



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2017 – 07:56 PM EDT

PDB ID : 5B5M  
Title : Crystal structure of the Sr-substituted LH1-RC complex from Tch. tepidum  
Authors : Wang-Otomo, Z.-Y.; Yu, L.-J.  
Deposited on : 2016-05-12  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029077



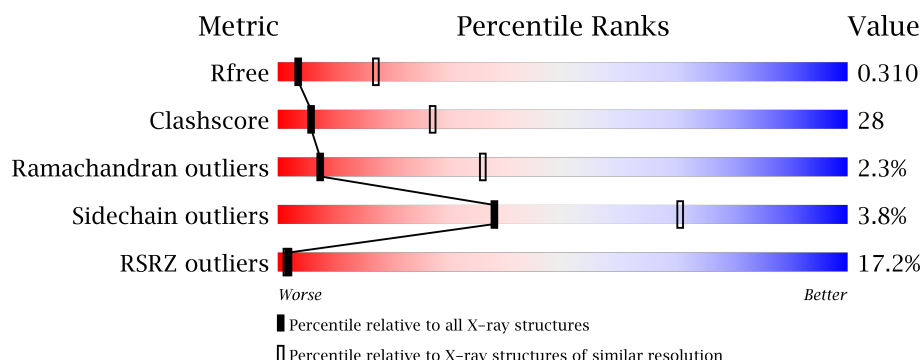
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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  $\geq 3$ , 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	C	333	<div> <div>11%</div> <div> <div></div> <div>52%</div> <div>36%</div> <div>6%</div> <div>5%</div> </div> </div>
1	o	333	<div> <div>14%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
2	L	281	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>44%</div> <div>5%</div> </div> </div>
2	x	281	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
3	M	319	<div> <div>4%</div> <div> <div></div> <div>43%</div> <div>50%</div> <div>6%</div> </div> </div>

*Continued on next page...*



Continued from previous page...

Mol	Chain	Length	Quality of chain
3	y	319	
4	H	259	
4	t	259	
5	1	61	
5	3	61	
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	AA	61	
5	AC	61	
5	AE	61	
5	AG	61	
5	AI	61	
5	AK	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
5	d	61	<div> <div>25%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
5	f	61	<div> <div>28%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
5	h	61	<div> <div>25%</div> <div>92%</div> <div>5%</div> <div>..</div> </div>
5	j	61	<div> <div>21%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
5	l	61	<div> <div>34%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
5	m	61	<div> <div>33%</div> <div>95%</div> <div>.</div> <div>..</div> </div>
5	p	61	<div> <div>31%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
5	r	61	<div> <div>23%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
5	u	61	<div> <div>28%</div> <div>95%</div> <div>.</div> <div>..</div> </div>
5	w	61	<div> <div>36%</div> <div>95%</div> <div>.</div> <div>..</div> </div>
6	0	47	<div> <div>19%</div> <div>53%</div> <div>30%</div> <div>.</div> <div>15%</div> </div>
6	2	47	<div> <div>13%</div> <div>49%</div> <div>36%</div> <div>.</div> <div>15%</div> </div>
6	4	47	<div> <div>4%</div> <div>66%</div> <div>19%</div> <div>.</div> <div>15%</div> </div>
6	6	47	<div> <div>11%</div> <div>60%</div> <div>26%</div> <div>.</div> <div>15%</div> </div>
6	8	47	<div> <div>26%</div> <div>62%</div> <div>23%</div> <div>.</div> <div>15%</div> </div>
6	AB	47	<div> <div>11%</div> <div>53%</div> <div>32%</div> <div>.</div> <div>15%</div> </div>
6	AD	47	<div> <div>9%</div> <div>60%</div> <div>26%</div> <div>.</div> <div>15%</div> </div>
6	AF	47	<div> <div>17%</div> <div>60%</div> <div>26%</div> <div>.</div> <div>15%</div> </div>
6	AH	47	<div> <div>15%</div> <div>53%</div> <div>32%</div> <div>.</div> <div>15%</div> </div>
6	AJ	47	<div> <div>17%</div> <div>47%</div> <div>34%</div> <div>.</div> <div>15%</div> </div>
6	AL	47	<div> <div>17%</div> <div>62%</div> <div>23%</div> <div>.</div> <div>15%</div> </div>
6	B	47	<div> <div>21%</div> <div>45%</div> <div>36%</div> <div>.</div> <div>15%</div> </div>
6	E	47	<div> <div>9%</div> <div>45%</div> <div>40%</div> <div>.</div> <div>15%</div> </div>
6	G	47	<div> <div>11%</div> <div>34%</div> <div>51%</div> <div>.</div> <div>15%</div> </div>
6	J	47	<div> <div>19%</div> <div>43%</div> <div>43%</div> <div>.</div> <div>15%</div> </div>

