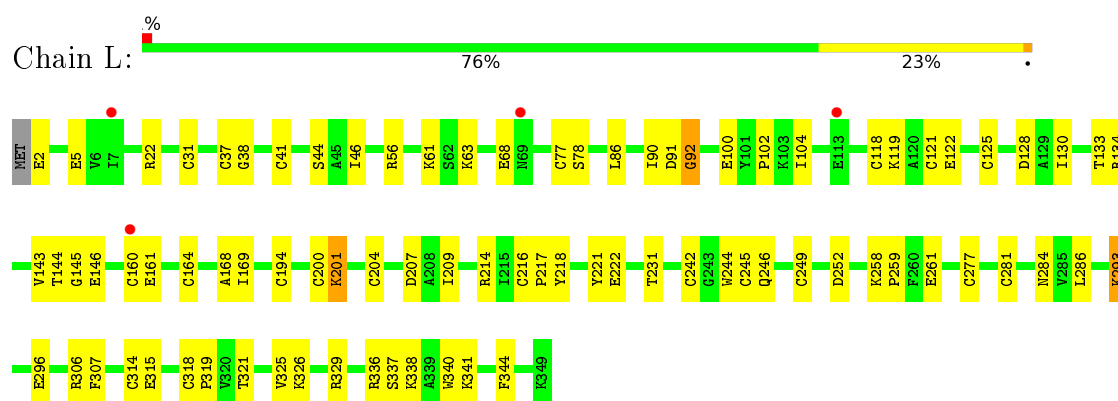
Chain u:  91% 7% .



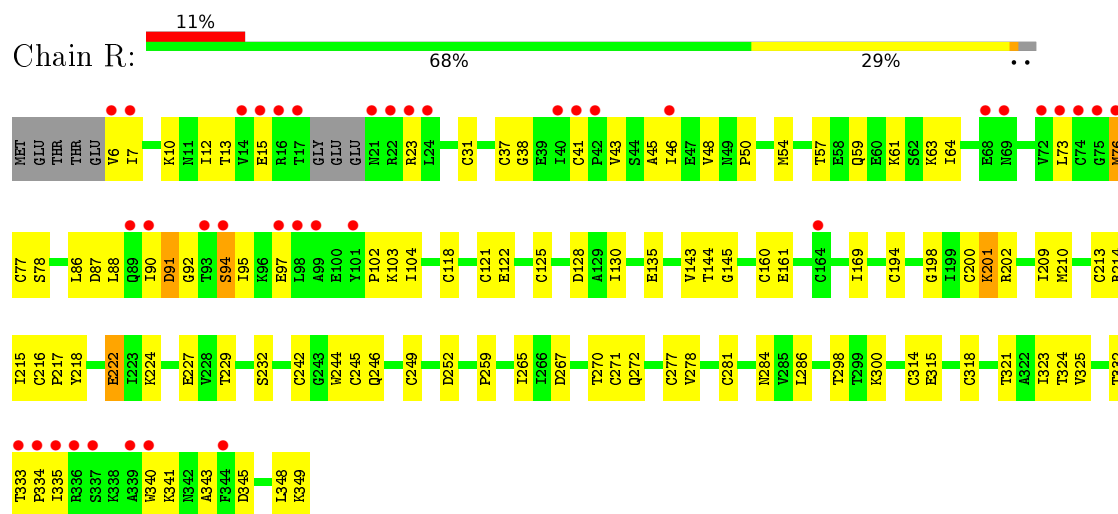
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF



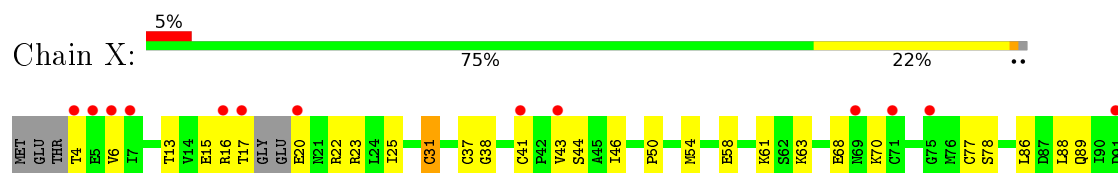
• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

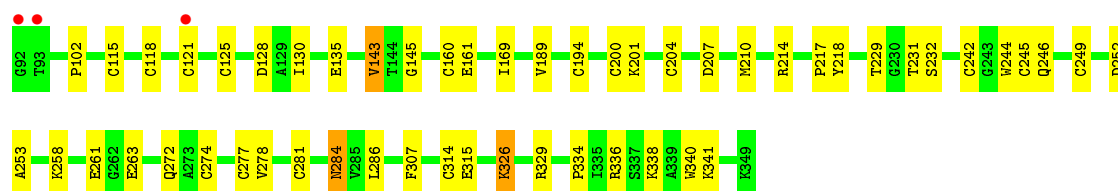


• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF

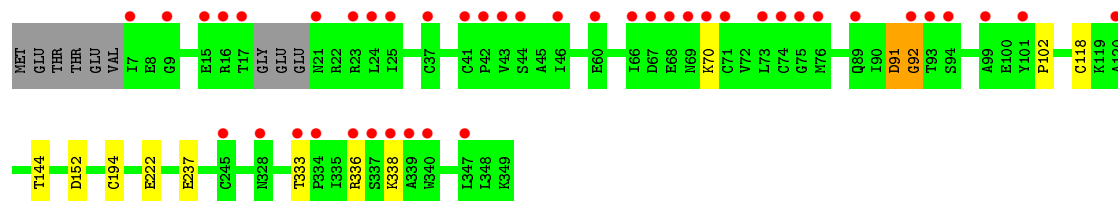


• Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdF





- 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

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

All (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
1	q	419	TRP	CE3-CZ3	-9.51	1.22	1.38
2	f	46	GLU	CD-OE1	-9.35	1.15	1.25
2	H	61	GLU	CD-OE1	-8.88	1.15	1.25
2	f	46	GLU	CD-OE2	-8.33	1.16	1.25
1	q	419	TRP	CG-CD1	8.07	1.48	1.36
6	v	23	ARG	NE-CZ	-7.72	1.23	1.33
1	q	423	LYS	CD-CE	-7.60	1.32	1.51
2	Z	424	LYS	CE-NZ	-7.51	1.30	1.49
2	Z	333	ARG	NE-CZ	-7.46	1.23	1.33
1	q	419	TRP	CD1-NE1	7.20	1.50	1.38
2	Z	333	ARG	CZ-NH1	-7.03	1.24	1.33
1	S	356	ARG	C-N	-6.91	1.18	1.34
6	R	97	GLU	CD-OE1	-6.73	1.18	1.25
2	T	428	TYR	CD1-CE1	-6.41	1.29	1.39
3	I	44	GLU	CD-OE1	-6.31	1.18	1.25
1	q	415	GLU	CB-CG	-6.27	1.40	1.52
1	A	558	LEU	CA-CB	6.26	1.68	1.53
3	I	237	GLU	CD-OE1	-6.26	1.18	1.25
6	v	349	LYS	CD-CE	-6.20	1.35	1.51
2	Z	24	GLU	CG-CD	6.05	1.61	1.51
6	v	23	ARG	CZ-NH2	-6.00	1.25	1.33
1	q	415	GLU	CG-CD	-5.99	1.43	1.51
6	X	326	LYS	CE-NZ	5.95	1.64	1.49
1	q	356	ARG	C-N	-5.94	1.20	1.34
1	A	559	PRO	C-O	5.80	1.34	1.23
2	T	428	TYR	CB-CG	-5.78	1.43	1.51
6	d	237	GLU	CD-OE1	-5.64	1.19	1.25
1	S	286	VAL	CB-CG2	5.56	1.64	1.52
6	v	143	VAL	CB-CG2	5.54	1.64	1.52
6	d	237	GLU	CD-OE2	-5.53	1.19	1.25
6	X	143	VAL	CB-CG2	5.44	1.64	1.52
6	p	180	SER	C-N	5.44	1.44	1.34
3	I	44	GLU	CD-OE2	-5.41	1.19	1.25
3	I	237	GLU	CD-OE2	-5.41	1.19	1.25
6	F	143	VAL	CB-CG2	5.39	1.64	1.52
1	A	559	PRO	N-CA	-5.38	1.38	1.47
2	Z	333	ARG	CZ-NH2	-5.35	1.26	1.33
2	r	58	LYS	CE-NZ	-5.21	1.36	1.49
6	R	143	VAL	CB-CG2	5.14	1.63	1.52
2	B	27	GLU	CD-OE1	-5.14	1.20	1.25
6	p	143	VAL	CB-CG2	5.09	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	143	VAL	CB-CG2	5.09	1.63	1.52
6	R	97	GLU	CD-OE2	-5.07	1.20	1.25
2	l	237	GLU	CD-OE2	5.05	1.31	1.25
1	q	286	VAL	CB-CG2	5.04	1.63	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	Y	221	LYS	CD-CE-NZ	-9.99	88.71	111.70
4	t	1	MET	CA-CB-CG	9.89	130.11	113.30
2	H	163	ARG	NE-CZ-NH1	-9.40	115.60	120.30
2	r	1	MET	CG-SD-CE	-8.77	86.16	100.20
1	S	569	LEU	CB-CG-CD2	-8.74	96.14	111.00
1	q	467	ILE	CG1-CB-CG2	-8.66	92.35	111.40
1	Y	300	ASP	CB-CG-OD2	8.63	126.06	118.30
2	T	428	TYR	CB-CG-CD1	-8.58	115.85	121.00
6	R	76	MET	CG-SD-CE	-8.21	87.06	100.20
2	H	163	ARG	NE-CZ-NH2	8.02	124.31	120.30
6	p	92	GLY	N-CA-C	7.57	132.03	113.10
6	R	73	LEU	CB-CG-CD2	7.56	123.86	111.00
1	Y	569	LEU	CA-CB-CG	7.39	132.29	115.30
1	q	423	LYS	CB-CA-C	-7.36	95.67	110.40
2	H	58	LYS	CD-CE-NZ	-7.22	95.10	111.70
2	r	333	ARG	CG-CD-NE	-7.20	96.67	111.80
6	R	61	LYS	CD-CE-NZ	-7.19	95.16	111.70
1	q	356	ARG	NE-CZ-NH2	7.14	123.87	120.30
6	L	92	GLY	N-CA-C	7.13	130.92	113.10
6	X	58	GLU	CB-CA-C	7.09	124.58	110.40
6	d	92	GLY	N-CA-C	7.08	130.80	113.10
3	C	230	ASP	CB-CG-OD1	6.79	124.41	118.30
1	q	300	ASP	CB-CG-OD2	6.68	124.31	118.30
1	k	283	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	M	478	ASP	CB-CG-OD1	6.51	124.16	118.30
1	M	300	ASP	CB-CG-OD1	6.50	124.15	118.30
1	q	423	LYS	CD-CE-NZ	-6.50	96.76	111.70
6	F	92	GLY	N-CA-C	6.48	129.31	113.10
1	q	419	TRP	CH2-CZ2-CE2	-6.42	110.98	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	125	GLU	CB-CA-C	6.27	122.94	110.40
1	e	426	VAL	CG1-CB-CG2	6.16	120.76	110.90
4	n	103	ILE	CA-CB-CG1	-6.13	99.35	111.00
1	M	478	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	S	221	LYS	CD-CE-NZ	6.12	125.78	111.70
2	T	428	TYR	CB-CG-CD2	6.04	124.62	121.00
2	r	58	LYS	CB-CG-CD	-5.97	96.08	111.60
6	X	58	GLU	N-CA-CB	-5.95	99.90	110.60
2	l	237	GLU	CG-CD-OE1	-5.87	106.56	118.30
4	t	86	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	k	496	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	Y	300	ASP	CB-CG-OD1	-5.83	113.05	118.30
3	m	122	ARG	NE-CZ-NH1	5.82	123.21	120.30
3	s	233	VAL	CG1-CB-CG2	5.72	120.06	110.90
6	R	97	GLU	CA-CB-CG	5.71	125.96	113.40
1	q	422	ARG	CB-CG-CD	-5.66	96.89	111.60
2	T	76	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	q	422	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	k	21	LYS	CD-CE-NZ	-5.58	98.86	111.70
2	B	27	GLU	CG-CD-OE1	5.56	129.42	118.30
2	T	428	TYR	CA-CB-CG	-5.56	102.84	113.40
2	r	61	GLU	CA-CB-CG	5.56	125.62	113.40
6	L	293	LYS	CD-CE-NZ	5.54	124.45	111.70
2	r	50	ARG	NE-CZ-NH2	5.50	123.05	120.30
2	Z	24	GLU	CG-CD-OE2	5.49	129.28	118.30
2	r	61	GLU	CG-CD-OE1	-5.46	107.38	118.30
1	S	505	LYS	CD-CE-NZ	-5.43	99.21	111.70
6	d	70	LYS	CB-CG-CD	-5.43	97.47	111.60
3	g	238	LEU	CB-CG-CD2	-5.38	101.86	111.00
2	r	421	LEU	CB-CG-CD2	-5.37	101.88	111.00
3	a	122	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	l	356	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	Z	24	GLU	CG-CD-OE1	-5.28	107.74	118.30
1	k	504	VAL	CG1-CB-CG2	5.27	119.34	110.90
3	O	238	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	M	568	MET	CA-CB-CG	5.24	122.20	113.30
3	U	141	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	q	419	TRP	CG-CD1-NE1	-5.18	104.92	110.10
3	m	230	ASP	CB-CG-OD2	5.15	122.94	118.30
6	R	61	LYS	CG-CD-CE	5.15	127.34	111.90
5	i	81	LEU	CB-CG-CD2	5.12	119.71	111.00
1	q	419	TRP	CZ3-CH2-CZ2	5.11	127.73	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	221	LYS	CB-CA-C	-5.09	100.22	110.40
1	q	422	ARG	CB-CA-C	5.08	120.56	110.40
6	d	333	THR	CA-CB-CG2	-5.08	105.29	112.40
6	v	23	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	N	173	GLU	CB-CA-C	-5.03	100.34	110.40
2	r	333	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (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
6	d	91	ASP	Peptide
1	k	83	PHE	Peptide
6	p	91	ASP	Peptide
6	v	91	ASP	Peptide

5.2 Too-close contacts

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.

All (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
1:Y:17:VAL:CG2	1:Y:20:GLU:OE1	2.02	1.06
1:S:81:GLU:OE1	1:S:103:ARG:NH2	1.94	1.00
2:Z:75:ALA:HB3	2:Z:424:LYS:HE3	1.42	0.99
1:Y:418:LYS:NZ	1:Y:422:ARG:HD3	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:158:VAL:HG12	1:S:221:LYS:NZ	1.79	0.98
1:Y:418:LYS:HZ3	1:Y:422:ARG:HH11	1.02	0.97
1:Y:418:LYS:HZ2	1:Y:422:ARG:HH11	1.10	0.97
3:C:231:ILE:HD11	3:C:238:LEU:HD12	1.49	0.94
1:Y:418:LYS:HZ2	1:Y:422:ARG:HD3	1.28	0.94
2:N:36:ARG:NH2	16:N:506:CL:CL	2.38	0.94
1:Y:418:LYS:HZ1	1:Y:422:ARG:HH11	0.96	0.93
2:T:76:LYS:NZ	2:T:428:TYR:OH	2.01	0.92
2:Z:71:ILE:HG22	2:Z:424:LYS:NZ	1.88	0.88
1:M:51:PRO:O	1:M:443:ARG:NH1	2.07	0.87
1:M:2:GLU:OE2	1:M:27:LYS:CB	2.23	0.86
2:Z:80:GLU:O	2:Z:82:LYS:NZ	2.10	0.84
6:L:216:CYS:HB3	6:R:216:CYS:HB3	1.58	0.83
6:R:224:LYS:NZ	6:R:227:GLU:OE1	2.11	0.82
3:C:31:ILE:HG22	3:C:35:LYS:HE2	1.62	0.82
1:Y:418:LYS:HZ3	1:Y:422:ARG:NH1	1.54	0.81
5:W:23:PRO:HG3	6:X:274:CYS:HB3	1.64	0.80
2:H:6:ASN:O	2:H:404:LYS:NZ	2.15	0.80
6:F:338:LYS:NZ	6:F:342:ASN:HD21	1.79	0.80
1:G:473:ASN:HB3	1:G:476:THR:HG22	1.64	0.80
2:Z:76:LYS:NZ	2:Z:80:GLU:OE2	2.15	0.79
2:Z:75:ALA:CB	2:Z:424:LYS:HE3	2.12	0.79
6:R:10:LYS:NZ	6:R:59:GLN:O	2.16	0.79
2:Z:24:GLU:OE2	2:Z:29:VAL:HG21	1.82	0.78
1:A:148:PHE:HE1	1:A:539:LYS:HG3	1.48	0.78
2:N:140:LYS:O	2:N:179:ARG:NH2	2.18	0.77
1:Y:418:LYS:NZ	1:Y:422:ARG:CD	2.47	0.77
6:R:145:GLY:HA2	6:R:214:ARG:HG3	1.66	0.77
6:F:144:THR:HG21	6:F:222:GLU:HB3	1.66	0.76
6:L:314:CYS:SG	6:L:315:GLU:N	2.58	0.76
1:M:497:LEU:HD21	1:M:502:ILE:HG12	1.68	0.75
3:C:2:SER:N	3:C:57:GLU:OE1	2.20	0.74
1:Y:418:LYS:HZ1	1:Y:422:ARG:NH1	1.56	0.74
6:L:242:CYS:SG	6:L:244:TRP:HD1	2.11	0.74
1:S:158:VAL:HG12	1:S:221:LYS:HZ1	1.50	0.74
2:B:204:ASP:OD2	2:B:260:ARG:N	2.15	0.74
2:Z:255:GLY:O	2:Z:259:SER:OG	2.05	0.73
1:S:158:VAL:HG12	1:S:221:LYS:HZ2	1.53	0.73
2:H:57:ARG:NH2	2:H:376:ALA:O	2.20	0.73
6:X:16:ARG:HH21	6:X:22:ARG:HG3	1.52	0.72
6:X:145:GLY:HA2	6:X:214:ARG:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:LEU:HA	1:G:218:VAL:HG22	1.71	0.72
2:N:141:ASN:HD22	2:N:170:PHE:H	1.36	0.72
1:M:2:GLU:OE2	1:M:27:LYS:HG3	1.88	0.72
1:G:286:VAL:HG12	1:G:423:LYS:HD2	1.71	0.72
6:R:6:VAL:HG22	6:R:13:THR:OG1	1.90	0.72
3:C:32:GLU:HG2	3:C:35:LYS:HE3	1.72	0.71
2:T:68:ASP:O	2:T:72:ASP:HB2	1.90	0.71
2:Z:71:ILE:HG22	2:Z:424:LYS:HZ1	1.53	0.71
3:C:4:ILE:HD13	3:C:65:ILE:HG23	1.72	0.71
6:L:144:THR:HG21	6:L:222:GLU:OE1	1.91	0.71
6:X:334:PRO:HB2	6:X:336:ARG:HH12	1.55	0.71
2:B:103:LEU:HD21	2:B:421:LEU:HD23	1.71	0.70
6:X:314:CYS:SG	6:X:315:GLU:N	2.64	0.70
2:Z:140:LYS:O	2:Z:179:ARG:NH2	2.24	0.70
6:F:145:GLY:HA2	6:F:214:ARG:HG3	1.74	0.70
2:B:323:GLU:OE2	3:C:97:TYR:OH	2.03	0.70
1:G:235:LEU:HD11	8:G:603:MFN:H11A	1.74	0.70
1:G:318:THR:HG22	1:G:320:ASP:N	2.00	0.70
2:B:59:ASN:HA	4:D:128:GLY:HA3	1.75	0.69
2:T:319:TYR:O	2:T:320:ASN:ND2	2.23	0.69
1:S:356:ARG:NH1	1:S:415:GLU:OE2	2.25	0.69
1:M:2:GLU:CD	1:M:27:LYS:HB2	2.13	0.69
2:T:59:ASN:O	2:T:61:GLU:N	2.23	0.69
2:B:72:ASP:OD1	2:B:428:TYR:OH	2.07	0.69
1:G:179:ILE:HB	1:G:230:LEU:HD12	1.74	0.69
3:O:170:LYS:NZ	3:O:236:GLU:OE2	2.25	0.69
5:W:18:CYS:HB2	5:W:67:CYS:HB2	1.74	0.69
6:R:15:GLU:CD	6:R:23:ARG:HH12	1.96	0.69
1:G:49:VAL:HG22	1:G:469:VAL:HG22	1.74	0.68
6:X:4:THR:N	6:X:68:GLU:OE2	2.27	0.68
2:H:358:ALA:HA	4:J:126:LYS:HD3	1.75	0.68
2:Z:6:ASN:O	2:Z:404:LYS:NZ	2.26	0.68
6:L:338:LYS:HD3	6:L:341:LYS:HE2	1.76	0.68
2:B:58:LYS:HD3	2:B:63:VAL:HG22	1.75	0.67
1:S:497:LEU:HD22	1:S:502:ILE:HG12	1.76	0.67
2:T:358:ALA:HA	4:V:126:LYS:HD3	1.77	0.67
6:L:145:GLY:HA2	6:L:214:ARG:HG3	1.77	0.67
3:C:70:ASP:OD2	3:C:91:ARG:NH1	2.27	0.67
4:D:73:GLU:OE1	17:D:201:HOH:O	2.13	0.67
1:M:2:GLU:OE1	1:M:35:VAL:HB	1.96	0.66
1:S:356:ARG:HH11	1:S:415:GLU:CD	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:LYS:HZ3	3:C:10:GLU:H	1.43	0.66
2:B:323:GLU:HG2	2:B:324:THR:HG23	1.76	0.66
6:F:338:LYS:HZ2	6:F:342:ASN:HD21	1.42	0.66
1:S:170:ARG:NH2	1:S:521:ASP:OD1	2.25	0.66
2:B:61:GLU:N	2:B:61:GLU:OE2	2.29	0.66
2:T:76:LYS:HD2	2:T:428:TYR:CE2	2.30	0.66
6:L:37:CYS:SG	6:L:46:ILE:HG21	2.35	0.66
5:E:44:ILE:HD11	5:E:47:ILE:HG12	1.78	0.65
5:K:80:GLU:OE1	6:L:61:LYS:NZ	2.30	0.65
3:U:36:ASN:OD1	3:U:47:LYS:NZ	2.29	0.65
3:C:32:GLU:CG	3:C:35:LYS:HE3	2.26	0.65
2:H:351:GLN:HG3	4:J:85:ASN:O	1.95	0.65
1:M:2:GLU:OE2	1:M:27:LYS:CG	2.43	0.65
6:X:16:ARG:NH2	6:X:20:GLU:O	2.28	0.65
5:E:18:CYS:HB2	5:E:67:CYS:HB2	1.79	0.65
6:X:6:VAL:CG1	6:X:13:THR:HB	2.26	0.65
3:I:66:LYS:HE3	3:I:68:ILE:HD11	1.78	0.65
2:T:140:LYS:O	2:T:179:ARG:NH2	2.28	0.65
6:R:315:GLU:OE2	6:R:325:VAL:N	2.24	0.65
2:B:371:PRO:HA	4:D:117:MET:HE1	1.79	0.65
6:R:135:GLU:OE2	6:R:229:THR:OG1	2.14	0.64
1:A:411:LEU:HD23	1:A:416:LEU:HG	1.79	0.64
6:R:267:ASP:OD1	6:R:270:THR:OG1	2.10	0.64
6:X:263:GLU:OE2	6:X:326:LYS:NZ	2.30	0.64
2:N:358:ALA:HA	4:P:126:LYS:HD3	1.78	0.64
6:F:314:CYS:SG	6:F:315:GLU:N	2.71	0.64
2:H:140:LYS:O	2:H:179:ARG:NH2	2.30	0.64
4:D:52:LYS:NZ	4:D:59:ASP:OD1	2.31	0.64
6:F:23:ARG:HD3	6:F:25:ILE:HD11	1.80	0.64
1:A:411:LEU:CD2	1:A:416:LEU:HG	2.27	0.64
2:B:53:LYS:HE3	2:B:64:GLU:CD	2.18	0.64
2:N:36:ARG:NH1	5:Q:12:CYS:O	2.31	0.64
6:R:77:CYS:SG	6:R:86:LEU:HD13	2.38	0.64
6:X:160:CYS:SG	6:X:169:ILE:HG21	2.38	0.63
2:T:69:GLU:O	2:T:73:LYS:HG2	1.99	0.63
6:R:7:ILE:HD11	6:R:12:ILE:HG23	1.81	0.63
2:T:222:ILE:O	2:T:232:ARG:NH1	2.23	0.63
6:X:4:THR:HG23	6:X:15:GLU:HB3	1.81	0.63
6:X:242:CYS:O	6:X:258:LYS:NZ	2.30	0.63
2:Z:75:ALA:HB2	2:Z:421:LEU:HD12	1.80	0.63
1:Y:418:LYS:HZ3	1:Y:422:ARG:CD	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:71:ILE:HG23	2:T:421:LEU:HG	1.81	0.62
2:B:333:ARG:NH2	2:B:359:GLU:OE1	2.32	0.62
2:T:158:PRO:O	5:W:15:CYS:HB2	1.99	0.62
1:A:377:PRO:HB2	1:A:440:GLN:HG2	1.82	0.62
1:Y:162:ALA:CB	1:Y:221:LYS:HE2	2.29	0.62
6:R:77:CYS:SG	6:R:78:SER:N	2.72	0.62
6:F:37:CYS:SG	6:F:46:ILE:HG21	2.39	0.62
4:J:10:THR:HG22	4:J:12:TRP:H	1.64	0.62
5:K:67:CYS:SG	5:K:68:VAL:N	2.72	0.62
3:O:232:GLU:CD	3:O:237:GLU:HG3	2.20	0.62
6:R:160:CYS:SG	6:R:169:ILE:HG21	2.40	0.62
1:M:405:ASN:HD21	1:M:430:ASP:CA	2.13	0.62
4:P:24:LYS:NZ	4:P:28:ASP:OD2	2.33	0.62
1:Y:17:VAL:HG23	1:Y:20:GLU:CD	2.11	0.62
3:O:210:VAL:HG11	3:O:238:LEU:HD21	1.82	0.61
1:Y:286:VAL:HG23	1:Y:423:LYS:HD2	1.81	0.61
5:K:6:LYS:HG2	5:K:79:GLU:OE1	1.98	0.61
4:P:10:THR:HG22	4:P:12:TRP:H	1.65	0.61
6:F:125:CYS:SG	6:F:128:ASP:N	2.73	0.61
2:T:424:LYS:O	2:T:428:TYR:HD1	1.84	0.61
1:Y:355:ALA:HB1	1:Y:416:LEU:HD23	1.81	0.61
2:Z:69:GLU:O	2:Z:73:LYS:HG2	2.00	0.61
1:S:443:ARG:NH2	1:S:470:TYR:OH	2.32	0.61
3:C:25:VAL:O	3:C:29:LYS:NZ	2.23	0.61
1:M:405:ASN:ND2	1:M:430:ASP:O	2.33	0.61
2:T:210:LEU:O	2:T:214:ARG:HG3	1.99	0.61
1:Y:565:LYS:HD2	1:Y:568:MET:CE	2.31	0.61
1:A:516:ARG:NH1	1:A:518:TYR:OH	2.33	0.61
1:Y:66:ASN:OD1	1:Y:69:ARG:NH1	2.32	0.61
1:Y:77:LYS:NZ	17:Y:703:HOH:O	2.32	0.61
5:Q:6:LYS:HD3	5:Q:79:GLU:OE1	2.00	0.61
1:A:148:PHE:CE1	1:A:539:LYS:HG3	2.34	0.61
6:R:37:CYS:SG	6:R:46:ILE:HG21	2.40	0.61
5:K:39:THR:OG1	17:K:201:HOH:O	2.15	0.61
6:R:121:CYS:SG	6:R:130:ILE:HG21	2.41	0.61
2:T:415:ARG:NH1	2:T:419:GLU:OE1	2.34	0.61
3:C:227:VAL:HG23	6:L:231:THR:CG2	2.31	0.60
2:T:428:TYR:CD1	2:T:428:TYR:N	2.63	0.60
1:M:5:ILE:HD11	1:M:469:VAL:HG21	1.82	0.60
1:G:434:THR:HG22	1:G:436:SER:H	1.66	0.60
1:G:84:LYS:HG3	1:G:85:GLY:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:224:LEU:HD22	1:S:520:VAL:HG11	1.84	0.60
3:C:63:GLU:N	3:C:63:GLU:OE1	2.29	0.60
1:A:36:SER:HG	1:A:38:SER:HG	1.39	0.60
6:X:43:VAL:HG11	6:X:70:LYS:O	2.02	0.59
5:W:80:GLU:HG2	6:X:61:LYS:HE2	1.83	0.59
6:L:77:CYS:SG	6:L:86:LEU:HD13	2.41	0.59
6:R:249:CYS:SG	6:R:252:ASP:N	2.74	0.59
2:T:163:ARG:NH1	17:T:601:HOH:O	2.09	0.59
2:N:158:PRO:O	5:Q:15:CYS:HB2	2.03	0.59
6:X:16:ARG:NH1	6:X:17:THR:O	2.35	0.59
1:M:492:ARG:HD2	1:M:492:ARG:O	2.02	0.59
1:G:224:LEU:HD22	1:G:520:VAL:HG11	1.84	0.59
1:M:159:ASP:OD1	1:M:221:LYS:NZ	2.28	0.59
1:S:99:MET:O	1:S:103:ARG:HG3	2.03	0.59
1:A:147:TRP:O	1:A:151:GLU:HG3	2.03	0.59
2:B:158:PRO:O	5:E:15:CYS:HB2	2.03	0.59
4:J:36:ASN:HB3	4:J:38:GLU:OE1	2.02	0.59
6:X:37:CYS:SG	6:X:46:ILE:HG21	2.42	0.59
1:Y:312:ASP:OD1	1:Y:394:ARG:NH2	2.33	0.59
1:M:360:PRO:HA	1:M:363:GLN:HE21	1.68	0.58
6:R:345:ASP:HA	6:R:348:LEU:CD1	2.32	0.58
6:X:135:GLU:HB2	6:X:229:THR:HG23	1.85	0.58
6:X:77:CYS:SG	6:X:78:SER:N	2.76	0.58
2:B:53:LYS:HE2	2:B:55:LEU:HD21	1.84	0.58
1:G:514:HIS:HB2	1:G:560:LYS:HZ1	1.68	0.58
6:L:160:CYS:SG	6:L:169:ILE:HG21	2.43	0.58
2:T:39:HIS:O	2:T:43:VAL:HG22	2.04	0.58
5:E:2:ALA:N	5:E:80:GLU:OE1	2.36	0.58
6:F:77:CYS:SG	6:F:78:SER:N	2.76	0.58
6:X:16:ARG:NH2	6:X:22:ARG:HG3	2.18	0.58
3:U:136:VAL:HB	3:U:162:ILE:HD12	1.86	0.58
3:C:32:GLU:HA	3:C:35:LYS:HD2	1.85	0.58
6:L:249:CYS:SG	6:L:252:ASP:N	2.77	0.58
1:M:359:VAL:O	1:M:363:GLN:HG3	2.03	0.58
1:M:403:MET:HE2	1:M:486:ILE:HG21	1.85	0.58
1:G:568:MET:O	1:G:569:LEU:HG	2.03	0.58
2:H:158:PRO:O	5:K:15:CYS:HB2	2.03	0.58
1:Y:418:LYS:HZ3	1:Y:422:ARG:CZ	2.14	0.58
1:G:514:HIS:HB2	1:G:560:LYS:NZ	2.18	0.57
6:L:160:CYS:SG	6:L:161:GLU:N	2.77	0.57
1:M:372:LEU:HD11	1:M:408:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:200:CYS:SG	6:R:201:LYS:N	2.77	0.57
6:F:160:CYS:SG	6:F:169:ILE:HG21	2.44	0.57
1:M:224:LEU:HD22	1:M:520:VAL:HG11	1.84	0.57
6:L:146:GLU:OE2	6:X:218:TYR:OH	2.19	0.57
1:M:2:GLU:OE1	1:M:35:VAL:HG12	2.04	0.57
2:N:233:GLU:O	2:N:237:GLU:HG3	2.02	0.57
1:A:538:SER:O	1:A:542:GLN:HG3	2.05	0.57
1:M:502:ILE:HG21	1:M:505:LYS:CE	2.35	0.57
1:Y:12:CYS:HB3	1:Y:17:VAL:CG1	2.34	0.57
1:A:69:ARG:NH2	1:A:128:GLU:OE1	2.34	0.57
5:E:53:VAL:HG21	11:E:101:SF4:S2	2.44	0.57
2:N:159:ARG:O	2:N:163:ARG:HG3	2.04	0.57
6:R:333:THR:HG23	6:R:334:PRO:HD2	1.85	0.57
1:G:414:GLY:O	1:G:415:GLU:HB2	2.03	0.57
2:N:333:ARG:NH1	2:N:359:GLU:OE2	2.37	0.57
6:X:77:CYS:SG	6:X:86:LEU:HD13	2.45	0.57
6:R:314:CYS:SG	6:R:315:GLU:N	2.77	0.57
1:S:414:GLY:O	1:S:415:GLU:HB2	2.04	0.57
5:W:18:CYS:SG	5:W:19:VAL:N	2.78	0.57
2:H:16:CYS:SG	2:H:163:ARG:NH2	2.78	0.57
1:S:102:TYR:O	1:S:106:GLN:HG3	2.04	0.57
2:B:347:ALA:HB2	2:B:371:PRO:HG2	1.87	0.57
2:B:53:LYS:HE3	2:B:64:GLU:OE2	2.04	0.57
5:Q:18:CYS:HB2	5:Q:67:CYS:HB2	1.87	0.57
2:B:424:LYS:NZ	2:B:427:GLU:OE1	2.29	0.56
2:H:223:LEU:HD11	3:I:270:PRO:HG3	1.87	0.56
2:H:58:LYS:NZ	2:H:63:VAL:HG11	2.20	0.56
6:R:213:CYS:SG	6:R:215:ILE:HD12	2.45	0.56
2:H:18:ASP:OD1	2:H:163:ARG:NH2	2.37	0.56
2:T:5:LYS:HG2	2:T:20:ILE:HD13	1.87	0.56
1:A:316:THR:OG1	1:A:349:VAL:O	2.18	0.56
6:R:160:CYS:SG	6:R:161:GLU:N	2.77	0.56
2:T:159:ARG:O	2:T:163:ARG:HG3	2.06	0.56
1:Y:311:LEU:HD22	1:Y:355:ALA:HB2	1.85	0.56
1:G:159:ASP:OD1	1:G:221:LYS:NZ	2.37	0.56
5:W:23:PRO:HG3	6:X:274:CYS:CB	2.34	0.56
2:N:72:ASP:HB2	2:N:424:LYS:NZ	2.21	0.56
2:T:428:TYR:HD1	2:T:428:TYR:H	1.54	0.56
2:B:52:LYS:HA	2:B:52:LYS:HE2	1.87	0.56
6:L:104:ILE:HD11	6:L:344:PHE:CE1	2.41	0.56
1:S:496:VAL:HB	1:S:504:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:169:ILE:HG12	6:X:189:VAL:HG22	1.86	0.56
1:M:2:GLU:OE1	1:M:35:VAL:CB	2.54	0.56
1:Y:103:ARG:NH2	1:Y:106:GLN:OE1	2.38	0.56
2:N:273:VAL:HG21	2:N:284:LEU:HD23	1.87	0.56
2:T:256:ILE:HG13	2:T:265:ASN:HB3	1.88	0.56
6:L:77:CYS:SG	6:L:78:SER:N	2.79	0.56
2:N:20:ILE:HB	2:N:32:ILE:HB	1.88	0.56
6:L:258:LYS:NZ	6:L:306:ARG:O	2.35	0.56
5:W:44:ILE:HD11	5:W:47:ILE:HG22	1.87	0.56
1:Y:231:HIS:NE2	1:Y:235:LEU:HD13	2.21	0.56
1:Y:6:LYS:HE2	1:Y:23:ASP:OD2	2.06	0.56
2:T:184:VAL:HG22	2:T:199:LEU:HD12	1.88	0.56
5:E:12:CYS:SG	5:E:53:VAL:HG23	2.46	0.55
1:G:473:ASN:HB3	1:G:476:THR:CG2	2.34	0.55
3:O:216:GLN:NE2	3:O:217:GLU:OE2	2.39	0.55
1:Y:411:LEU:CD2	1:Y:416:LEU:HG	2.36	0.55
2:B:5:LYS:HG2	2:B:20:ILE:HD13	1.88	0.55
5:K:69:GLU:OE1	6:L:56:ARG:NE	2.37	0.55
1:M:377:PRO:HB2	1:M:440:GLN:HG2	1.88	0.55
5:Q:10:GLU:CD	5:Q:10:GLU:H	2.09	0.55
6:R:103:LYS:H	6:R:333:THR:HB	1.70	0.55
5:Q:67:CYS:SG	5:Q:68:VAL:N	2.79	0.55
1:S:249:ASP:O	1:S:252:LYS:HG2	2.06	0.55
1:M:497:LEU:CD2	1:M:502:ILE:HG12	2.36	0.55
1:M:523:GLN:HG3	1:M:568:MET:HG3	1.89	0.55
3:C:9:LYS:NZ	3:C:10:GLU:HB3	2.22	0.55
1:M:3:TYR:HB2	1:M:26:VAL:CG2	2.37	0.55
1:M:456:LYS:HE3	1:M:466:ASP:OD2	2.07	0.55
3:C:227:VAL:HG22	6:L:133:THR:HG21	1.88	0.55
6:F:200:CYS:SG	6:F:201:LYS:N	2.80	0.55
2:T:154:MET:HG2	2:T:161:MET:HE1	1.88	0.55
1:S:551:TYR:HB3	1:S:552:PRO:HD3	1.88	0.55
1:Y:99:MET:O	1:Y:103:ARG:HG2	2.07	0.55
1:M:405:ASN:HD21	1:M:430:ASP:HA	1.72	0.54
2:Z:55:LEU:HD21	2:Z:64:GLU:HG2	1.88	0.54
3:O:216:GLN:HG2	3:O:217:GLU:HG3	1.89	0.54
6:R:48:VAL:HG22	6:R:64:ILE:HD12	1.87	0.54
2:B:53:LYS:N	2:B:53:LYS:HD3	2.21	0.54
6:R:265:ILE:HB	6:R:324:THR:HG23	1.89	0.54
1:Y:355:ALA:HB3	1:Y:415:GLU:OE1	2.07	0.54
2:Z:71:ILE:HG22	2:Z:424:LYS:HZ3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:121:CYS:SG	6:X:130:ILE:HG21	2.46	0.54
2:B:56:ILE:HD13	2:B:73:LYS:HD2	1.89	0.54
3:C:136:VAL:HB	3:C:162:ILE:HG22	1.89	0.54
6:R:37:CYS:HB2	6:R:77:CYS:HB2	1.89	0.54
1:Y:55:ASP:O	1:Y:113:MET:HG2	2.08	0.54
1:Y:235:LEU:HD11	8:Y:603:MFN:H11A	1.89	0.54
6:X:43:VAL:CG1	6:X:70:LYS:HB3	2.37	0.54
1:M:2:GLU:OE1	1:M:35:VAL:CG1	2.56	0.54
3:O:83:MET:HG2	3:O:102:MET:HG3	1.90	0.54
3:O:232:GLU:OE1	3:O:237:GLU:HA	2.08	0.54
2:T:277:ASN:HA	2:T:280:ALA:O	2.08	0.54
6:F:338:LYS:HZ3	6:F:342:ASN:HD21	1.54	0.53
1:G:496:VAL:HB	1:G:504:VAL:HB	1.90	0.53
1:M:356:ARG:NE	1:M:415:GLU:OE1	2.41	0.53
6:X:261:GLU:HB2	6:X:329:ARG:HB3	1.90	0.53