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
6	N	47	
6	P	47	
6	R	47	
6	T	47	
6	V	47	
6	X	47	
6	Z	47	
6	c	47	
6	e	47	
6	g	47	
6	i	47	
6	k	47	
6	n	47	
6	q	47	
6	s	47	
6	v	47	
6	z	47	

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
10	BPH	x	302	-	-	-	X
11	UQ8	L	304	-	-	-	X
11	UQ8	x	304	-	-	-	X
12	PEF	A	101	-	-	-	X
12	PEF	y	408	-	-	-	X
14	MQ8	M	403	-	-	-	X
14	MQ8	y	403	-	-	-	X
15	CRT	2	101	-	-	-	X

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CRT	4	101	-	-	-	X
15	CRT	6	101	-	-	-	X
15	CRT	8	101	-	-	-	X
15	CRT	9	102	-	-	-	X
15	CRT	A	103	-	-	-	X
15	CRT	AC	101	-	-	-	X
15	CRT	AD	102	-	-	-	X
15	CRT	AE	103	-	-	-	X
15	CRT	AH	102	-	-	-	X
15	CRT	AJ	101	-	-	-	X
15	CRT	AL	101	-	-	-	X
15	CRT	E	101	-	-	-	X
15	CRT	G	101	-	-	-	X
15	CRT	J	101	-	-	-	X
15	CRT	M	404	-	-	-	X
15	CRT	N	101	-	-	X	X
15	CRT	P	102	-	-	-	X
15	CRT	R	101	-	-	-	X
15	CRT	T	101	-	-	-	X
15	CRT	U	102	-	-	-	X
15	CRT	X	101	-	-	-	X
15	CRT	Z	101	-	-	-	X
15	CRT	c	101	-	-	-	X
15	CRT	e	101	-	-	-	X
15	CRT	f	102	-	-	-	X
15	CRT	i	101	-	-	-	X
15	CRT	k	101	-	-	-	X
15	CRT	n	101	-	-	-	X
15	CRT	p	103	-	-	-	X
15	CRT	s	101	-	-	-	X
15	CRT	v	101	-	-	-	X
15	CRT	y	404	-	-	-	X
15	CRT	z	101	-	-	-	X
16	PO4	H	302	-	-	-	X
7	HEM	C	502	-	-	-	X
7	HEM	o	501	-	-	-	X
7	HEM	o	502	-	-	-	X
7	HEM	o	503	-	-	-	X
7	HEM	o	504	-	-	-	X
9	BCL	0	101	-	-	-	X
9	BCL	4	102	-	-	-	X
9	BCL	5	102	-	-	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCL	AB	101	-	-	-	X
9	BCL	AC	102	-	-	-	X
9	BCL	AE	104	-	-	-	X
9	BCL	AH	101	-	-	-	X
9	BCL	AI	101	-	-	-	X
9	BCL	AK	101	-	-	-	X
9	BCL	D	101	-	-	X	-
9	BCL	D	102	-	-	-	X
9	BCL	F	101	-	-	-	X
9	BCL	J	102	-	-	-	X
9	BCL	K	101	-	-	-	X
9	BCL	N	102	-	-	-	X
9	BCL	O	101	-	-	-	X
9	BCL	U	101	-	-	X	-
9	BCL	W	101	-	-	X	-
9	BCL	Z	102	-	-	-	X
9	BCL	e	102	-	-	-	X
9	BCL	r	101	-	-	-	X
9	BCL	s	102	-	-	-	X
9	BCL	w	101	-	-	-	X
9	BCL	y	401	-	-	-	X
9	BCL	z	102	-	-	-	X



## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 51893 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			
1	o	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			
2	x	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	318	Total	C	N	O	S	0	0	0
			2546	1710	416	409	11			
3	y	318	Total	C	N	O	S	0	0	0
			2546	1710	416	409	11			

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	0	0	0
			1982	1275	339	363	5			
4	t	258	Total	C	N	O	S	0	0	0
			1982	1275	339	363	5			

- Molecule 5 is a protein called LH1 alpha polypeptide.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	D	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	F	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	I	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	K	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	O	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	Q	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	S	60	Total 481	C 318	N 78	O 83	S 2	0	1	0
5	U	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	W	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	Y	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	1	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	3	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	5	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	7	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	9	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	m	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	p	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	r	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	u	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	w	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	AA	60	Total 475	C 315	N 77	O 81	S 2	0	0	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	AE	60	Total	C	N	O	S	0	1	0
			481	318	78	83	2			
5	AG	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	AI	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	AK	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	d	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	f	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	h	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	j	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	l	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	E	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	G	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	J	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	N	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	P	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	R	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	T	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	V	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	Z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	2	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	4	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	6	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	8	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	0	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	n	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	q	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	s	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	v	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AB	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AD	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AF	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AH	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AJ	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AL	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	e	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	g	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	i	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

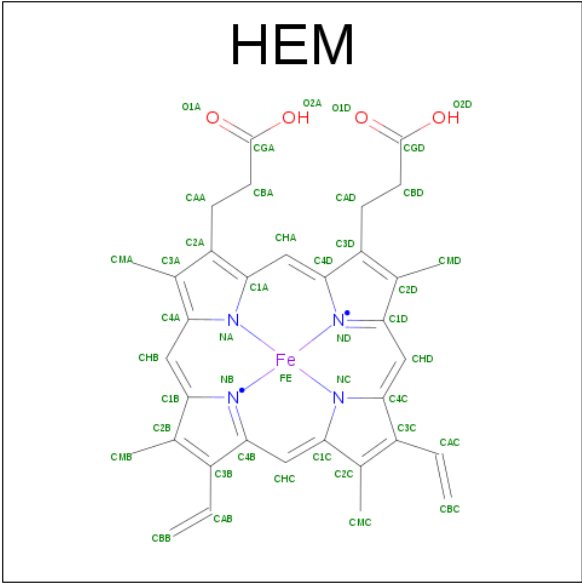
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	k	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	c	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	o	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	o	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	o	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	o	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is STRONTIUM ION (three-letter code: SR) (formula: Sr).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	1	Total 1	Sr 1	0	0
8	h	1	Total 1	Sr 1	0	0
8	AC	1	Total 1	Sr 1	0	0
8	W	1	Total 1	Sr 1	0	0
8	o	1	Total 1	Sr 1	0	0
8	S	1	Total 1	Sr 1	0	0
8	f	1	Total 1	Sr 1	0	0
8	AK	1	Total 1	Sr 1	0	0
8	p	1	Total 1	Sr 1	0	0
8	AE	1	Total 1	Sr 1	0	0
8	w	2	Total 2	Sr 2	0	0
8	A	1	Total 1	Sr 1	0	0
8	5	2	Total 2	Sr 2	0	0
8	x	2	Total 2	Sr 2	0	0
8	AA	1	Total 1	Sr 1	0	0
8	j	1	Total 1	Sr 1	0	0
8	1	1	Total 1	Sr 1	0	0
8	D	1	Total 1	Sr 1	0	0
8	I	1	Total 1	Sr 1	0	0
8	U	1	Total 1	Sr 1	0	0
8	r	1	Total 1	Sr 1	0	0
8	9	1	Total 1	Sr 1	0	0