1:Y:213:LYS:O	1:Y:217:GLU:HG3	2.08	0.53
2:H:32:ILE:HB	2:H:65:VAL:HG21	39.14	0.53
2:N:413:SER:OG	2:N:416:GLU:HG3	2.08	0.53
2:T:424:LYS:O	2:T:428:TYR:CD1	2.61	0.53
1:A:124:HIS:NE2	1:A:128:GLU:OE2	2.41	0.53
6:R:318:CYS:SG	6:R:321:THR:N	2.82	0.53
6:X:6:VAL:HG12	6:X:13:THR:HB	1.90	0.53
1:Y:411:LEU:HD23	1:Y:416:LEU:HG	1.90	0.53
3:O:216:GLN:HE21	3:O:217:GLU:HG3	1.73	0.53
6:R:345:ASP:HA	6:R:348:LEU:HD12	1.90	0.53
5:W:6:LYS:HD3	5:W:79:GLU:OE1	2.07	0.53
2:B:234:GLN:NE2	2:B:237:GLU:OE1	2.42	0.53
4:D:86:ARG:HD2	4:D:124:TYR:OH	2.08	0.53
6:X:338:LYS:HZ2	6:X:341:LYS:HE2	1.73	0.53
6:F:148:GLU:HG3	6:F:210:MET:HB3	1.91	0.53
6:L:200:CYS:SG	6:L:201:LYS:N	2.82	0.53
1:M:403:MET:CE	1:M:486:ILE:HG21	2.38	0.53
1:A:7:ASN:HB3	1:A:21:LYS:HE3	1.90	0.53
6:L:242:CYS:SG	6:L:244:TRP:CD1	2.98	0.53
2:Z:252:PHE:HE1	2:Z:284:LEU:HD13	1.74	0.53
2:B:252:PHE:HB2	2:B:256:ILE:HD11	1.91	0.53
6:L:277:CYS:SG	6:L:286:LEU:HD13	2.48	0.53
2:N:347:ALA:HB2	2:N:371:PRO:HG2	1.91	0.53
6:X:231:THR:HG22	6:X:232:SER:H	1.74	0.53
6:L:214:ARG:NH1	6:L:222:GLU:OE2	2.42	0.53
1:Y:17:VAL:CB	1:Y:20:GLU:OE1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:6:VAL:HG22	6:F:13:THR:HB	1.91	0.52
1:M:153:LEU:HD13	1:M:214:GLY:HA3	1.91	0.52
3:O:231:ILE:HG13	3:O:238:LEU:HB2	1.92	0.52
6:R:242:CYS:SG	6:R:244:TRP:HD1	2.32	0.52
2:B:159:ARG:O	2:B:163:ARG:HG3	2.09	0.52
3:C:201:GLY:HA3	3:C:204:MET:HE2	1.91	0.52
6:F:245:CYS:SG	6:F:246:GLN:N	2.81	0.52
6:F:318:CYS:SG	6:F:321:THR:N	2.82	0.52
5:K:12:CYS:SG	5:K:52:VAL:HA	2.49	0.52
1:M:287:SER:OG	1:M:423:LYS:O	2.20	0.52
1:A:99:MET:O	1:A:103:ARG:HG3	2.10	0.52
6:L:218:TYR:OH	6:X:214:ARG:NH2	2.41	0.52
6:L:104:ILE:HG23	6:L:259:PRO:HB3	1.89	0.52
1:M:102:TYR:O	1:M:106:GLN:HG3	2.10	0.52
3:U:204:MET:SD	3:U:256:GLY:HA3	2.50	0.52
1:Y:455:THR:HB	1:Y:464:ASP:OD1	2.09	0.52
6:F:249:CYS:SG	6:F:252:ASP:N	2.82	0.52
1:G:148:PHE:CE1	1:G:539:LYS:HE2	2.44	0.52
2:N:252:PHE:HB2	2:N:256:ILE:HD11	1.92	0.52
1:Y:418:LYS:NZ	1:Y:422:ARG:CZ	2.65	0.52
6:L:119:LYS:HD2	6:L:134:ARG:CZ	2.39	0.52
2:N:277:ASN:HA	2:N:280:ALA:O	2.09	0.52
6:R:341:LYS:NZ	6:R:345:ASP:OD2	2.39	0.52
1:A:102:TYR:O	1:A:106:GLN:HG3	2.09	0.52
1:G:71:TYR:HA	2:H:127:GLN:HG2	1.92	0.52
2:H:252:PHE:HB2	2:H:256:ILE:HD11	1.90	0.52
2:H:255:GLY:O	2:H:259:SER:OG	2.24	0.52
1:S:318:THR:HG23	1:S:320:ASP:H	1.75	0.52
1:Y:221:LYS:O	1:Y:567:VAL:HG21	2.09	0.52
1:Y:162:ALA:HB1	1:Y:222:LEU:HD21	1.91	0.52
2:T:347:ALA:HB2	2:T:371:PRO:HG2	1.92	0.52
6:X:160:CYS:HB2	6:X:200:CYS:HB2	1.92	0.52
1:Y:235:LEU:HD12	1:Y:275:HIS:CE1	2.45	0.52
2:Z:75:ALA:HB2	2:Z:421:LEU:CD1	2.40	0.52
4:D:34:GLN:HA	4:D:65:VAL:HG23	1.92	0.52
6:R:104:ILE:CG2	6:R:259:PRO:HB3	2.39	0.52
3:U:63:GLU:H	3:U:63:GLU:CD	2.14	0.52
2:B:413:SER:OG	2:B:416:GLU:HG3	2.11	0.51
6:F:77:CYS:SG	6:F:86:LEU:HD13	2.50	0.51
2:N:351:GLN:HG2	2:N:352:ARG:N	2.24	0.51
5:W:67:CYS:SG	5:W:68:VAL:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ILE:HB	2:B:32:ILE:HB	1.93	0.51
3:C:32:GLU:CD	3:C:35:LYS:HE3	2.31	0.51
5:K:24:VAL:O	5:K:28:ARG:HG3	2.10	0.51
6:L:261:GLU:HB2	6:L:329:ARG:HB3	1.93	0.51
6:L:121:CYS:SG	6:L:122:GLU:N	2.84	0.51
6:F:41:CYS:SG	6:F:44:SER:N	2.84	0.51
6:R:104:ILE:HG22	6:R:259:PRO:HB3	1.93	0.51
6:X:281:CYS:SG	6:X:284:ASN:N	2.83	0.51
4:J:10:THR:HG22	4:J:12:TRP:N	2.25	0.51
2:N:95:GLU:O	2:N:99:VAL:HG23	2.11	0.51
3:O:254:ALA:O	3:O:255:LYS:HE2	2.11	0.51
6:R:332:THR:HG21	6:R:335:ILE:HD11	1.93	0.51
1:S:235:LEU:HD11	8:S:603:MFN:H11A	1.92	0.51
1:Y:64:LYS:HD3	1:Y:317:MET:HB2	1.91	0.51
2:Z:20:ILE:HB	2:Z:32:ILE:HB	1.93	0.51
5:E:18:CYS:SG	5:E:19:VAL:N	2.83	0.51
6:L:160:CYS:SG	6:L:169:ILE:HD13	2.51	0.51
6:R:91:ASP:N	6:R:92:GLY:HA2	2.25	0.51
1:Y:318:THR:HG21	8:Y:603:MFN:O1	2.11	0.51
4:J:38:GLU:H	4:J:38:GLU:CD	2.13	0.51
6:R:232:SER:O	3:U:229:LYS:HD3	2.10	0.51
1:S:377:PRO:HB2	1:S:440:GLN:HG2	1.92	0.51
1:Y:473:ASN:HB3	1:Y:476:THR:OG1	2.10	0.51
1:A:535:ASN:O	1:A:539:LYS:HG2	2.11	0.50
6:L:125:CYS:SG	6:L:128:ASP:N	2.84	0.50
1:M:442:THR:C	1:M:443:ARG:HD2	2.31	0.50
6:X:200:CYS:SG	6:X:201:LYS:N	2.84	0.50
2:B:2:GLU:OE1	2:B:2:GLU:HA	2.11	0.50
1:G:31:ILE:HG23	1:G:54:VAL:HG12	18.35	0.50
6:L:37:CYS:SG	6:L:38:GLY:N	2.85	0.50
2:N:320:ASN:ND2	3:O:97:TYR:OH	2.30	0.50
6:R:125:CYS:SG	6:R:128:ASP:N	2.85	0.50
6:R:7:ILE:HG13	6:R:12:ILE:HG12	1.93	0.50
3:U:210:VAL:HG22	3:U:259:TYR:HB2	1.93	0.50
2:B:58:LYS:HD3	2:B:63:VAL:CG2	2.42	0.50
4:D:10:THR:HG22	4:D:12:TRP:H	1.76	0.50
2:H:20:ILE:HB	2:H:32:ILE:HB	1.93	0.50
3:I:6:LEU:HB2	3:I:69:ILE:HG12	1.92	0.50
6:L:37:CYS:HB2	6:L:77:CYS:HB2	1.93	0.50
1:M:175:TYR:HD2	1:M:176:THR:HG22	1.76	0.50
2:T:253:GLY:O	2:T:256:ILE:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:280:THR:HG23	1:G:281:THR:HG23	1.92	0.50
6:R:245:CYS:SG	6:R:246:GLN:N	2.84	0.50
1:S:385:ASP:OD2	8:S:603:MFN:H12A	2.11	0.50
2:T:165:VAL:O	2:T:179:ARG:NH1	2.41	0.50
6:X:245:CYS:SG	6:X:246:GLN:N	2.84	0.50
3:C:204:MET:SD	3:C:256:GLY:HA3	2.52	0.50
3:C:27:ALA:O	3:C:29:LYS:HE3	2.12	0.50
5:E:64:CYS:SG	5:E:66:THR:OG1	2.66	0.50
2:H:347:ALA:HB2	2:H:371:PRO:HG2	1.94	0.50
1:M:497:LEU:HD23	1:M:502:ILE:HA	1.92	0.50
1:Y:102:TYR:O	1:Y:106:GLN:HG3	2.11	0.50
3:C:155:HIS:ND1	3:C:174:LYS:HE2	2.27	0.50
2:Z:71:ILE:C	2:Z:424:LYS:HZ2	2.15	0.50
6:F:200:CYS:SG	6:F:209:ILE:HG21	2.53	0.49
2:T:256:ILE:HG23	2:T:266:ILE:CD1	2.42	0.49
6:R:332:THR:HG23	6:R:333:THR:O	2.12	0.49
6:R:90:ILE:HD12	6:R:95:ILE:HG22	1.94	0.49
6:X:249:CYS:SG	6:X:252:ASP:N	2.85	0.49
6:F:160:CYS:SG	6:F:169:ILE:HD13	2.53	0.49
6:F:277:CYS:SG	6:F:286:LEU:HD13	2.53	0.49
3:O:204:MET:SD	3:O:256:GLY:HA3	2.52	0.49
5:Q:38:PRO:HG2	5:Q:47:ILE:HD11	1.93	0.49
2:Z:118:CYS:SG	13:Z:504:MGD:S12	3.11	0.49
2:Z:56:ILE:HD12	2:Z:65:VAL:HG21	1.95	0.49
2:B:205:ARG:NH2	3:C:217:GLU:OE2	2.45	0.49
6:F:104:ILE:HG23	6:F:259:PRO:HB3	1.94	0.49
2:T:320:ASN:OD1	3:U:97:TYR:OH	2.21	0.49
2:N:216:CYS:HB2	2:N:222:ILE:HD11	1.94	0.49
1:S:497:LEU:CD2	1:S:502:ILE:HG12	2.42	0.49
6:F:169:ILE:HG12	6:F:189:VAL:HG22	1.94	0.49
1:M:3:TYR:HB2	1:M:26:VAL:HG22	1.93	0.49
3:O:232:GLU:OE1	3:O:237:GLU:HG3	2.12	0.49
5:Q:71:CYS:SG	5:Q:74:ASP:N	2.85	0.49
2:T:324:THR:O	2:T:324:THR:HG22	2.13	0.49
1:Y:318:THR:OG1	1:Y:324:GLU:OE2	2.20	0.49
1:A:162:ALA:HA	1:A:218:VAL:HG13	1.95	0.49
2:H:277:ASN:HA	2:H:280:ALA:O	2.12	0.49
6:L:100:GLU:HG3	6:L:336:ARG:HH22	1.78	0.49
6:L:31:CYS:SG	6:L:63:LYS:HD3	2.52	0.49
1:S:336:ALA:HB3	1:S:348:VAL:HB	1.95	0.49
2:H:32:ILE:HB	2:H:65:VAL:CG2	38.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:231:ILE:O	3:O:231:ILE:HG13	2.13	0.49
3:O:231:ILE:O	3:O:232:GLU:OE1	2.31	0.49
3:O:232:GLU:HG3	3:O:237:GLU:HA	1.95	0.49
2:H:222:ILE:O	2:H:232:ARG:NH2	2.45	0.49
1:M:175:TYR:HD2	1:M:176:THR:CG2	2.26	0.49
1:Y:565:LYS:HD2	1:Y:568:MET:HE2	1.94	0.49
6:F:121:CYS:SG	6:F:130:ILE:HG21	2.52	0.48
6:L:318:CYS:SG	6:L:321:THR:N	2.86	0.48
1:M:175:TYR:OH	1:M:450:LEU:O	2.28	0.48
2:Z:277:ASN:HA	2:Z:280:ALA:O	2.13	0.48
1:M:356:ARG:NH1	1:M:415:GLU:OE2	2.45	0.48
3:O:174:LYS:HA	3:O:193:GLU:HB2	1.95	0.48
4:P:117:MET:HB3	4:P:118:PRO:HD3	1.94	0.48
2:T:154:MET:HG2	2:T:161:MET:CE	2.43	0.48
2:T:369:ARG:NH2	2:T:374:GLU:OE2	2.47	0.48
2:T:22:LYS:NZ	5:W:49:GLU:OE1	2.37	0.48
1:G:4:ILE:HG23	1:G:6:LYS:HE3	1.95	0.48
6:L:293:LYS:HE3	6:L:296:GLU:OE1	2.12	0.48
6:L:281:CYS:SG	6:L:284:ASN:N	2.87	0.48
1:Y:443:ARG:NH2	1:Y:470:TYR:OH	2.41	0.48
4:D:110:THR:OG1	4:D:112:GLU:OE2	2.30	0.48
1:M:318:THR:HG22	1:M:324:GLU:OE1	2.13	0.48
6:R:15:GLU:HB2	6:R:23:ARG:NH2	2.28	0.48
1:S:59:HIS:HD1	1:S:64:LYS:HZ1	1.62	0.48
6:X:135:GLU:HB2	6:X:229:THR:CG2	2.42	0.48
6:X:41:CYS:SG	6:X:44:SER:N	2.87	0.48
6:F:264:LEU:N	6:F:305:GLU:OE1	2.47	0.48
3:O:225:LEU:HD11	3:O:246:GLU:HB2	1.96	0.48
3:U:160:ASN:OD1	3:U:178:ASN:HB3	2.13	0.48
6:X:37:CYS:SG	6:X:38:GLY:N	2.87	0.48
1:S:231:HIS:CE1	1:S:235:LEU:HD13	2.48	0.48
1:G:293:ALA:HA	1:G:374:ILE:HD11	1.96	0.48
13:H:503:MGD:S13	4:J:9:ARG:NH1	2.82	0.48
3:I:106:LYS:HG2	17:I:401:HOH:O	2.14	0.48
1:S:473:ASN:HB3	1:S:476:THR:OG1	2.14	0.48
3:U:127:GLU:HG3	3:U:153:THR:HB	1.96	0.48
5:E:80:GLU:OE1	5:E:81:LEU:HD23	2.14	0.48
6:F:334:PRO:HB2	6:F:336:ARG:NH2	2.29	0.48
4:V:117:MET:HB3	4:V:118:PRO:HD3	1.95	0.48
6:X:204:CYS:SG	6:X:207:ASP:N	2.87	0.48
6:X:242:CYS:SG	6:X:244:TRP:HD1	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:121:CYS:SG	6:L:130:ILE:HG21	2.54	0.48
1:A:318:THR:HG23	1:A:320:ASP:H	1.78	0.47
3:U:68:ILE:HD12	3:U:91:ARG:NH2	2.29	0.47
6:F:204:CYS:SG	6:F:207:ASP:N	2.87	0.47
3:O:201:GLY:HA3	3:O:204:MET:HE2	1.95	0.47
1:Y:439:ALA:O	1:Y:443:ARG:HB2	2.14	0.47
1:A:170:ARG:NH2	1:A:521:ASP:OD1	2.32	0.47
3:C:225:LEU:HD12	3:C:244:LYS:HE2	1.96	0.47
6:F:49:ASN:OD1	6:F:61:LYS:HD2	2.14	0.47
3:I:189:LEU:HD22	3:I:234:ASP:HB2	1.96	0.47
1:M:526:GLU:HG3	1:M:527:SER:N	2.28	0.47
1:S:472:ILE:HD13	1:S:486:ILE:HD13	1.95	0.47
6:X:37:CYS:HB2	6:X:77:CYS:HB2	1.95	0.47
1:Y:551:TYR:HB3	1:Y:552:PRO:HD3	1.96	0.47
6:L:200:CYS:SG	6:L:209:ILE:HG21	2.54	0.47
1:M:434:THR:O	1:M:438:ILE:HG23	2.14	0.47
1:M:111:THR:OG1	1:M:456:LYS:HE2	2.15	0.47
1:S:148:PHE:CE2	1:S:536:VAL:HG22	2.49	0.47
1:Y:323:MET:HE1	8:Y:603:MFN:C5	2.45	0.47
2:Z:288:ARG:HG2	2:Z:396:MET:HB2	1.97	0.47
1:A:1:MET:HG2	1:A:3:TYR:CE2	2.50	0.47
4:D:32:ILE:HD12	4:D:65:VAL:HG21	1.96	0.47
5:E:12:CYS:SG	5:E:52:VAL:HA	2.55	0.47
6:F:212:VAL:HG11	6:R:218:TYR:CE1	2.49	0.47
4:V:11:ILE:HG12	5:W:13:HIS:CE1	2.50	0.47
2:B:338:MET:HE2	2:B:357:MET:HG2	1.96	0.47
2:B:385:VAL:HG23	13:B:503:MGD:O6	2.15	0.47
2:N:141:ASN:HD22	2:N:170:PHE:N	2.09	0.47
6:R:38:GLY:HA2	6:R:46:ILE:HB	1.96	0.47
6:X:50:PRO:O	6:X:54:MET:HG2	2.15	0.47
1:G:231:HIS:CE1	1:G:235:LEU:HD13	2.50	0.47
6:R:348:LEU:C	6:R:349:LYS:HG3	2.34	0.47
6:F:37:CYS:HB2	6:F:77:CYS:HB2	1.96	0.47
4:J:82:PRO:O	4:J:86:ARG:HG2	2.15	0.47
6:L:5:GLU:HB2	6:L:68:GLU:HG3	1.97	0.47
1:M:103:ARG:HA	1:M:106:GLN:HG3	1.97	0.47
6:X:125:CYS:SG	6:X:128:ASP:N	2.87	0.47
1:Y:162:ALA:HB3	1:Y:221:LYS:HE2	1.96	0.47
2:B:375:MET:O	4:D:126:LYS:HE3	2.14	0.47
6:R:277:CYS:SG	6:R:286:LEU:HD13	2.55	0.47
1:S:540:PHE:HA	1:S:544:TYR:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:CYS:SG	5:E:68:VAL:N	2.87	0.47
2:N:371:PRO:HB3	4:P:121:MET:SD	2.55	0.47
6:R:37:CYS:SG	6:R:38:GLY:N	2.88	0.47
5:W:12:CYS:SG	5:W:52:VAL:HA	2.54	0.47
1:Y:207:THR:OG1	1:Y:210:GLU:HG3	2.14	0.47
2:B:344:ASP:OD1	2:B:372:THR:OG1	2.20	0.46
6:R:76:MET:HE1	6:R:343:ALA:HB3	1.98	0.46
2:Z:159:ARG:O	2:Z:163:ARG:HG3	2.14	0.46
1:G:3:TYR:CE1	1:G:40:LYS:HD2	2.51	0.46
2:H:68:ASP:N	2:H:68:ASP:OD1	2.48	0.46
3:I:204:MET:SD	3:I:256:GLY:HA3	2.55	0.46
1:M:502:ILE:HG21	1:M:505:LYS:HE2	1.98	0.46
1:M:551:TYR:HB3	1:M:552:PRO:HD3	1.97	0.46
1:S:115:ALA:HA	1:S:140:TYR:CD2	2.50	0.46
1:Y:159:ASP:HA	1:Y:221:LYS:NZ	2.30	0.46
4:J:52:LYS:HD2	4:J:61:VAL:HG22	1.97	0.46
5:K:44:ILE:HD11	5:K:47:ILE:HG22	1.96	0.46
1:M:505:LYS:HE3	1:M:505:LYS:HB2	1.69	0.46
2:N:182:ILE:HG12	2:N:197:ILE:HB	1.97	0.46
3:O:160:ASN:OD1	3:O:178:ASN:HB3	2.15	0.46
2:N:375:MET:O	4:P:126:LYS:HE3	2.15	0.46
1:Y:523:GLN:HE22	1:Y:568:MET:CE	2.28	0.46
2:H:11:PHE:CE2	2:H:37:ILE:HG21	2.50	0.46
3:I:182:GLY:HA3	3:I:209:ILE:HD11	1.97	0.46
4:J:117:MET:HB3	4:J:118:PRO:HD3	1.97	0.46
6:L:164:CYS:SG	6:L:168:ALA:N	2.78	0.46
1:M:2:GLU:HG2	1:M:27:LYS:CB	2.44	0.46
6:R:315:GLU:HA	6:R:323:ILE:HG23	1.96	0.46
6:R:23:ARG:O	6:R:88:LEU:HA	2.14	0.46
1:M:99:MET:O	1:M:103:ARG:HG3	2.14	0.46
1:A:272:VAL:HG23	1:A:370:LEU:HD13	1.96	0.46
1:G:2:GLU:CG	1:G:27:LYS:HD2	2.45	0.46
1:M:398:VAL:O	1:M:402:LEU:HG	2.15	0.46
5:Q:18:CYS:SG	5:Q:19:VAL:N	2.88	0.46
2:B:327:ASN:O	2:B:331:GLN:HG3	2.15	0.46
5:Q:78:LEU:HD12	6:R:57:THR:HG21	1.98	0.46
6:R:43:VAL:HG13	6:R:45:ALA:HB2	1.97	0.46
1:A:46:GLY:O	17:A:701:HOH:O	2.20	0.46
1:G:217:GLU:HG3	1:G:254:ILE:HD13	1.97	0.46
3:I:201:GLY:HA3	3:I:204:MET:HE2	1.98	0.46
1:M:502:ILE:HG21	1:M:505:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:210:VAL:HG11	3:O:238:LEU:CD2	2.46	0.46
6:R:271:CYS:SG	6:R:300:LYS:HD2	2.56	0.46
6:R:50:PRO:O	6:R:54:MET:HG2	2.16	0.46
1:A:115:ALA:HA	1:A:140:TYR:CD2	2.51	0.46
2:T:11:PHE:CE2	2:T:37:ILE:HG21	2.51	0.46
2:T:36:ARG:NH1	5:W:12:CYS:O	2.49	0.46
3:U:201:GLY:HA3	3:U:204:MET:HE2	1.98	0.46
1:A:33:GLU:HG2	1:A:34:SER:N	2.31	0.46
2:B:50:ARG:O	2:B:52:LYS:HD2	2.15	0.46
2:B:68:ASP:OD1	2:B:68:ASP:N	2.49	0.46
3:C:32:GLU:HA	3:C:35:LYS:CD	2.46	0.46
4:D:34:GLN:HB2	4:D:77:TYR:HB3	1.96	0.46
1:M:71:TYR:HA	2:N:127:GLN:HG2	1.97	0.46
4:V:55:SER:HB3	4:V:105:VAL:HG12	1.97	0.46
2:Z:270:ILE:HG12	2:Z:284:LEU:HD21	1.98	0.46
3:C:57:GLU:HG2	3:C:58:PRO:O	2.15	0.45
1:G:310:THR:HB	1:G:394:ARG:HD2	1.98	0.45
1:G:505:LYS:HB2	1:G:510:VAL:HG11	1.97	0.45
3:I:143:ASP:OD1	3:I:144:TRP:N	2.49	0.45
6:L:315:GLU:OE2	6:L:325:VAL:N	2.48	0.45
1:S:411:LEU:O	1:S:416:LEU:HB2	2.16	0.45
6:L:217:PRO:HG3	6:X:217:PRO:HG3	1.97	0.45
1:Y:159:ASP:OD1	1:Y:221:LYS:NZ	2.49	0.45
2:B:53:LYS:CD	2:B:53:LYS:N	2.79	0.45
6:L:204:CYS:SG	6:L:207:ASP:N	2.90	0.45
1:Y:231:HIS:ND1	1:Y:271:HIS:CE1	2.84	0.45
2:B:277:ASN:HA	2:B:280:ALA:O	2.15	0.45
6:F:242:CYS:SG	6:F:244:TRP:HD1	2.39	0.45
4:P:10:THR:HG22	4:P:12:TRP:N	2.30	0.45
6:R:87:ASP:OD2	6:R:94:SER:OG	2.34	0.45
1:Y:17:VAL:HA	1:Y:20:GLU:OE1	2.16	0.45
2:Z:238:ALA:O	2:Z:242:LEU:HG	2.16	0.45
2:B:84:PRO:HG2	2:B:109:ALA:HB2	1.97	0.45
6:F:160:CYS:SG	6:F:161:GLU:N	2.89	0.45
2:H:344:ASP:OD1	2:H:372:THR:OG1	2.23	0.45
6:L:102:PRO:HG2	6:L:340:TRP:CE3	2.52	0.45
1:M:235:LEU:HD11	8:M:603:MFN:H11A	1.98	0.45
3:O:3:GLU:HG2	3:O:66:LYS:HD3	1.98	0.45
2:T:73:LYS:HG2	2:T:73:LYS:H	1.56	0.45
2:Z:23:VAL:HG22	2:Z:28:ILE:CD1	2.47	0.45
1:A:309:ILE:HA	1:A:309:ILE:HD13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASN:HB2	2:B:323:GLU:HB3	1.99	0.45
1:G:411:LEU:O	1:G:416:LEU:HB2	2.15	0.45
1:S:48:ILE:HD12	1:S:472:ILE:HG23	1.97	0.45
1:M:369:GLU:OE2	1:M:425:THR:HG22	2.16	0.45
3:O:189:LEU:HD13	3:O:233:VAL:HG11	1.98	0.45
1:S:148:PHE:HE2	1:S:536:VAL:HA	1.81	0.45
6:X:31:CYS:SG	6:X:63:LYS:HD3	2.56	0.45
2:H:89:TRP:CH2	2:H:100:GLY:HA3	2.51	0.45
1:M:502:ILE:HD13	1:M:505:LYS:HE2	1.99	0.45
6:R:200:CYS:SG	6:R:209:ILE:HG21	2.56	0.45
6:R:41:CYS:SG	6:R:43:VAL:HG12	2.56	0.45
1:A:7:ASN:CB	1:A:21:LYS:HE3	2.46	0.45
1:M:82:LYS:HD3	1:M:88:ALA:HB2	1.98	0.45
3:O:238:LEU:HA	3:O:239:PRO:HD3	1.88	0.45
1:A:191:GLY:N	2:B:281:LYS:HG3	2.32	0.45
2:B:361:PRO:HA	2:B:377:ASP:OD2	2.17	0.45
1:G:124:HIS:HE1	1:G:128:GLU:OE2	2.00	0.45
1:M:14:LEU:HD13	1:M:458:HIS:HB3	1.99	0.45
6:X:16:ARG:HH21	6:X:22:ARG:CG	2.25	0.45
2:Z:149:TRP:O	2:Z:252:PHE:HA	2.17	0.45
1:G:3:TYR:CZ	1:G:40:LYS:HD2	2.52	0.45
3:I:66:LYS:HG2	3:I:68:ILE:HD11	1.98	0.45
4:J:78:ILE:HG22	4:J:84:ALA:HB2	1.99	0.45
2:Z:75:ALA:HB1	2:Z:425:VAL:CG2	2.47	0.45
2:B:358:ALA:HA	4:D:126:LYS:HD3	1.98	0.44
1:G:282:TRP:HB3	8:G:603:MFN:O6	2.17	0.44
1:S:4:ILE:HG13	1:S:6:LYS:HG2	1.98	0.44
6:F:324:THR:O	6:F:324:THR:HG22	5.05	0.44
1:M:64:LYS:HG2	1:M:317:MET:HB2	2.00	0.44
2:Z:55:LEU:CD2	2:Z:64:GLU:HG2	2.47	0.44
1:G:4:ILE:HG22	1:G:40:LYS:O	2.17	0.44
1:G:448:LYS:HA	1:G:453:SER:OG	2.17	0.44
2:H:2:GLU:HB2	2:H:23:VAL:HG13	1.98	0.44
2:H:58:LYS:HZ2	2:H:63:VAL:HG11	1.83	0.44
2:H:55:LEU:HD23	2:H:64:GLU:HA	2.00	0.44
2:Z:16:CYS:SG	2:Z:163:ARG:NH1	2.91	0.44
6:X:277:CYS:HB2	6:X:314:CYS:HB2	1.98	0.44
6:X:334:PRO:CB	6:X:336:ARG:HH12	2.28	0.44
2:Z:28:ILE:HD11	2:Z:407:VAL:HG13	1.98	0.44
4:D:117:MET:HB3	4:D:118:PRO:HD3	1.99	0.44
6:F:71:CYS:SG	6:F:73:LEU:HG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:344:THR:OG1	1:M:345:GLY:N	2.50	0.44
2:N:6:ASN:O	2:N:404:LYS:NZ	2.44	0.44
6:R:277:CYS:SG	6:R:278:VAL:N	2.90	0.44
1:G:64:LYS:HG2	1:G:317:MET:HB2	1.98	0.44
1:M:75:ASP:O	1:M:78:ARG:HG2	2.18	0.44
2:N:292:ASN:OD1	2:N:295:GLY:HA3	2.18	0.44
6:R:277:CYS:HB2	6:R:314:CYS:HB2	1.98	0.44
3:U:81:GLN:HG2	3:U:82:GLU:HG3	1.99	0.44
6:X:277:CYS:SG	6:X:278:VAL:N	2.91	0.44
4:D:78:ILE:HG22	4:D:84:ALA:HB2	1.99	0.44
2:H:110:VAL:HG22	2:H:311:ASP:HA	2.00	0.44
4:J:22:ASP:OD1	4:J:22:ASP:N	2.48	0.44
6:L:245:CYS:SG	6:L:246:GLN:N	2.90	0.44
1:M:2:GLU:HG2	1:M:27:LYS:HA	1.98	0.44
2:N:15:LEU:HD23	2:N:401:ILE:HD12	1.99	0.44
2:T:210:LEU:HD13	2:T:268:THR:HG23	2.00	0.44
1:Y:565:LYS:HD2	1:Y:568:MET:HE1	1.99	0.44
1:A:386:SER:HA	1:A:387:PRO:HA	1.83	0.44
1:A:71:TYR:HA	2:B:127:GLN:HG2	2.00	0.44
1:G:443:ARG:NH2	1:G:470:TYR:OH	2.49	0.44
1:M:537:GLU:HG2	1:M:541:LYS:HE3	1.99	0.44
2:N:5:LYS:HG2	2:N:20:ILE:HD12	1.99	0.44
4:V:1:MET:HE2	4:V:43:LEU:HD13	2.00	0.44
2:B:167:ALA:O	2:B:179:ARG:NH2	2.47	0.44
1:G:57:HIS:CE1	1:G:115:ALA:HB1	2.53	0.44
1:M:124:HIS:NE2	1:M:128:GLU:OE2	2.51	0.44
1:M:496:VAL:HB	1:M:504:VAL:HB	1.99	0.44
6:X:160:CYS:SG	6:X:161:GLU:N	2.91	0.44
5:E:25:ASN:HB3	5:E:32:VAL:HG11	1.99	0.43
6:F:95:ILE:HG13	6:F:96:LYS:HD3	1.99	0.43
1:G:244:THR:OG1	1:G:275:HIS:HB3	2.16	0.43
1:G:280:THR:HG22	1:G:284:ASP:OD2	2.18	0.43
5:K:18:CYS:HB2	5:K:67:CYS:HB2	2.00	0.43
1:Y:496:VAL:HB	1:Y:504:VAL:HB	2.00	0.43
2:B:57:ARG:C	2:B:58:LYS:HD2	2.39	0.43
3:C:16:LEU:HD23	3:C:41:HIS:HB2	2.00	0.43
1:G:3:TYR:CD1	1:G:40:LYS:HB2	2.51	0.43
5:K:5:LEU:HD21	5:K:76:ILE:HD11	2.00	0.43
2:T:333:ARG:NH1	2:T:359:GLU:OE1	2.49	0.43
6:X:277:CYS:SG	6:X:286:LEU:HD13	2.58	0.43
6:F:164:CYS:SG	6:F:168:ALA:N	2.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:ALA:HA	13:H:503:MGD:N3	2.33	0.43
1:M:376:ASN:ND2	1:M:378:GLU:H	2.16	0.43
2:B:58:LYS:N	2:B:58:LYS:HD2	2.33	0.43
6:F:242:CYS:O	6:F:307:PHE:HA	2.18	0.43
5:K:23:PRO:HG2	6:L:319:PRO:HG2	2.01	0.43
6:L:242:CYS:O	6:L:307:PHE:HA	2.19	0.43
4:P:6:ASN:O	4:P:77:TYR:HA	2.18	0.43
6:R:102:PRO:HG2	6:R:340:TRP:CE3	2.53	0.43
6:R:31:CYS:SG	6:R:63:LYS:HD3	2.58	0.43
1:S:88:ALA:HB1	2:T:317:PRO:HD3	2.00	0.43
4:V:6:ASN:O	4:V:77:TYR:HA	2.18	0.43
6:X:43:VAL:HG12	6:X:70:LYS:HB3	2.00	0.43
1:Y:286:VAL:HG22	1:Y:423:LYS:HB3	2.01	0.43
3:O:11:GLN:HE22	3:O:76:THR:CG2	2.32	0.43
1:Y:71:TYR:HA	2:Z:127:GLN:HG2	2.01	0.43
6:F:217:PRO:HG3	6:R:217:PRO:HG3	2.00	0.43
1:G:293:ALA:HB1	1:G:374:ILE:HG13	1.99	0.43
3:I:269:ALA:HA	3:I:270:PRO:HD3	1.69	0.43
2:N:74:ALA:HB1	2:N:363:ILE:HD13	2.01	0.43
2:N:174:ARG:NH2	6:R:298:THR:OG1	2.51	0.43
1:S:103:ARG:O	1:S:107:MET:HG2	2.18	0.43
2:T:149:TRP:O	2:T:252:PHE:HA	2.18	0.43
2:T:68:ASP:OD1	2:T:68:ASP:N	2.52	0.43
1:Y:469:VAL:HG22	1:Y:495:CYS:HB3	1.99	0.43
5:W:25:ASN:HB3	5:W:32:VAL:HG11	2.00	0.43
6:X:88:LEU:HD23	6:X:89:GLN:N	2.33	0.43
1:G:411:LEU:HG	1:G:416:LEU:HG	2.01	0.43
1:G:551:TYR:HB3	1:G:552:PRO:HD3	2.01	0.43
1:M:244:THR:OG1	1:M:275:HIS:HB3	2.19	0.43
2:N:72:ASP:HB2	2:N:424:LYS:HZ2	1.84	0.43
1:S:151:GLU:O	1:S:155:GLU:HG2	2.19	0.43
1:S:84:LYS:HB2	1:S:84:LYS:HE2	1.92	0.43
2:Z:346:GLY:O	2:Z:354:LEU:HD21	2.19	0.43
1:A:180:VAL:HA	1:A:231:HIS:HB3	2.00	0.43
4:D:48:GLY:HA2	4:D:63:LYS:HD2	2.00	0.43
6:F:37:CYS:SG	6:F:38:GLY:N	2.91	0.43
5:K:18:CYS:SG	5:K:19:VAL:N	2.92	0.43
6:L:221:TYR:CE1	6:X:210:MET:HG2	2.54	0.43
1:M:4:ILE:HD13	1:M:35:VAL:CG2	2.48	0.43
4:P:1:MET:HE2	4:P:1:MET:HB3	1.78	0.43
4:P:78:ILE:HG22	4:P:84:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:78:ILE:HG22	4:V:84:ALA:HB2	2.01	0.43
1:Y:231:HIS:CE1	1:Y:235:LEU:HD13	2.54	0.43
2:B:89:TRP:CH2	2:B:100:GLY:HA3	2.54	0.43
3:C:48:LEU:HD23	3:C:52:PHE:HB2	2.01	0.43
2:H:149:TRP:O	2:H:252:PHE:HA	2.18	0.43
2:H:351:GLN:HE21	4:J:86:ARG:C	2.21	0.43
6:L:337:SER:O	6:L:341:LYS:HG3	2.19	0.43
3:U:16:LEU:HB2	3:U:76:THR:HG23	2.01	0.43
5:W:76:ILE:C	5:W:77:ARG:HG2	2.40	0.43
6:X:20:GLU:OE1	6:X:22:ARG:NE	2.50	0.43
1:Y:222:LEU:C	1:Y:567:VAL:HG23	2.39	0.43
6:F:213:CYS:SG	6:F:215:ILE:HD13	2.59	0.42
1:G:88:ALA:HB1	2:H:317:PRO:HD3	2.00	0.42
2:T:89:TRP:CH2	2:T:100:GLY:HA3	2.54	0.42
2:B:428:TYR:N	2:B:428:TYR:CD2	2.87	0.42
2:B:8:VAL:HA	2:B:17:ASP:HA	2.00	0.42
6:F:94:SER:OG	6:F:96:LYS:HG2	2.19	0.42
2:H:86:MET:SD	2:H:103:LEU:HD22	2.58	0.42
6:R:76:MET:CE	6:R:343:ALA:HB3	2.50	0.42
2:T:289:GLY:HA3	13:T:504:MGD:C13	2.49	0.42
1:Y:23:ASP:OD2	17:Y:701:HOH:O	2.20	0.42
1:Y:64:LYS:HE2	1:Y:318:THR:C	2.39	0.42
2:Z:15:LEU:HD23	2:Z:401:ILE:HD12	2.02	0.42
1:A:31:ILE:HD11	1:A:467:ILE:HD11	2.01	0.42
3:C:182:GLY:HA3	3:C:209:ILE:HD11	2.01	0.42
5:E:71:CYS:SG	5:E:74:ASP:N	2.93	0.42
1:G:226:HIS:ND1	1:G:450:LEU:HD23	2.35	0.42
2:H:84:PRO:HG2	2:H:109:ALA:HB2	2.01	0.42
2:N:366:GLU:OE1	2:N:367:PRO:HD2	2.19	0.42
1:A:384:THR:O	1:A:389:ALA:HB3	2.20	0.42
6:R:198:GLY:O	6:R:202:ARG:HG3	2.19	0.42
2:Z:56:ILE:HG12	2:Z:378:ILE:HG12	2.01	0.42
1:A:37:ASP:OD1	1:A:37:ASP:N	2.50	0.42
3:I:16:LEU:HD12	3:I:76:THR:HG22	2.01	0.42
1:M:438:ILE:HA	1:M:441:ILE:HG12	2.01	0.42
1:M:163:ALA:HB2	1:M:528:ILE:HG22	2.01	0.42
1:S:244:THR:OG1	1:S:275:HIS:HB3	2.18	0.42
1:S:107:MET:HE1	1:S:393:THR:HA	2.02	0.42
2:B:424:LYS:HD2	2:B:428:TYR:CE2	2.55	0.42
1:G:540:PHE:HA	1:G:544:TYR:HB2	2.01	0.42
1:M:232:CYS:HB2	1:M:275:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:438:ILE:HG13	1:M:439:ALA:N	2.34	0.42
6:R:281:CYS:SG	6:R:284:ASN:N	2.92	0.42
1:S:6:LYS:HZ2	1:S:6:LYS:HB3	1.85	0.42
6:X:23:ARG:CZ	6:X:25:ILE:HD11	2.49	0.42
1:Y:231:HIS:HE1	8:Y:603:MFN:N1	2.18	0.42
2:Z:58:LYS:HD2	2:Z:58:LYS:HA	1.73	0.42
5:E:74:ASP:HB3	5:E:77:ARG:HE	1.85	0.42
1:G:61:ALA:HA	1:G:128:GLU:OE1	2.20	0.42
6:L:104:ILE:HD11	6:L:344:PHE:HE1	1.83	0.42
1:M:4:ILE:HD12	1:M:25:CYS:HA	2.02	0.42
2:N:299:VAL:HG22	2:N:302:TRP:CH2	2.54	0.42
6:R:46:ILE:HG23	6:R:64:ILE:HG23	2.02	0.42
1:A:219:ASN:OD1	1:A:224:LEU:HD12	2.20	0.42
2:B:328:ASP:N	2:B:328:ASP:OD1	2.51	0.42
1:M:162:ALA:HA	1:M:218:VAL:HG13	2.02	0.42
1:M:282:TRP:CZ2	8:M:603:MFN:H152	2.55	0.42
3:O:99:GLY:O	3:O:102:MET:HB2	2.20	0.42
3:U:61:ALA:HB1	3:U:63:GLU:OE2	2.19	0.42
1:Y:136:ASP:OD2	1:Y:456:LYS:NZ	2.51	0.42
2:Z:333:ARG:HD2	2:Z:333:ARG:HH11	1.53	0.42
1:S:5:ILE:HD12	1:S:5:ILE:N	4.38	0.42
2:T:8:VAL:HA	2:T:17:ASP:HA	2.01	0.42
1:A:244:THR:OG1	1:A:275:HIS:HB3	2.20	0.42
2:H:159:ARG:O	2:H:163:ARG:HG3	2.19	0.42
2:N:223:LEU:HD23	2:N:224:TYR:CZ	2.54	0.42
4:P:82:PRO:O	4:P:86:ARG:HG2	2.20	0.42
6:R:270:THR:O	6:R:272:GLN:NE2	2.48	0.42
2:T:375:MET:O	4:V:126:LYS:HE3	2.20	0.42
1:Y:235:LEU:CD1	8:Y:603:MFN:H11A	2.50	0.42
6:F:23:ARG:O	6:F:88:LEU:HD12	2.20	0.41
6:F:277:CYS:SG	6:F:278:VAL:N	2.93	0.41
1:G:356:ARG:HD3	1:G:415:GLU:HG3	2.02	0.41
1:M:143:PHE:CE2	1:M:168:LEU:HD23	2.55	0.41
2:N:35:CYS:SG	2:N:36:ARG:N	2.93	0.41
1:S:289:ALA:HB2	1:S:366:ILE:HG23	2.01	0.41
1:A:8:GLY:O	1:A:21:LYS:HA	2.20	0.41
2:B:93:GLU:HB3	2:B:385:VAL:HG11	2.03	0.41
3:C:70:ASP:OD2	3:C:91:ARG:HD2	2.20	0.41
6:X:4:THR:CG2	6:X:15:GLU:HB3	2.49	0.41
2:Z:118:CYS:SG	14:Z:505:H2S:S	3.18	0.41
6:R:315:GLU:OE2	6:R:324:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:160:CYS:SG	6:X:169:ILE:HD13	2.59	0.41
1:M:316:THR:HB	8:M:603:MFN:H5	2.02	0.41
2:T:235:ILE:O	2:T:239:VAL:HG23	2.20	0.41
2:B:40:SER:OG	4:D:15:GLN:HG3	2.20	0.41
6:R:121:CYS:SG	6:R:122:GLU:N	2.94	0.41
8:S:603:MFN:H261	8:S:603:MFN:C34	2.51	0.41
2:Z:299:VAL:HG22	2:Z:302:TRP:CZ2	2.55	0.41
1:A:207:THR:OG1	1:A:210:GLU:HG3	2.21	0.41
1:A:283:ARG:HE	1:A:283:ARG:HB3	1.73	0.41
5:E:23:PRO:HG2	6:F:319:PRO:HG2	2.02	0.41
6:F:96:LYS:HD3	6:F:96:LYS:N	2.36	0.41
2:N:210:LEU:HD13	2:N:268:THR:HG23	2.02	0.41
1:S:154:LYS:HE2	1:S:205:ASP:O	2.21	0.41
2:T:338:MET:HE2	2:T:357:MET:HG2	2.03	0.41
6:X:242:CYS:O	6:X:307:PHE:HA	2.21	0.41
2:Z:8:VAL:HA	2:Z:17:ASP:HA	2.01	0.41
2:B:428:TYR:HD2	2:B:428:TYR:N	2.18	0.41
1:G:356:ARG:HG2	1:G:356:ARG:H	1.63	0.41
6:L:22:ARG:HG2	6:L:90:ILE:CD1	2.50	0.41
2:N:141:ASN:ND2	2:N:170:PHE:H	2.09	0.41
3:O:16:LEU:HD12	3:O:76:THR:HG22	2.02	0.41
5:Q:12:CYS:SG	5:Q:52:VAL:HA	2.61	0.41
5:Q:80:GLU:HG3	5:Q:81:LEU:HG	2.01	0.41
2:T:20:ILE:HB	2:T:32:ILE:HB	2.03	0.41
2:T:323:GLU:OE1	3:U:97:TYR:OH	2.38	0.41
2:Z:254:MET:HA	2:Z:257:THR:OG1	2.21	0.41
2:Z:72:ASP:HA	2:Z:424:LYS:CD	2.51	0.41
1:A:4:ILE:HD11	1:A:23:ASP:HB3	2.03	0.41
1:M:162:ALA:HB1	1:M:222:LEU:HD11	2.03	0.41
6:R:214:ARG:NH1	6:R:222:GLU:OE2	2.53	0.41
3:U:166:MET:HB3	3:U:185:MET:HG3	2.03	0.41
6:X:102:PRO:HG2	6:X:340:TRP:CE3	2.55	0.41
1:Y:529:TYR:CE2	1:Y:533:LEU:HD11	2.56	0.41
1:A:269:ALA:O	1:A:304:ILE:HA	2.21	0.41
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.83	0.41
2:H:159:ARG:NH1	2:H:163:ARG:HH21	2.17	0.41
5:K:71:CYS:SG	5:K:74:ASP:N	2.94	0.41
2:N:89:TRP:CH2	2:N:100:GLY:HA3	2.56	0.41
3:U:177:VAL:HG22	3:U:196:VAL:HG22	2.03	0.41
2:T:205:ARG:NH2	3:U:217:GLU:OE2	2.53	0.41
1:M:48:ILE:HD12	1:M:472:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:69:ILE:HD12	3:O:90:VAL:HG22	2.03	0.41
2:T:415:ARG:NH1	2:T:416:GLU:HG2	2.36	0.41
1:Y:36:SER:OG	1:Y:38:SER:OG	2.31	0.41
2:B:53:LYS:HD3	2:B:53:LYS:H	1.85	0.41
3:C:106:LYS:NZ	3:C:108:THR:OG1	2.44	0.41
3:C:231:ILE:HG13	3:C:238:LEU:HB2	2.03	0.41
1:G:84:LYS:HG3	1:G:85:GLY:H	1.84	0.41
1:S:523:GLN:NE2	1:S:569:LEU:H	2.19	0.41
5:W:23:PRO:HB3	6:X:272:GLN:HB2	2.02	0.41
1:Y:384:THR:HG23	1:Y:395:TYR:CE1	2.56	0.41
1:Y:441:ILE:HG13	1:Y:442:THR:HG23	2.01	0.41
2:Z:139:VAL:HG13	2:Z:249:ILE:HG21	2.02	0.41
3:C:16:LEU:HD22	3:C:39:ILE:HD12	2.03	0.40
6:F:227:GLU:O	6:F:227:GLU:HG3	2.21	0.40
2:H:8:VAL:HA	2:H:17:ASP:HA	2.03	0.40
3:O:38:GLN:HG3	3:O:45:VAL:HG13	2.03	0.40
1:S:136:ASP:OD2	1:S:456:LYS:NZ	2.52	0.40
1:A:118:PRO:HG2	1:A:121:LEU:HD12	2.03	0.40
1:A:323:MET:HE1	8:A:603:MFN:C5	2.51	0.40
1:G:144:GLY:HA3	1:G:179:ILE:HG23	2.03	0.40
1:G:520:VAL:HG12	1:G:522:THR:HG23	2.02	0.40
2:H:375:MET:O	4:J:126:LYS:HE3	2.21	0.40
6:L:326:LYS:NZ	6:L:326:LYS:HB3	2.36	0.40
1:M:439:ALA:O	1:M:443:ARG:HB2	2.20	0.40
2:N:255:GLY:O	2:N:259:SER:OG	2.20	0.40
6:F:31:CYS:SG	6:F:63:LYS:HD3	2.61	0.40
1:M:31:ILE:HG23	1:M:54:VAL:HG12	18.29	0.40
1:Y:167:TRP:CD1	1:Y:533:LEU:HD21	2.57	0.40
2:B:374:GLU:HG3	4:D:117:MET:HE1	2.04	0.40
3:C:32:GLU:HA	3:C:35:LYS:CE	2.51	0.40
4:J:34:GLN:HB2	4:J:77:TYR:HB3	2.03	0.40
2:H:351:GLN:HG2	4:J:86:ARG:O	2.22	0.40
1:M:443:ARG:HD2	1:M:443:ARG:N	2.35	0.40
1:M:526:GLU:CG	1:M:527:SER:N	2.84	0.40
2:N:5:LYS:HD3	5:Q:39:THR:HG22	2.03	0.40
6:X:249:CYS:SG	6:X:253:ALA:N	2.82	0.40
2:Z:89:TRP:CH2	2:Z:100:GLY:HA3	2.57	0.40
1:A:496:VAL:HB	1:A:504:VAL:HB	2.03	0.40
2:H:124:LEU:HD21	2:H:321:PRO:HG2	2.04	0.40
2:H:286:PRO:HG2	2:H:288:ARG:HD3	2.02	0.40
3:I:5:ILE:N	3:I:5:ILE:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:41:CYS:SG	6:L:44:SER:N	2.95	0.40
2:T:223:LEU:HD23	2:T:224:TYR:CZ	2.56	0.40
2:T:76:LYS:HD2	2:T:428:TYR:CZ	2.56	0.40
2:Z:286:PRO:HG2	2:Z:288:ARG:HD3	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:336:ARG:NH1	1:e:526:GLU:OE1[1_544]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
6	F	92	GLY
1	G	415	GLU
6	L	92	GLY
1	S	415	GLU
2	T	60	GLY
6	d	92	GLY
6	p	92	GLY
6	v	92	GLY
2	B	59	ASN
2	T	59	ASN
2	N	59	ASN
2	T	382	PRO
2	Z	382	PRO
2	r	382	PRO
2	B	382	PRO
2	H	382	PRO
2	N	382	PRO
2	f	382	PRO
2	l	382	PRO
1	G	84	LYS
6	d	102	PRO
2	H	25	GLY
2	f	25	GLY
2	r	307	PRO
2	T	307	PRO