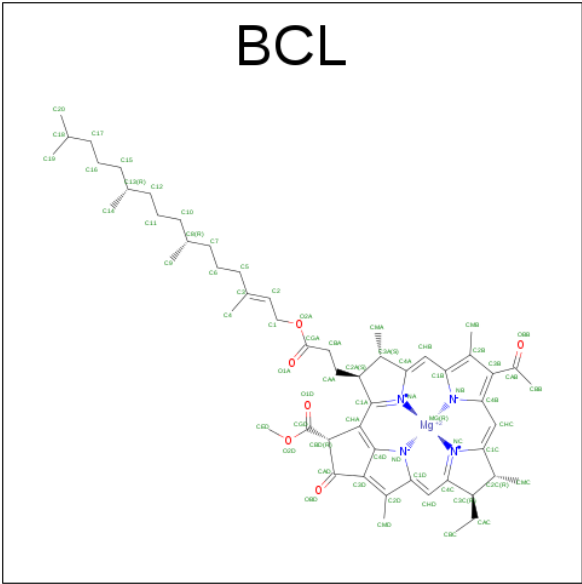
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	2	Total 2	Sr 2	0	0
8	m	1	Total 1	Sr 1	0	0
8	Q	1	Total 1	Sr 1	0	0
8	d	1	Total 1	Sr 1	0	0
8	AI	2	Total 2	Sr 2	0	0
8	C	1	Total 1	Sr 1	0	0
8	7	1	Total 1	Sr 1	0	0
8	O	1	Total 1	Sr 1	0	0
8	Y	1	Total 1	Sr 1	0	0
8	l	1	Total 1	Sr 1	0	0
8	F	1	Total 1	Sr 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	J	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	N	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	P	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	T	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	U	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	V	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	W	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	X	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	4	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	7	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	8	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	9	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	0	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	x	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	x	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	x	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	y	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	m	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	m	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	p	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	p	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	r	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	s	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	v	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	w	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AA	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	d	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	e	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

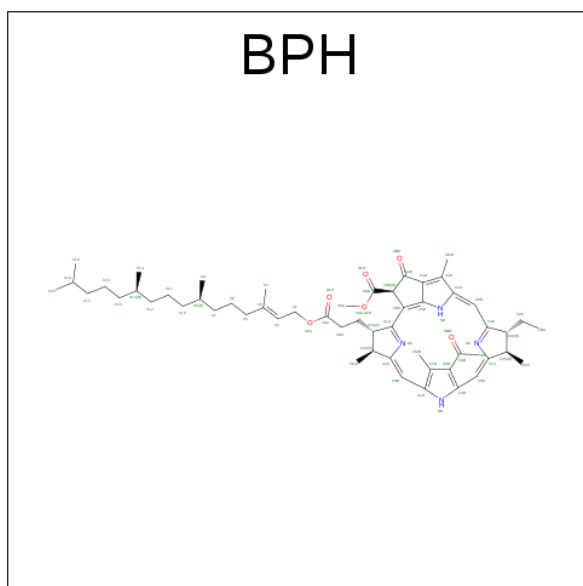
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	f	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	g	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	h	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	i	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	j	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	k	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	l	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	c	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		
10	x	1	Total	C	N	O	0	0
			65	55	4	6		