5.3.2 Protein sidechains ⓘ

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	A	231	HIS
1	A	380	VAL
1	A	407	TYR
2	B	20	ILE
2	B	27	GLU
2	B	35	CYS
2	B	53	LYS
2	B	57	ARG
2	B	68	ASP
2	B	82	LYS

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Mol	Chain	Res	Type
2	B	281	LYS
2	B	302	TRP
2	B	308	TYR
2	B	351	GLN
2	B	397	GLU
2	B	410	ASP
3	C	237	GLU
3	C	264	CYS
4	D	117	MET
5	E	15	CYS
5	E	22	CYS
5	E	46	MET
5	E	61	CYS
6	F	31	CYS
6	F	118	CYS
6	F	143	VAL
6	F	194	CYS
6	F	210	MET
6	F	222	GLU
6	F	240	VAL
6	F	306	ARG
6	F	328	ASN
1	G	71	TYR
1	G	231	HIS
1	G	323	MET
1	G	380	VAL
1	G	407	TYR
1	G	505	LYS
2	H	35	CYS
2	H	58	LYS
2	H	68	ASP
2	H	302	TRP
2	H	308	TYR
2	H	397	GLU
2	H	411	LEU
3	I	44	GLU
3	I	187	ASN
3	I	264	CYS
4	J	129	GLN
5	K	22	CYS
5	K	46	MET
5	K	61	CYS

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Mol	Chain	Res	Type
5	K	69	GLU
6	L	2	GLU
6	L	118	CYS
6	L	194	CYS
6	L	201	LYS
1	M	71	TYR
1	M	222	LEU
1	M	231	HIS
1	M	405	ASN
1	M	407	TYR
1	M	492	ARG
1	M	523	GLN
1	M	568	MET
2	N	35	CYS
2	N	36	ARG
2	N	281	LYS
2	N	302	TRP
2	N	308	TYR
2	N	351	GLN
2	N	397	GLU
3	O	151	THR
3	O	232	GLU
3	O	264	CYS
5	Q	15	CYS
5	Q	22	CYS
5	Q	46	MET
5	Q	61	CYS
6	R	94	SER
6	R	118	CYS
6	R	144	THR
6	R	194	CYS
6	R	201	LYS
6	R	210	MET
6	R	222	GLU
1	S	71	TYR
1	S	231	HIS
1	S	286	VAL
1	S	356	ARG
1	S	380	VAL
1	S	406	LYS
1	S	407	TYR
1	S	482	GLU

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Mol	Chain	Res	Type
1	S	512	SER
2	T	20	ILE
2	T	35	CYS
2	T	68	ASP
2	T	302	TRP
2	T	308	TYR
2	T	351	GLN
2	T	397	GLU
2	T	421	LEU
3	U	187	ASN
3	U	223	LYS
3	U	264	CYS
4	V	2	ARG
4	V	11	ILE
4	V	129	GLN
5	W	5	LEU
5	W	15	CYS
5	W	22	CYS
5	W	46	MET
5	W	61	CYS
5	W	69	GLU
6	X	31	CYS
6	X	115	CYS
6	X	118	CYS
6	X	143	VAL
6	X	194	CYS
6	X	284	ASN
1	Y	71	TYR
1	Y	286	VAL
1	Y	407	TYR
1	Y	418	LYS
2	Z	35	CYS
2	Z	52	LYS
2	Z	58	LYS
2	Z	302	TRP
2	Z	308	TYR
2	Z	351	GLN
2	Z	397	GLU
3	a	187	ASN
3	a	231	ILE
3	a	236	GLU
3	a	237	GLU

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Mol	Chain	Res	Type
3	a	264	CYS
5	c	22	CYS
5	c	46	MET
5	c	61	CYS
5	c	63	LYS
6	d	91	ASP
6	d	118	CYS
6	d	144	THR
6	d	152	ASP
6	d	194	CYS
6	d	222	GLU
6	d	336	ARG
6	d	338	LYS
1	e	71	TYR
1	e	83	PHE
1	e	231	HIS
1	e	273	GLN
1	e	283	ARG
1	e	286	VAL
1	e	407	TYR
1	e	456	LYS
1	e	482	GLU
2	f	20	ILE
2	f	35	CYS
2	f	68	ASP
2	f	308	TYR
2	f	339	MET
2	f	351	GLN
2	f	397	GLU
2	f	421	LEU
3	g	60	ASP
3	g	236	GLU
4	h	2	ARG
5	i	15	CYS
5	i	22	CYS
5	i	46	MET
5	i	61	CYS
6	j	79	SER
6	j	118	CYS
6	j	154	CYS
6	j	194	CYS
6	j	201	LYS

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Mol	Chain	Res	Type
6	j	224	LYS
6	j	299	THR
6	j	338	LYS
1	k	71	TYR
1	k	354	SER
1	k	407	TYR
1	k	423	LYS
2	l	35	CYS
2	l	68	ASP
2	l	302	TRP
2	l	308	TYR
2	l	351	GLN
2	l	397	GLU
3	m	11	GLN
3	m	237	GLU
3	m	264	CYS
4	n	2	ARG
4	n	117	MET
5	o	15	CYS
5	o	22	CYS
5	o	46	MET
5	o	61	CYS
6	p	93	THR
6	p	118	CYS
6	p	142	LEU
6	p	194	CYS
6	p	299	THR
6	p	300	LYS
6	p	336	ARG
6	p	349	LYS
1	q	22	MET
1	q	36	SER
1	q	71	TYR
1	q	380	VAL
1	q	407	TYR
2	r	35	CYS
2	r	53	LYS
2	r	58	LYS
2	r	68	ASP
2	r	83	ARG
2	r	281	LYS
2	r	302	TRP

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Mol	Chain	Res	Type
2	r	308	TYR
2	r	351	GLN
2	r	354	LEU
2	r	397	GLU
3	s	55	SER
3	s	233	VAL
3	s	264	CYS
4	t	117	MET
5	u	5	LEU
5	u	15	CYS
5	u	22	CYS
5	u	46	MET
5	u	61	CYS
5	u	69	GLU
6	v	21	ASN
6	v	23	ARG
6	v	31	CYS
6	v	58	GLU
6	v	118	CYS
6	v	142	LEU
6	v	143	VAL
6	v	154	CYS
6	v	194	CYS
6	v	210	MET
6	v	336	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	342	ASN
1	G	106	GLN
1	G	523	GLN
2	H	234	GLN
2	H	297	ASN
1	M	253	ASN
1	M	363	GLN
1	M	376	ASN
1	M	405	ASN
2	N	141	ASN
3	O	216	GLN
1	S	523	GLN
1	Y	15	ASN

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Mol	Chain	Res	Type
1	Y	410	ASN
1	Y	523	GLN
3	a	265	ASN
6	d	246	GLN
6	d	268	GLN
2	f	44	HIS
1	k	7	ASN
1	k	106	GLN
1	k	126	HIS
1	q	253	ASN
2	r	332	ASN
3	s	81	GLN
6	v	21	ASN
6	v	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	S	178	KCX	CE-NZ-CX	-2.13	121.29	123.53
1	S	178	KCX	O-C-CA	-2.08	120.13	125.72
1	q	178	KCX	O-C-CA	-2.08	120.14	125.72
1	A	178	KCX	O-C-CA	-2.08	120.14	125.72
1	q	178	KCX	CE-NZ-CX	-2.06	121.36	123.53

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SF4	v	508	6	-	0/0/48/48	0/6/5/5

All (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
8	S	603	MFN	C23-N4	-3.28	1.41	1.46
8	e	603	MFN	C23-N4	-3.15	1.42	1.46
8	A	603	MFN	C23-N4	-2.66	1.42	1.46
8	M	603	MFN	C19-N3	-2.64	1.42	1.46
8	q	603	MFN	C19-N3	-2.11	1.43	1.46
8	G	603	MFN	C19-N3	-2.09	1.43	1.46
8	q	603	MFN	C26-C25	2.02	1.55	1.51
8	A	603	MFN	C27-C26	2.06	1.59	1.52
8	e	603	MFN	C26-C25	2.14	1.55	1.51
8	S	603	MFN	C13-C4	2.17	1.55	1.50
8	G	603	MFN	C13-C4	2.18	1.55	1.50
8	M	603	MFN	C13-C4	2.18	1.55	1.50
8	G	603	MFN	C26-C25	2.19	1.55	1.51
8	e	603	MFN	C17-C16	2.21	1.55	1.51
8	A	603	MFN	O2-C9	2.22	1.43	1.37
8	S	603	MFN	C26-C25	2.22	1.55	1.51
8	q	603	MFN	C13-C4	2.31	1.55	1.50
8	e	603	MFN	C10-C9	2.41	1.43	1.38
8	A	603	MFN	C26-C25	2.45	1.56	1.51
8	k	603	MFN	C10-C9	2.49	1.43	1.38
8	G	603	MFN	C17-C16	2.51	1.56	1.51
8	G	603	MFN	C10-C9	2.53	1.43	1.38
8	S	603	MFN	C10-C9	2.53	1.43	1.38
8	Y	603	MFN	C17-C16	2.54	1.56	1.51
8	Y	603	MFN	C10-C9	2.55	1.43	1.38
8	q	603	MFN	C17-C16	2.57	1.56	1.51
8	A	603	MFN	C17-C16	2.58	1.56	1.51
8	q	603	MFN	C10-C9	2.59	1.43	1.38
8	A	603	MFN	C13-C4	2.59	1.56	1.50
8	k	603	MFN	C17-C16	2.64	1.56	1.51
13	B	503	MGD	C5-C4	2.68	1.46	1.40
8	M	603	MFN	C10-C9	2.71	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	603	MFN	C17-C16	2.76	1.56	1.51
8	M	603	MFN	C17-C16	2.76	1.56	1.51
8	k	603	MFN	C8-C9	2.81	1.44	1.38
13	B	504	MGD	C5-C4	2.81	1.46	1.40
13	T	503	MGD	C5-C4	2.81	1.46	1.40
8	A	603	MFN	C10-C9	2.84	1.44	1.38
13	r	503	MGD	C5-C4	2.84	1.46	1.40
8	Y	603	MFN	C8-C9	2.85	1.44	1.38
13	f	504	MGD	C5-C4	2.87	1.47	1.40
8	G	603	MFN	C8-C9	2.88	1.44	1.38
8	M	603	MFN	C8-C9	2.88	1.44	1.38
13	l	504	MGD	C5-C4	2.88	1.47	1.40
13	Z	503	MGD	C5-C4	2.89	1.47	1.40
13	r	504	MGD	C5-C4	2.89	1.47	1.40
13	H	503	MGD	C5-C4	2.90	1.47	1.40
13	N	503	MGD	C5-C4	2.90	1.47	1.40
8	e	603	MFN	C8-C9	2.92	1.44	1.38
13	N	504	MGD	C5-C4	2.93	1.47	1.40
13	Z	504	MGD	C5-C4	2.94	1.47	1.40
13	T	504	MGD	C5-C4	2.95	1.47	1.40
13	l	503	MGD	C5-C4	2.95	1.47	1.40
8	A	603	MFN	C8-C9	2.96	1.44	1.38
13	f	503	MGD	C5-C4	2.97	1.47	1.40
8	S	603	MFN	C8-C9	2.99	1.44	1.38
8	q	603	MFN	C8-C9	3.03	1.44	1.38
13	H	504	MGD	C5-C4	3.05	1.47	1.40
13	l	503	MGD	C16-C21	3.42	1.47	1.41
13	Z	503	MGD	C16-C21	3.44	1.47	1.41
13	H	504	MGD	C16-C21	3.49	1.48	1.41
13	N	503	MGD	C16-C21	3.53	1.48	1.41
13	f	503	MGD	C16-C21	3.54	1.48	1.41
13	H	503	MGD	C16-C21	3.55	1.48	1.41
13	B	503	MGD	C16-C21	3.58	1.48	1.41
13	T	504	MGD	C16-C21	3.61	1.48	1.41
13	r	503	MGD	C16-C21	3.63	1.48	1.41
13	B	503	MGD	C6-C5	3.65	1.48	1.41
13	f	504	MGD	C16-C21	3.66	1.48	1.41
13	l	504	MGD	C16-C21	3.66	1.48	1.41
13	B	504	MGD	C6-C5	3.70	1.48	1.41
13	H	504	MGD	C6-C5	3.72	1.48	1.41
13	T	503	MGD	C16-C21	3.72	1.48	1.41
13	B	504	MGD	C16-C21	3.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	504	MGD	C6-C5	3.75	1.48	1.41
13	r	504	MGD	C6-C5	3.76	1.48	1.41
13	N	504	MGD	C16-C21	3.77	1.48	1.41
13	Z	504	MGD	C6-C5	3.78	1.49	1.41
13	T	503	MGD	C6-C5	3.79	1.49	1.41
13	H	503	MGD	C6-C5	3.79	1.49	1.41
13	Z	504	MGD	C16-C21	3.81	1.48	1.41
13	T	504	MGD	C6-C5	3.82	1.49	1.41
13	N	503	MGD	C6-C5	3.83	1.49	1.41
13	l	504	MGD	C6-C5	3.85	1.49	1.41
13	f	504	MGD	C6-C5	3.87	1.49	1.41
13	r	503	MGD	C6-C5	3.87	1.49	1.41
13	f	503	MGD	C6-C5	3.88	1.49	1.41
13	Z	503	MGD	C6-C5	3.88	1.49	1.41
13	r	504	MGD	C16-C21	3.89	1.48	1.41
13	l	503	MGD	C6-C5	3.95	1.49	1.41
8	k	603	MFN	C25-N4	4.28	1.42	1.34
8	Y	603	MFN	C25-N4	4.35	1.42	1.34
8	M	603	MFN	C25-N4	4.52	1.43	1.34
13	H	504	MGD	C17-C16	4.62	1.48	1.41
8	G	603	MFN	C25-N4	4.64	1.43	1.34
13	l	504	MGD	C17-C16	4.72	1.48	1.41
8	q	603	MFN	C25-N4	4.84	1.43	1.34
13	B	503	MGD	C17-C16	4.88	1.48	1.41
13	T	503	MGD	C17-C16	4.90	1.48	1.41
8	e	603	MFN	C25-N4	4.91	1.44	1.34
8	S	603	MFN	C25-N4	4.92	1.44	1.34
13	H	503	MGD	C17-C16	4.93	1.48	1.41
13	N	503	MGD	C17-C16	4.93	1.48	1.41
8	e	603	MFN	C16-N2	4.94	1.45	1.33
13	Z	503	MGD	C17-C16	4.95	1.48	1.41
8	S	603	MFN	C16-N2	4.99	1.45	1.33
8	q	603	MFN	C16-N2	5.01	1.45	1.33
8	G	603	MFN	C16-N2	5.01	1.45	1.33
13	l	503	MGD	C17-C16	5.05	1.48	1.41
13	T	504	MGD	C17-C16	5.05	1.48	1.41
13	f	504	MGD	C17-C16	5.07	1.48	1.41
8	A	603	MFN	C25-N4	5.12	1.44	1.34
8	k	603	MFN	C16-N2	5.12	1.45	1.33
8	Y	603	MFN	C16-N2	5.14	1.45	1.33
13	f	503	MGD	C17-C16	5.18	1.48	1.41
8	M	603	MFN	C16-N2	5.19	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	r	503	MGD	C17-C16	5.24	1.48	1.41
13	Z	504	MGD	C17-C16	5.25	1.48	1.41
13	B	504	MGD	C17-C16	5.27	1.48	1.41
8	A	603	MFN	C16-N2	5.36	1.46	1.33
13	r	504	MGD	C17-C16	5.47	1.49	1.41
13	N	504	MGD	C17-C16	5.50	1.49	1.41
8	M	603	MFN	C21-N3	5.80	1.45	1.34
8	G	603	MFN	C21-N3	5.88	1.46	1.34
8	q	603	MFN	C21-N3	6.11	1.46	1.34
8	A	603	MFN	C21-N3	6.24	1.46	1.34
8	Y	603	MFN	C21-N3	6.32	1.46	1.34
8	k	603	MFN	C21-N3	6.39	1.47	1.34
8	S	603	MFN	C21-N3	6.96	1.48	1.34
8	e	603	MFN	C21-N3	6.96	1.48	1.34