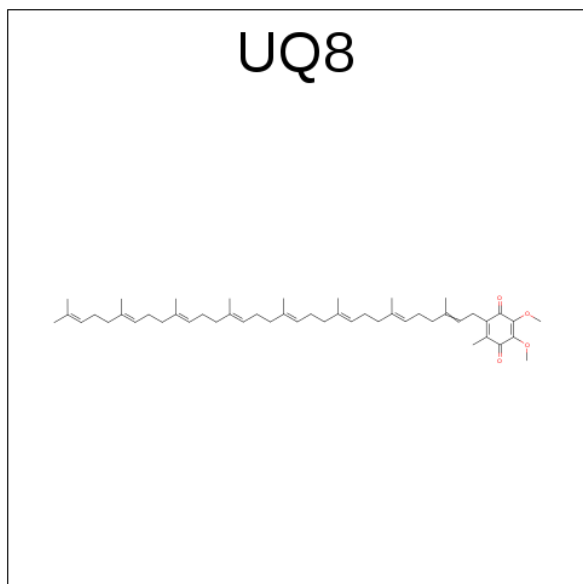
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	y	1	Total	C	N	O	0	0
			65	55	4	6		

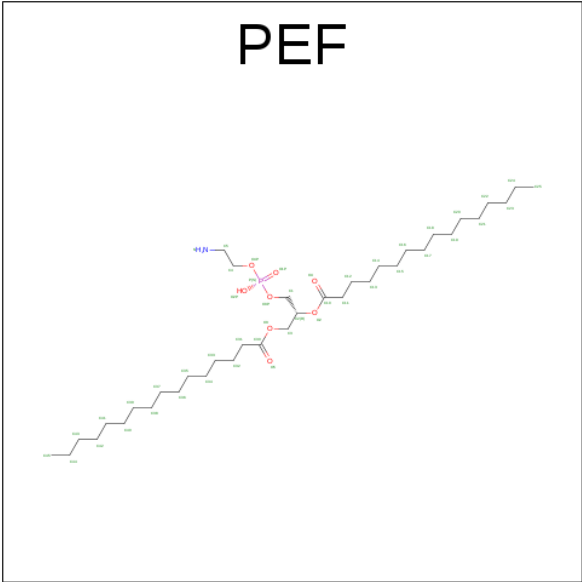
- Molecule 11 is Ubiquinone-8 (three-letter code: UQ8) (formula: C<sub>49</sub>H<sub>74</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			53	49	4		
11	x	1	Total	C	O	0	0
			53	49	4		

- Molecule 12 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	L	1	Total	C	N	O	P	0	0
			12	5	1	5	1		
12	M	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	M	1	Total	C	N	O	P	0	0
			16	7	1	7	1		
12	M	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	x	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	y	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	y	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	y	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	t	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	t	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

Continued on next page...



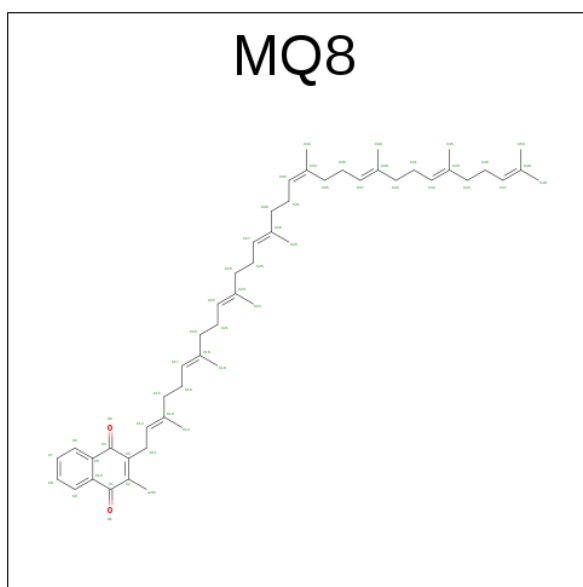
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	m	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	p	1	Total	C	N	O	P	0	0
			16	7	1	7	1		