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
13	B	504	MGD	C1'-N9-C4	-5.76	120.37	126.81
8	S	603	MFN	C24-C23-N4	-5.72	101.52	112.93
8	M	603	MFN	C20-C19-N3	-5.70	101.55	112.93
8	M	603	MFN	C8-C9-C10	-5.61	111.20	120.18
8	q	603	MFN	C8-C9-C10	-5.53	111.34	120.18
8	G	603	MFN	C8-C9-C10	-5.44	111.49	120.18
13	N	504	MGD	C4'-O4'-C1'	-5.38	103.94	109.64
8	q	603	MFN	C20-C19-N3	-5.30	102.35	112.93
8	Y	603	MFN	C8-C9-C10	-5.24	111.80	120.18
8	k	603	MFN	C8-C9-C10	-5.23	111.81	120.18
8	S	603	MFN	C8-C9-C10	-5.20	111.86	120.18
13	f	504	MGD	C1'-N9-C4	-5.18	121.03	126.81
13	T	503	MGD	C1'-N9-C4	-5.17	121.04	126.81
8	M	603	MFN	C24-C23-N4	-4.97	103.00	112.93
8	e	603	MFN	C8-C9-C10	-4.93	112.30	120.18
13	Z	504	MGD	C4'-O4'-C1'	-4.90	104.45	109.64
8	k	603	MFN	C26-C25-N4	-4.78	107.81	115.85
8	A	603	MFN	C20-C19-N3	-4.72	103.52	112.93
13	f	503	MGD	C1'-N9-C4	-4.60	121.67	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	603	MFN	C20-C19-N3	-4.55	103.86	112.93
8	k	603	MFN	C20-C19-N3	-4.42	104.11	112.93
8	Y	603	MFN	C22-C14-C23	-4.39	104.69	113.05
8	M	603	MFN	C22-C14-C23	-4.38	104.71	113.05
13	B	504	MGD	C6-C5-C4	-4.35	115.89	120.86
13	r	504	MGD	C1'-N9-C4	-4.34	121.96	126.81
8	G	603	MFN	C22-C14-C23	-4.32	104.83	113.05
8	q	603	MFN	C22-C14-C23	-4.31	104.84	113.05
13	T	503	MGD	C6-C5-C4	-4.30	115.95	120.86
8	M	603	MFN	C26-C27-C28	-4.30	102.92	113.92
13	N	504	MGD	C1'-N9-C4	-4.30	122.01	126.81
13	r	503	MGD	C1'-N9-C4	-4.24	122.08	126.81
13	f	504	MGD	C6-C5-C4	-4.21	116.05	120.86
13	f	503	MGD	N3-C2-N1	-4.21	121.83	127.56
13	H	504	MGD	C4'-O4'-C1'	-4.19	105.20	109.64
13	f	503	MGD	C5-C6-N1	-4.18	118.05	123.52
13	T	504	MGD	C1'-N9-C4	-4.17	122.16	126.81
13	f	503	MGD	C6-C5-C4	-4.17	116.10	120.86
13	B	503	MGD	N3-C2-N1	-4.14	121.93	127.56
13	r	504	MGD	N3-C2-N1	-4.13	121.94	127.56
13	T	503	MGD	N3-C2-N1	-4.12	121.95	127.56
13	r	503	MGD	N3-C2-N1	-4.12	121.95	127.56
13	N	504	MGD	C6-C5-C4	-4.12	116.15	120.86
13	f	504	MGD	N3-C2-N1	-4.11	121.96	127.56
13	l	504	MGD	C1'-N9-C4	-4.11	122.22	126.81
13	B	503	MGD	C6-C5-C4	-4.09	116.18	120.86
13	Z	503	MGD	C6-C5-C4	-4.08	116.19	120.86
13	l	504	MGD	C4'-O4'-C1'	-4.08	105.32	109.64
13	Z	503	MGD	N3-C2-N1	-4.07	122.02	127.56
13	H	504	MGD	C5-C6-N1	-4.07	118.20	123.52
13	f	504	MGD	C5-C6-N1	-4.06	118.21	123.52
13	r	503	MGD	C6-C5-C4	-4.05	116.23	120.86
13	r	504	MGD	C6-C5-C4	-4.01	116.28	120.86
13	Z	504	MGD	N3-C2-N1	-4.00	122.12	127.56
13	l	503	MGD	N3-C2-N1	-3.96	122.17	127.56
13	H	503	MGD	N3-C2-N1	-3.95	122.18	127.56
13	H	504	MGD	N3-C2-N1	-3.95	122.19	127.56
13	Z	503	MGD	C1'-N9-C4	-3.94	122.41	126.81
13	B	504	MGD	N3-C2-N1	-3.94	122.20	127.56
13	l	504	MGD	N3-C2-N1	-3.94	122.20	127.56
13	l	504	MGD	C6-C5-C4	-3.93	116.36	120.86
13	N	503	MGD	N3-C2-N1	-3.93	122.21	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	504	MGD	N3-C2-N1	-3.93	122.21	127.56
13	T	503	MGD	C5-C6-N1	-3.93	118.39	123.52
13	N	503	MGD	C6-C5-C4	-3.92	116.38	120.86
13	B	504	MGD	C5-C6-N1	-3.92	118.40	123.52
13	l	504	MGD	C5-C6-N1	-3.89	118.44	123.52
13	H	503	MGD	C6-C5-C4	-3.88	116.42	120.86
8	Y	603	MFN	C20-C19-N3	-3.87	105.20	112.93
13	N	504	MGD	C5-C6-N1	-3.85	118.49	123.52
13	H	504	MGD	C6-C5-C4	-3.82	116.49	120.86
13	B	503	MGD	C1'-N9-C4	-3.82	122.55	126.81
13	T	504	MGD	N3-C2-N1	-3.81	122.37	127.56
13	T	504	MGD	C5-C6-N1	-3.79	118.56	123.52
13	Z	504	MGD	C5-C6-N1	-3.79	118.57	123.52
13	l	503	MGD	C6-C5-C4	-3.76	116.56	120.86
13	Z	504	MGD	C6-C5-C4	-3.76	116.56	120.86
13	N	503	MGD	C1'-N9-C4	-3.76	122.61	126.81
13	T	504	MGD	C6-C5-C4	-3.72	116.60	120.86
13	r	503	MGD	C5-C6-N1	-3.72	118.66	123.52
13	H	503	MGD	C5-C6-N1	-3.72	118.66	123.52
8	Y	603	MFN	C24-C23-N4	-3.69	105.57	112.93
13	T	504	MGD	C4'-O4'-C1'	-3.65	105.77	109.64
13	r	504	MGD	C5-C6-N1	-3.63	118.77	123.52
13	H	504	MGD	C1'-N9-C4	-3.59	122.80	126.81
8	e	603	MFN	O2-C13-C4	-3.55	99.03	109.17
13	N	503	MGD	C5-C6-N1	-3.54	118.90	123.52
13	H	503	MGD	C1'-N9-C4	-3.49	122.91	126.81
13	B	504	MGD	C4'-O4'-C1'	-3.48	105.96	109.64
13	l	503	MGD	C5-C6-N1	-3.48	118.98	123.52
13	f	504	MGD	C4'-O4'-C1'	-3.45	105.98	109.64
13	Z	503	MGD	C5-C6-N1	-3.43	119.03	123.52
13	r	504	MGD	C4'-O4'-C1'	-3.41	106.03	109.64
8	A	603	MFN	C24-C23-N4	-3.40	106.15	112.93
8	k	603	MFN	O2-C13-C4	-3.25	99.89	109.17
13	B	503	MGD	C5-C6-N1	-3.20	119.34	123.52
8	S	603	MFN	O2-C13-C4	-3.14	100.21	109.17
8	Y	603	MFN	O2-C13-C4	-3.11	100.29	109.17
13	l	503	MGD	C1'-N9-C4	-2.99	123.47	126.81
8	G	603	MFN	O2-C13-C4	-2.93	100.82	109.17
13	Z	504	MGD	C1'-N9-C4	-2.80	123.69	126.81
8	M	603	MFN	O2-C13-C4	-2.72	101.42	109.17
8	G	603	MFN	C26-C27-C28	-2.64	107.16	113.92
8	S	603	MFN	O3-C16-N2	-2.58	117.84	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	603	MFN	C26-C27-C28	-2.45	107.65	113.92
8	M	603	MFN	C22-C21-N3	-2.42	111.78	115.85
8	q	603	MFN	C26-C27-C28	-2.40	107.77	113.92
8	M	603	MFN	C26-C25-N4	-2.36	111.87	115.85
8	k	603	MFN	O3-C16-N2	-2.29	118.41	122.96
8	A	603	MFN	C27-C26-C25	-2.29	108.02	113.26
8	M	603	MFN	O3-C16-N2	-2.25	118.49	122.96
8	A	603	MFN	C22-C14-C23	-2.19	108.88	113.05
8	q	603	MFN	O3-C16-N2	-2.16	118.67	122.96
8	Y	603	MFN	C31-C32-C33	-2.09	108.60	113.91
13	r	503	MGD	O11-C23-C14	-2.09	107.54	108.96
8	G	603	MFN	C31-C32-C33	-2.08	108.63	113.91
8	G	603	MFN	C24-C23-N4	-2.07	108.80	112.93
8	M	603	MFN	C14-C23-N4	-2.04	106.73	109.92
13	H	503	MGD	O11-C23-C14	-2.04	107.57	108.96
13	N	503	MGD	C16-C21-N22	2.00	120.09	118.19
13	Z	503	MGD	C16-C21-N22	2.05	120.14	118.19
8	A	603	MFN	C17-C16-N2	2.07	120.06	116.46
8	q	603	MFN	C3-C4-C5	2.08	108.03	104.75
8	e	603	MFN	C18-C19-N3	2.09	113.19	109.92
8	M	603	MFN	C7-C8-C9	2.14	122.40	119.74
8	Y	603	MFN	C18-C19-N3	2.14	113.26	109.92
8	G	603	MFN	C3-C4-C5	2.15	108.14	104.75
13	T	504	MGD	C16-C21-N22	2.16	120.25	118.19
13	B	503	MGD	C16-C21-N22	2.16	120.25	118.19
8	A	603	MFN	C19-N3-C21	2.16	126.48	121.76
8	e	603	MFN	C11-C10-C9	2.17	122.44	119.74
8	M	603	MFN	C3-C4-C5	2.19	108.20	104.75
13	B	504	MGD	O4'-C1'-N9	2.20	112.26	108.11
13	H	504	MGD	C16-C21-N22	2.22	120.30	118.19
8	k	603	MFN	C17-C16-N2	2.32	120.50	116.46
8	S	603	MFN	C3-C4-C5	2.34	108.44	104.75
13	r	503	MGD	C16-C21-N22	2.34	120.42	118.19
8	M	603	MFN	C27-C26-C25	2.35	118.63	113.26
13	N	504	MGD	C16-C21-N22	2.36	120.44	118.19
8	A	603	MFN	C18-C19-N3	2.36	113.62	109.92
8	k	603	MFN	O9-C25-C26	2.37	126.07	121.97
13	B	504	MGD	C16-C21-N22	2.40	120.47	118.19
8	k	603	MFN	C14-C23-N4	2.42	113.70	109.92
13	l	504	MGD	C16-C21-N22	2.43	120.50	118.19
8	Y	603	MFN	C11-C10-C9	2.43	122.77	119.74
8	k	603	MFN	C11-C10-C9	2.44	122.78	119.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	r	504	MGD	O4'-C1'-N9	2.44	112.72	108.11
8	Y	603	MFN	C3-C4-C5	2.46	108.62	104.75
8	k	603	MFN	C3-C4-C5	2.50	108.69	104.75
8	S	603	MFN	C11-C10-C9	2.54	122.91	119.74
8	G	603	MFN	C11-C10-C9	2.55	122.92	119.74
8	e	603	MFN	C3-C4-C5	2.56	108.78	104.75
13	r	504	MGD	N22-C21-N20	2.58	120.73	116.62
8	M	603	MFN	C19-N3-C21	2.60	127.42	121.76
13	N	504	MGD	C17-C16-C21	2.60	116.90	114.61
13	f	504	MGD	C16-C21-N22	2.62	120.68	118.19
13	Z	504	MGD	C16-C21-N22	2.69	120.74	118.19
8	k	603	MFN	C14-C22-C21	2.69	119.41	113.26
13	r	504	MGD	C16-C21-N22	2.72	120.78	118.19
13	r	504	MGD	C17-C16-C21	2.73	117.02	114.61
13	N	504	MGD	N22-C21-N20	2.76	121.02	116.62
8	q	603	MFN	C11-C10-C9	2.77	123.20	119.74
13	T	504	MGD	O4'-C1'-N9	2.78	113.36	108.11
8	M	603	MFN	C11-C10-C9	2.89	123.34	119.74
13	l	504	MGD	N22-C21-N20	2.91	121.25	116.62
13	l	503	MGD	C17-C16-C21	2.92	117.18	114.61
13	l	504	MGD	C19-N20-C21	2.96	121.27	114.63
13	f	504	MGD	O4'-C1'-N9	2.98	113.74	108.11
13	N	503	MGD	C19-N20-C21	2.98	121.33	114.63
13	T	504	MGD	C19-N20-C21	2.99	121.34	114.63
8	Y	603	MFN	C19-N3-C21	3.01	128.33	121.76
13	B	504	MGD	C19-N20-C21	3.01	121.40	114.63
13	Z	504	MGD	N22-C21-N20	3.02	121.43	116.62
8	A	603	MFN	C26-C25-N4	3.02	120.92	115.85
13	T	503	MGD	C19-N20-C21	3.02	121.42	114.63
13	r	503	MGD	C19-N20-C21	3.03	121.44	114.63
8	k	603	MFN	C18-C19-N3	3.03	114.66	109.92
13	N	504	MGD	C19-N20-C21	3.04	121.45	114.63
13	r	504	MGD	C19-N20-C21	3.04	121.47	114.63
13	r	503	MGD	N22-C21-N20	3.06	121.50	116.62
13	B	503	MGD	C19-N20-C21	3.07	121.53	114.63
8	A	603	MFN	C11-C10-C9	3.09	123.59	119.74
13	H	503	MGD	C19-N20-C21	3.10	121.59	114.63
13	f	503	MGD	C19-N20-C21	3.10	121.60	114.63
13	f	503	MGD	C17-C16-C21	3.12	117.36	114.61
13	l	503	MGD	C19-N20-C21	3.13	121.66	114.63
13	B	504	MGD	N22-C21-N20	3.14	121.62	116.62
13	H	504	MGD	C19-N20-C21	3.15	121.71	114.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	503	MGD	C19-N20-C21	3.16	121.72	114.63
13	Z	504	MGD	C19-N20-C21	3.16	121.73	114.63
13	l	503	MGD	N22-C21-N20	3.17	121.66	116.62
13	f	504	MGD	C19-N20-C21	3.17	121.75	114.63
13	f	503	MGD	N22-C21-N20	3.26	121.81	116.62
13	f	504	MGD	N22-C21-N20	3.27	121.82	116.62
8	S	603	MFN	C18-C19-N3	3.27	115.03	109.92
13	Z	504	MGD	C17-C16-C21	3.27	117.49	114.61
13	N	503	MGD	N22-C21-N20	3.31	121.90	116.62
13	l	504	MGD	O4'-C1'-N9	3.32	114.39	108.11
13	H	503	MGD	C17-C16-C21	3.35	117.56	114.61
8	e	603	MFN	C19-N3-C21	3.35	129.07	121.76
13	B	503	MGD	N22-C21-N20	3.39	122.01	116.62
13	H	504	MGD	N22-C21-N20	3.41	122.05	116.62
13	r	503	MGD	C17-C16-C21	3.42	117.62	114.61
13	T	504	MGD	N22-C21-N20	3.48	122.16	116.62
13	T	503	MGD	N22-C21-N20	3.48	122.16	116.62
13	H	503	MGD	N22-C21-N20	3.54	122.26	116.62
13	N	503	MGD	C17-C16-C21	3.55	117.74	114.61
13	l	504	MGD	C17-C16-C21	3.57	117.75	114.61
13	B	504	MGD	C17-C16-C21	3.57	117.75	114.61
13	Z	503	MGD	N22-C21-N20	3.57	122.30	116.62
13	Z	503	MGD	C17-C16-C21	3.66	117.83	114.61
13	T	503	MGD	C17-C16-C21	3.66	117.83	114.61
13	B	503	MGD	C17-C16-C21	3.68	117.85	114.61
13	H	504	MGD	C17-C16-C21	3.92	118.06	114.61
13	Z	504	MGD	O4'-C1'-N9	3.97	115.60	108.11
13	f	504	MGD	C17-C16-C21	4.05	118.17	114.61
13	T	504	MGD	C17-C16-C21	4.23	118.34	114.61
13	N	504	MGD	O4'-C1'-N9	4.26	116.16	108.11
8	k	603	MFN	C27-C26-C25	4.28	123.05	113.26
13	H	504	MGD	O4'-C1'-N9	4.39	116.41	108.11
8	S	603	MFN	C19-N3-C21	4.51	131.61	121.76
13	B	503	MGD	C6-N1-C2	4.96	121.69	115.88
13	l	503	MGD	C6-N1-C2	5.03	121.78	115.88
13	N	503	MGD	C6-N1-C2	5.06	121.82	115.88
13	Z	503	MGD	C6-N1-C2	5.15	121.91	115.88
13	H	503	MGD	C6-N1-C2	5.26	122.05	115.88
13	T	504	MGD	C6-N1-C2	5.33	122.13	115.88
13	f	504	MGD	C17-N18-C19	5.37	122.17	115.88
13	Z	504	MGD	C6-N1-C2	5.42	122.23	115.88
13	r	503	MGD	C6-N1-C2	5.43	122.25	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	503	MGD	C17-N18-C19	5.45	122.27	115.88
13	r	504	MGD	C6-N1-C2	5.46	122.28	115.88
13	l	504	MGD	C6-N1-C2	5.53	122.37	115.88
13	N	504	MGD	C6-N1-C2	5.55	122.39	115.88
13	T	504	MGD	C17-N18-C19	5.57	122.40	115.88
13	H	504	MGD	C17-N18-C19	5.59	122.44	115.88
13	B	504	MGD	C6-N1-C2	5.63	122.47	115.88
13	B	504	MGD	C17-N18-C19	5.71	122.58	115.88
13	l	503	MGD	C17-N18-C19	5.72	122.58	115.88
13	H	503	MGD	C17-N18-C19	5.75	122.62	115.88
13	T	503	MGD	C6-N1-C2	5.75	122.62	115.88
13	H	504	MGD	C6-N1-C2	5.76	122.63	115.88
13	N	503	MGD	C17-N18-C19	5.78	122.66	115.88
13	r	504	MGD	C17-N18-C19	5.79	122.67	115.88
13	B	503	MGD	C17-N18-C19	5.79	122.67	115.88
13	Z	504	MGD	C17-N18-C19	5.87	122.76	115.88
13	f	504	MGD	C6-N1-C2	5.88	122.77	115.88
13	N	504	MGD	C17-N18-C19	5.90	122.79	115.88
13	r	503	MGD	C17-N18-C19	5.93	122.83	115.88
13	f	503	MGD	C17-N18-C19	5.95	122.85	115.88
13	l	504	MGD	C17-N18-C19	5.97	122.87	115.88
13	T	503	MGD	C17-N18-C19	6.06	122.99	115.88
13	f	503	MGD	C6-N1-C2	6.09	123.02	115.88

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
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, 95th 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