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	x	1	Total	Fe	0	0
			1	1		
13	L	1	Total	Fe	0	0
			1	1		

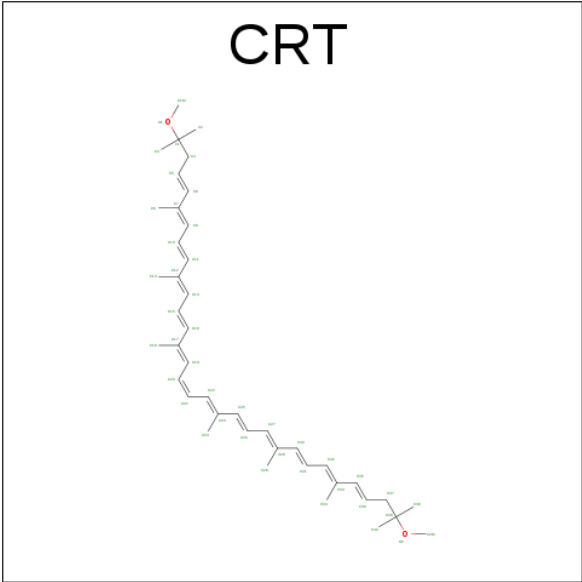
- Molecule 14 is MENAQUINONE 8 (three-letter code: MQ8) (formula: C<sub>51</sub>H<sub>72</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			53	51	2		
14	y	1	Total	C	O	0	0
			53	51	2		

- Molecule 15 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			44	42	2		
15	A	1	Total	C	O	0	0
			44	42	2		
15	E	1	Total	C	O	0	0
			44	42	2		
15	G	1	Total	C	O	0	0
			44	42	2		
15	J	1	Total	C	O	0	0
			44	42	2		
15	N	1	Total	C	O	0	0
			44	42	2		
15	P	1	Total	C	O	0	0
			44	42	2		
15	R	1	Total	C	O	0	0
			44	42	2		
15	T	1	Total	C	O	0	0
			44	42	2		
15	U	1	Total	C	O	0	0
			44	42	2		
15	X	1	Total	C	O	0	0
			44	42	2		
15	Z	1	Total	C	O	0	0
			44	42	2		
15	2	1	Total	C	O	0	0
			44	42	2		
15	4	1	Total	C	O	0	0
			44	42	2		

Continued on next page...