All (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

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Mol	Chain	Res	Type	RSRZ
3	U	235	GLY	6.5
1	k	462	GLY	6.4
6	R	17	THR	6.2
1	k	6	LYS	6.1
6	d	17	THR	6.0
6	j	7	ILE	6.0
6	d	99	ALA	5.9
6	d	75	GLY	5.9
6	R	6	VAL	5.8
6	d	76	MET	5.8
6	j	4	THR	5.8
2	B	45	ALA	5.7
6	X	4	THR	5.6
3	g	234	ASP	5.5
1	M	8	GLY	5.4
6	R	15	GLU	5.3
1	Y	3	TYR	5.2
1	G	32	VAL	5.1
1	Y	84	LYS	5.1
6	R	334	PRO	5.0
1	Y	35	VAL	5.0
6	R	21	ASN	5.0
1	M	156	GLY	5.0
6	X	92	GLY	5.0
3	s	32	GLU	4.9
3	U	231	ILE	4.9
3	s	37	ILE	4.8
3	s	52	PHE	4.8
1	k	486	ILE	4.8
6	X	7	ILE	4.7
1	q	419	TRP	4.7
6	d	334	PRO	4.7
6	R	337	SER	4.7
2	l	55	LEU	4.6
1	k	35	VAL	4.6
6	p	2	GLU	4.6
6	R	97	GLU	4.6
6	R	7	ILE	4.5
2	r	430	ALA	4.5
6	d	245	CYS	4.4
1	G	25	CYS	4.4
6	R	99	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
6	d	42	PRO	4.4
1	Y	41	VAL	4.4
3	C	61	ALA	4.3
1	Y	4	ILE	4.3
1	q	467	ILE	4.3
1	M	345	GLY	4.2
1	S	569	LEU	4.2
1	G	505	LYS	4.2
6	F	25	ILE	4.2
6	d	69	ASN	4.2
6	j	92	GLY	4.2
3	g	37	ILE	4.1
1	Y	24	ILE	4.1
1	M	4	ILE	4.1
2	T	428	TYR	4.1
3	s	65	ILE	4.0
4	P	45	ILE	4.0
1	k	569	LEU	4.0
5	c	2	ALA	4.0
4	h	65	VAL	4.0
1	Y	36	SER	4.0
6	R	340	TRP	4.0
3	s	28	GLY	4.0
6	R	333	THR	4.0
2	Z	61	GLU	4.0
5	Q	2	ALA	4.0
1	M	39	ALA	3.9
6	R	336	ARG	3.9
3	s	5	ILE	3.9
2	Z	410	ASP	3.9
3	g	233	VAL	3.9
1	M	346	SER	3.9
6	X	43	VAL	3.9
2	r	293	VAL	3.8
3	C	60	ASP	3.8
6	R	42	PRO	3.8
6	d	41	CYS	3.8
1	k	479	PRO	3.8
1	G	477	VAL	3.8
1	Y	65	VAL	3.8
2	T	123	VAL	3.8
1	M	38	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	l	294	THR	3.7
1	k	9	PHE	3.7
3	s	68	ILE	3.7
6	R	74	CYS	3.7
1	M	24	ILE	3.7
6	d	71	CYS	3.7
1	S	67	VAL	3.6
1	k	22	MET	3.6
6	d	46	ILE	3.6
1	M	465	ALA	3.6
1	G	83	PHE	3.6
1	M	502	ILE	3.6
3	C	68	ILE	3.6
1	k	42	ILE	3.6
6	R	41	CYS	3.6
2	r	61	GLU	3.6
1	k	40	LYS	3.6
6	X	5	GLU	3.5
6	v	179	ALA	3.5
3	C	52	PHE	3.5
1	M	3	TYR	3.5
1	M	528	ILE	3.5
3	U	238	LEU	3.5
1	Y	474	PRO	3.5
3	s	234	ASP	3.5
3	g	237	GLU	3.5
2	r	294	THR	3.5
3	O	2	SER	3.5
2	N	123	VAL	3.5
2	r	424	LYS	3.5
4	D	1	MET	3.5
6	d	89	GLN	3.4
1	M	23	ASP	3.4
3	C	2	SER	3.4
4	b	127	VAL	3.4
1	M	41	VAL	3.4
3	C	234	ASP	3.4
6	R	24	LEU	3.4
1	k	25	CYS	3.4
6	d	74	CYS	3.4
3	C	37	ILE	3.4
2	B	59	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
3	s	61	ALA	3.4
2	H	225	ASP	3.4
2	Z	27	GLU	3.3
3	g	34	ILE	3.3
6	d	339	ALA	3.3
1	M	71	TYR	3.3
6	d	16	ARG	3.3
1	G	28	ASP	3.3
1	G	35	VAL	3.3
1	G	37	ASP	3.3
6	d	337	SER	3.3
1	k	44	ALA	3.3
1	G	156	GLY	3.3
2	H	23	VAL	3.3
2	l	293	VAL	3.3
4	h	109	PRO	3.3
2	Z	428	TYR	3.3
6	F	16	ARG	3.3
3	a	2	SER	3.3
1	M	9	PHE	3.2
2	r	45	ALA	3.2
6	F	68	GLU	3.2
2	B	123	VAL	3.2
1	A	506	ASP	3.2
1	M	116	ALA	3.2
1	M	70	MET	3.2
3	C	71	GLY	3.2
6	d	92	GLY	3.2
1	S	83	PHE	3.2
1	M	64	LYS	3.2
6	j	167	ASP	3.2
2	B	44	HIS	3.2
6	d	120	ALA	3.2
2	B	336	ASP	3.2
2	l	430	ALA	3.2
6	d	333	THR	3.2
2	l	63	VAL	3.2
1	M	120	LEU	3.1
1	q	255	LYS	3.1
6	R	73	LEU	3.1
6	R	339	ALA	3.1
4	J	129	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
6	d	70	LYS	3.1
1	Y	67	VAL	3.1
1	e	316	THR	3.1
6	d	7	ILE	3.1
3	U	239	PRO	3.1
1	Y	116	ALA	3.1
6	d	9	GLY	3.1
3	I	5	ILE	3.1
1	Y	37	ASP	3.1
1	Y	2	GLU	3.1
1	M	347	GLY	3.1
2	l	75	ALA	3.1
2	l	297	ASN	3.1
6	R	93	THR	3.1
1	A	567	VAL	3.1
1	k	159	ASP	3.1
1	e	65	VAL	3.1
2	H	293	VAL	3.1
1	q	28	ASP	3.0
2	H	16	CYS	3.0
3	U	54	VAL	3.0
6	R	22	ARG	3.0
6	R	90	ILE	3.0
6	F	71	CYS	3.0
1	M	336	ALA	3.0
3	C	35	LYS	3.0
6	p	71	CYS	3.0
1	k	475	GLU	3.0
6	R	76	MET	3.0
1	Y	60	ILE	3.0
6	F	9	GLY	3.0
6	R	75	GLY	3.0
1	M	63	ALA	3.0
6	R	89	GLN	3.0
1	G	493	ALA	3.0
2	l	114	THR	3.0
1	M	121	LEU	3.0
2	r	407	VAL	2.9
6	j	5	GLU	2.9
3	C	231	ILE	2.9
1	Y	58	SER	2.9
1	k	7	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	Z	229	GLY	2.9
3	U	233	VAL	2.9
6	R	16	ARG	2.9
1	Y	465	ALA	2.9
3	s	36	ASN	2.9
6	j	93	THR	2.9
2	f	299	VAL	2.9
1	k	568	MET	2.9
1	Y	415	GLU	2.9
2	H	296	PHE	2.9
6	p	69	ASN	2.9
1	Y	121	LEU	2.9
6	F	77	CYS	2.9
2	l	23	VAL	2.9
1	Y	346	SER	2.9
5	W	81	LEU	2.9
1	G	27	LYS	2.9
2	T	116	SER	2.9
2	Z	424	LYS	2.9
1	q	41	VAL	2.9
1	G	34	SER	2.9
1	M	27	LYS	2.9
2	H	294	THR	2.9
6	d	340	TRP	2.9
2	Z	407	VAL	2.8
3	g	2	SER	2.8
1	Y	338	CYS	2.8
6	v	7	ILE	2.8
6	R	164	CYS	2.8
6	j	77	CYS	2.8
4	t	128	GLY	2.8
6	d	328	ASN	2.8
1	Y	96	SER	2.8
1	M	26	VAL	2.8
3	s	58	PRO	2.8
1	k	39	ALA	2.8
1	M	317	MET	2.8
2	Z	302	TRP	2.8
2	Z	226	GLU	2.8
1	G	4	ILE	2.8
1	k	435	PHE	2.8
6	d	338	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	r	114	THR	2.8
3	s	60	ASP	2.8
3	U	240	GLY	2.8
1	S	70	MET	2.8
1	k	84	LYS	2.8
2	Z	123	VAL	2.8
2	H	62	PHE	2.8
2	r	62	PHE	2.8
2	l	24	GLU	2.8
4	t	1	MET	2.8
1	q	43	ASP	2.8
2	N	297	ASN	2.8
6	p	60	GLU	2.8
1	Y	340	VAL	2.7
1	e	338	CYS	2.7
1	q	19	GLY	2.7
2	Z	305	GLY	2.7
2	f	61	GLU	2.7
3	s	10	GLU	2.7
5	o	43	GLU	2.7
1	e	70	MET	2.7
1	Y	31	ILE	2.7
1	Y	39	ALA	2.7
1	Y	528	ILE	2.7
2	N	394	TYR	2.7
2	Z	294	THR	2.7
2	f	223	LEU	2.7
1	M	2	GLU	2.7
1	k	41	VAL	2.7
1	q	477	VAL	2.7
2	H	2	GLU	2.7
2	T	223	LEU	2.7
2	Z	394	TYR	2.7
4	J	108	ILE	2.7
1	A	338	CYS	2.7
1	q	259	ALA	2.7
2	l	225	ASP	2.7
3	m	234	ASP	2.7
2	N	124	LEU	2.7
3	C	49	GLY	2.7
3	C	237	GLU	2.7
3	g	239	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
6	d	23	ARG	2.7
1	Y	477	VAL	2.7
1	k	506	ASP	2.7
1	Y	160	ALA	2.7
2	H	222	ILE	2.7
2	H	297	ASN	2.7
4	h	44	GLY	2.7
6	j	91	ASP	2.7
3	U	46	VAL	2.7
5	W	2	ALA	2.7
6	d	25	ILE	2.7
2	N	295	GLY	2.7
2	l	67	TYR	2.7
3	g	74	TYR	2.7
1	G	70	MET	2.7
2	r	63	VAL	2.6
3	g	46	VAL	2.6
4	t	123	VAL	2.6
6	j	43	VAL	2.6
1	G	44	ALA	2.6
2	B	53	LYS	2.6
2	Z	301	THR	2.6
3	U	269	ALA	2.6
6	X	17	THR	2.6
2	T	286	PRO	2.6
1	Y	375	ASP	2.6
1	Y	25	CYS	2.6
2	f	297	ASN	2.6
6	X	71	CYS	2.6
1	Y	23	ASP	2.6
6	d	94	SER	2.6
1	Y	61	ALA	2.6
1	k	477	VAL	2.6
2	T	44	HIS	2.6
3	I	269	ALA	2.6
1	M	60	ILE	2.6
2	N	133	ILE	2.6
3	I	270	PRO	2.6
3	s	31	ILE	2.6
6	F	349	LYS	2.6
1	Y	33	GLU	2.6
2	Z	236	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	f	46	GLU	2.6
6	F	97	GLU	2.6
1	M	6	LYS	2.6
2	N	307	PRO	2.6
2	T	131	TYR	2.6
1	Y	124	HIS	2.6
1	e	319	ALA	2.6
2	l	61	GLU	2.6
6	v	97	GLU	2.6
1	e	465	ALA	2.6
4	V	67	ALA	2.6
1	Y	26	VAL	2.6
1	M	396	PRO	2.6
3	C	34	ILE	2.6
1	k	43	ASP	2.6
1	k	347	GLY	2.6
2	N	305	GLY	2.6
2	l	288	ARG	2.6
3	s	235	GLY	2.6
6	R	23	ARG	2.6
1	M	35	VAL	2.5
2	Z	135	THR	2.5
2	l	16	CYS	2.5
2	r	300	CYS	2.5
4	V	96	ALA	2.5
6	v	71	CYS	2.5
5	K	81	LEU	2.5
6	d	73	LEU	2.5
1	M	36	SER	2.5
3	g	235	GLY	2.5
6	X	75	GLY	2.5
1	k	3	TYR	2.5
1	A	336	ALA	2.5
1	M	185	THR	2.5
1	M	65	VAL	2.5
2	Z	400	PRO	2.5
1	G	24	ILE	2.5
1	k	68	GLY	2.5
6	X	91	ASP	2.5
1	M	480	SER	2.5
1	k	70	MET	2.5
1	q	36	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	39	ALA	2.5
3	g	59	ALA	2.5
1	k	67	VAL	2.5
5	W	53	VAL	2.5
6	R	98	LEU	2.5
1	M	239	GLY	2.5
2	f	47	GLY	2.5
3	U	5	ILE	2.5
6	X	69	ASN	2.5
1	M	338	CYS	2.5
1	Y	40	LYS	2.5
1	M	316	THR	2.5
1	M	531	GLU	2.5
2	N	288	ARG	2.5
4	n	2	ARG	2.5
6	p	99	ALA	2.5
1	A	340	VAL	2.5
1	e	43	ASP	2.5
1	k	497	LEU	2.5
6	d	24	LEU	2.5
1	S	16	GLY	2.5
1	Y	8	GLY	2.5
2	T	297	ASN	2.5
6	d	66	ILE	2.5
6	d	37	CYS	2.5
1	M	28	ASP	2.5
1	M	29	GLY	2.5
1	Y	345	GLY	2.5
1	e	67	VAL	2.5
1	k	407	TYR	2.5
2	N	132	PRO	2.5
2	T	225	ASP	2.5
2	N	294	THR	2.5
4	D	64	ALA	2.5
3	C	235	GLY	2.5
1	k	120	LEU	2.5
2	B	67	TYR	2.5
2	H	299	VAL	2.5
3	C	63	GLU	2.5
6	X	20	GLU	2.5
1	M	429	ILE	2.5
1	Y	336	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	r	286	PRO	2.5
2	r	381	PRO	2.5
2	N	237	GLU	2.5
1	e	237	HIS	2.4
2	f	394	TYR	2.4
3	C	65	ILE	2.4
5	c	43	GLU	2.4
6	L	69	ASN	2.4
1	k	319	ALA	2.4
2	Z	299	VAL	2.4
1	A	155	GLU	2.4
2	N	302	TRP	2.4
2	l	62	PHE	2.4
6	R	46	ILE	2.4
2	Z	307	PRO	2.4
1	Y	59	HIS	2.4
2	f	228	ALA	2.4
2	l	215	ALA	2.4
6	F	93	THR	2.4
2	N	284	LEU	2.4
2	l	399	VAL	2.4
4	n	127	VAL	2.4
1	Y	43	ASP	2.4
3	U	74	TYR	2.4
1	k	83	PHE	2.4
3	U	79	ILE	2.4
1	k	409	MET	2.4
3	U	56	GLY	2.4
1	M	474	PRO	2.4
2	r	307	PRO	2.4
3	g	32	GLU	2.4
1	S	43	ASP	2.4
1	A	348	VAL	2.4
2	f	123	VAL	2.4
1	M	483	TYR	2.4
4	t	42	GLN	2.4
2	f	130	GLY	2.4
3	C	5	ILE	2.4
3	a	105	GLY	2.4
3	s	89	ILE	2.4
6	d	101	TYR	2.4
2	N	398	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	k	338	CYS	2.4
5	E	12	CYS	2.4
6	d	68	GLU	2.4
2	l	116	SER	2.4
6	R	94	SER	2.4
1	Y	66	ASN	2.4
2	r	295	GLY	2.4
1	M	84	LYS	2.4
6	j	70	LYS	2.4
3	g	7	THR	2.4
2	r	124	LEU	2.4
1	e	567	VAL	2.4
2	Z	23	VAL	2.4
1	Y	70	MET	2.4
1	Y	119	PRO	2.4
1	k	474	PRO	2.4
3	g	31	ILE	2.4
2	f	62	PHE	2.4
6	R	101	TYR	2.4
1	G	43	ASP	2.4
2	T	324	THR	2.4
1	G	33	GLU	2.4
2	T	126	LEU	2.4
6	L	160	CYS	2.4
1	q	567	VAL	2.3
1	Y	237	HIS	2.3
1	q	405	ASN	2.3
2	B	124	LEU	2.3
2	l	396	MET	2.3
3	a	44	GLU	2.3
6	R	344	PHE	2.3
1	M	115	ALA	2.3
3	C	106	LYS	2.3
1	G	38	SER	2.3
1	G	462	GLY	2.3
1	Y	62	GLY	2.3
2	B	126	LEU	2.3
2	T	61	GLU	2.3
6	p	8	GLU	2.3
1	k	32	VAL	2.3
1	Y	64	LYS	2.3
6	R	335	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	435	PHE	2.3
2	Z	90	SER	2.3
2	r	394	TYR	2.3
3	s	74	TYR	2.3
2	T	124	LEU	2.3
3	s	63	GLU	2.3
4	b	129	GLN	2.3
1	k	48	ILE	2.3
1	M	58	SER	2.3
1	k	494	ALA	2.3
1	q	44	ALA	2.3
4	D	44	GLY	2.3
2	l	428	TYR	2.3
1	q	418	LYS	2.3
6	j	42	PRO	2.3
1	M	348	VAL	2.3
2	B	297	ASN	2.3
3	g	152	ILE	2.3
1	M	96	SER	2.3
1	q	63	ALA	2.3
2	N	134	CYS	2.3
2	Z	94	CYS	2.3
6	d	347	LEU	2.3
1	e	340	VAL	2.3
1	e	347	GLY	2.3
2	l	398	GLY	2.3
3	C	111	GLY	2.3
1	M	31	ILE	2.3
3	C	31	ILE	2.3
3	C	26	PHE	2.3
2	l	13	GLY	2.2
1	G	528	ILE	2.2
1	M	486	ILE	2.2
1	M	318	THR	2.2
3	C	32	GLU	2.2
6	p	3	THR	2.2
2	Z	15	LEU	2.2
2	l	126	LEU	2.2
4	n	43	LEU	2.2
2	Z	308	TYR	2.2
1	Y	19	GLY	2.2
2	N	298	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	41	VAL	2.2
2	Z	396	MET	2.2
2	l	1	MET	2.2
6	F	72	VAL	2.2
6	F	128	ASP	2.2
1	k	24	ILE	2.2
4	P	96	ALA	2.2
1	Y	476	THR	2.2
4	t	97	THR	2.2
1	e	120	LEU	2.2
2	l	422	LEU	2.2
1	M	479	PRO	2.2
6	j	21	ASN	2.2
1	G	502	ILE	2.2
1	e	422	ARG	2.2
6	d	93	THR	2.2
2	l	412	LEU	2.2
4	P	38	GLU	2.2
6	R	69	ASN	2.2
6	d	67	ASP	2.2
1	k	11	TYR	2.2
2	H	308	TYR	2.2
1	A	70	MET	2.2
1	M	340	VAL	2.2
1	k	504	VAL	2.2
1	M	344	THR	2.2
1	Y	344	THR	2.2
1	k	27	LYS	2.2
4	V	44	GLY	2.2
6	p	336	ARG	2.2
1	k	530	SER	2.2
1	k	33	GLU	2.2
4	b	64	ALA	2.2
6	d	60	GLU	2.2
2	Z	133	ILE	2.2
3	g	70	ASP	2.2
2	N	421	LEU	2.2
3	a	189	LEU	2.2
3	g	58	PRO	2.2
4	V	98	PRO	2.2
2	T	394	TYR	2.2
4	D	47	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	3	THR	2.2
2	N	25	GLY	2.2
2	N	296	PHE	2.2
2	Z	295	GLY	2.2
2	l	137	GLY	2.2
1	Y	20	GLU	2.2
1	S	94	VAL	2.1
1	q	37	ASP	2.1
2	l	425	VAL	2.1
3	I	233	VAL	2.1
1	M	473	ASN	2.1
5	i	2	ALA	2.1
3	O	89	ILE	2.1
3	g	231	ILE	2.1
6	p	13	THR	2.1
6	v	219	GLY	2.1
2	Z	24	GLU	2.1
2	r	427	GLU	2.1
6	d	15	GLU	2.1
1	M	497	LEU	2.1
6	X	121	CYS	2.1
2	r	377	ASP	2.1
1	M	501	GLU	2.1
2	N	226	GLU	2.1
2	T	115	ALA	2.1
3	g	71	GLY	2.1
2	f	286	PRO	2.1
2	f	126	LEU	2.1
1	k	488	GLU	2.1
3	I	232	GLU	2.1
2	H	396	MET	2.1
6	d	21	ASN	2.1
1	M	46	GLY	2.1
2	N	120	GLY	2.1
1	A	67	VAL	2.1
1	M	32	VAL	2.1
6	j	349	LYS	2.1
1	S	4	ILE	2.1
2	f	307	PRO	2.1
2	r	133	ILE	2.1
1	Y	120	LEU	2.1
1	Y	38	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	Y	482	GLU	2.1
2	H	116	SER	2.1
2	H	288	ARG	2.1
3	s	230	ASP	2.1
1	S	336	ALA	2.1
1	k	140	TYR	2.1
2	r	123	VAL	2.1
6	d	43	VAL	2.1
6	F	17	THR	2.1
2	Z	134	CYS	2.1
4	t	103	ILE	2.1
1	q	283	ARG	2.1
1	q	422	ARG	2.1
2	Z	69	GLU	2.1
3	g	33	GLU	2.1
1	M	294	ASP	2.1
2	H	58	LYS	2.1
2	N	225	ASP	2.1
4	D	128	GLY	2.1
1	G	65	VAL	2.1
1	M	544	TYR	2.1
1	Y	360	PRO	2.1
1	k	348	VAL	2.1
1	k	461	VAL	2.1
2	l	115	ALA	2.1
2	r	428	TYR	2.1
3	C	74	TYR	2.1
1	A	43	ASP	2.1
1	k	28	ASP	2.1
2	H	133	ILE	2.1
5	u	81	LEU	2.1
6	X	41	CYS	2.1
6	v	77	CYS	2.1
1	Y	68	GLY	2.1
4	n	42	GLN	2.1
6	L	113	GLU	2.1
1	G	474	PRO	2.1
2	f	326	ALA	2.1
1	G	23	ASP	2.1
2	B	410	ASP	2.1
2	Z	225	ASP	2.1
2	l	319	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	s	191	ILE	2.1
1	G	530	SER	2.1
2	r	55	LEU	2.1
6	d	44	SER	2.1
1	q	345	GLY	2.1
2	T	289	GLY	2.1
2	f	300	CYS	2.1
2	l	12	CYS	2.1
6	R	68	GLU	2.1
3	g	229	LYS	2.1
6	j	16	ARG	2.1
6	v	349	LYS	2.1
1	M	37	ASP	2.0
1	k	393	THR	2.0
1	k	524	VAL	2.0
4	D	62	VAL	2.0
2	f	131	TYR	2.0
6	F	64	ILE	2.0
2	T	130	GLY	2.0
1	Y	6	LYS	2.0
1	G	568	MET	2.0
1	M	506	ASP	2.0
1	q	70	MET	2.0
4	n	1	MET	2.0
4	t	49	ASP	2.0
1	S	259	ALA	2.0
3	s	8	PRO	2.0
1	Y	125	THR	2.0
2	f	301	THR	2.0
4	t	95	THR	2.0
6	j	17	THR	2.0
6	p	153	THR	2.0
2	l	66	SER	2.0
4	V	42	GLN	2.0
3	m	235	GLY	2.0
6	X	16	ARG	2.0
3	U	234	ASP	2.0
1	G	479	PRO	2.0
2	H	64	GLU	2.0
4	D	38	GLU	2.0
1	A	25	CYS	2.0
1	k	61	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	r	115	ALA	2.0
2	N	135	THR	2.0
5	i	64	CYS	2.0
6	F	194	CYS	2.0
6	X	93	THR	2.0
1	k	410	ASN	2.0
5	c	42	VAL	2.0
6	R	72	VAL	2.0
1	M	62	GLY	2.0
1	k	528	ILE	2.0
2	B	285	ILE	2.0
6	L	7	ILE	2.0
6	R	40	ILE	2.0
1	k	483	TYR	2.0
2	l	136	PHE	2.0
2	l	296	PHE	2.0
1	k	21	LYS	2.0
1	q	84	LYS	2.0
3	C	58	PRO	2.0
4	P	42	GLN	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

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

6.5 Other polymers

There are no such residues in this entry.