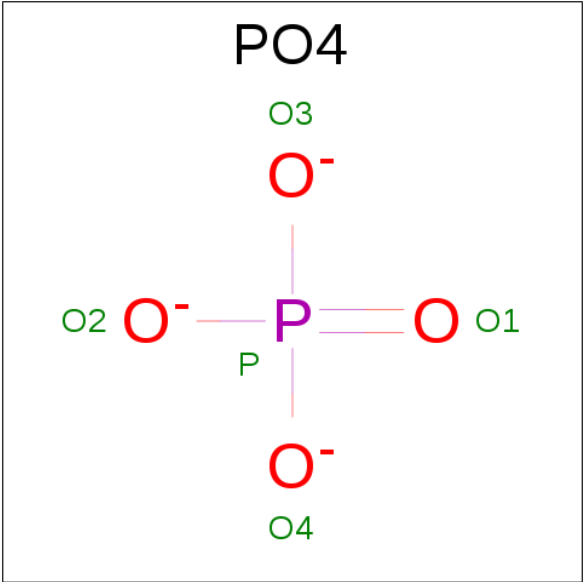


*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	6	1	Total	C	O	0	0
			44	42	2		
15	8	1	Total	C	O	0	0
			44	42	2		
15	9	1	Total	C	O	0	0
			44	42	2		
15	y	1	Total	C	O	0	0
			44	42	2		
15	n	1	Total	C	O	0	0
			44	42	2		
15	p	1	Total	C	O	0	0
			44	42	2		
15	s	1	Total	C	O	0	0
			44	42	2		
15	v	1	Total	C	O	0	0
			44	42	2		
15	z	1	Total	C	O	0	0
			44	42	2		
15	AC	1	Total	C	O	0	0
			44	42	2		
15	AD	1	Total	C	O	0	0
			44	42	2		
15	AE	1	Total	C	O	0	0
			44	42	2		
15	AH	1	Total	C	O	0	0
			44	42	2		
15	AJ	1	Total	C	O	0	0
			44	42	2		
15	AL	1	Total	C	O	0	0
			44	42	2		
15	e	1	Total	C	O	0	0
			44	42	2		
15	f	1	Total	C	O	0	0
			44	42	2		
15	i	1	Total	C	O	0	0
			44	42	2		
15	k	1	Total	C	O	0	0
			44	42	2		
15	c	1	Total	C	O	0	0
			44	42	2		

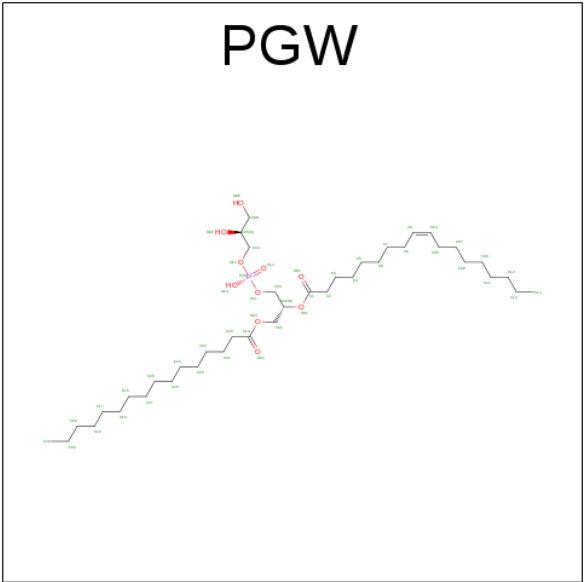
- Molecule 16 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	M	1	Total	O	P	0	0
			5	4	1		
16	H	1	Total	O	P	0	0
			5	4	1		
16	y	1	Total	O	P	0	0
			5	4	1		
16	t	1	Total	O	P	0	0
			5	4	1		

- Molecule 17 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	S	1	Total	C	O	P	0	0
			21	10	10	1		
17	AE	1	Total	C	O	P	0	0
			21	10	10	1		

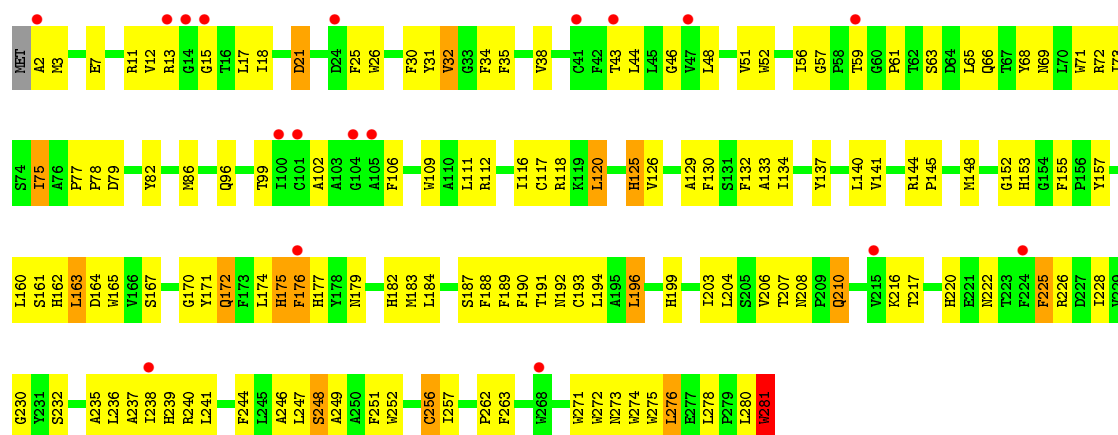
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	1	Total	O	0	0
			1	1		
18	L	1	Total	O	0	0
			1	1		
18	W	1	Total	O	0	0
			1	1		
18	o	1	Total	O	0	0
			1	1		
18	x	1	Total	O	0	0
			1	1		
18	AI	1	Total	O	0	0
			1	1		

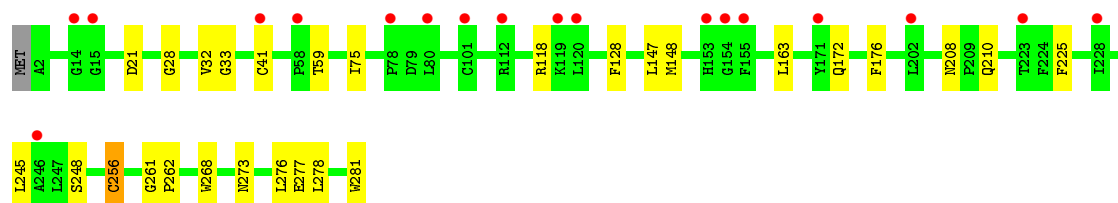
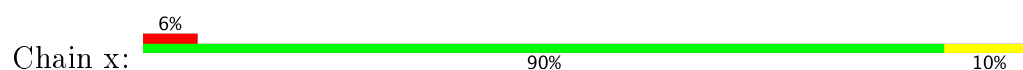




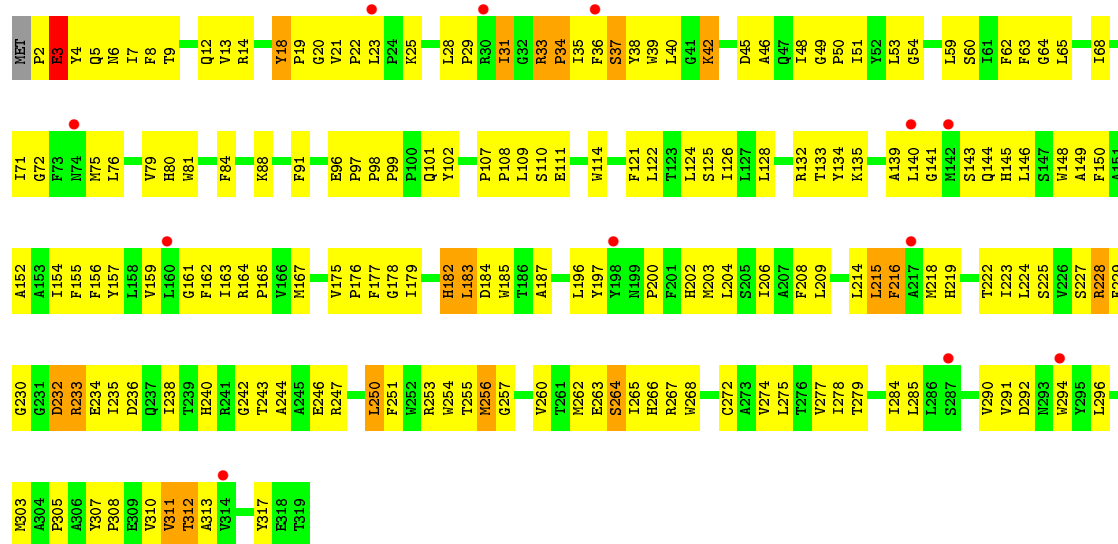
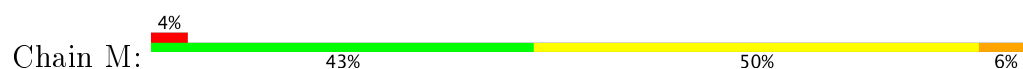




• Molecule 2: Photosynthetic reaction center L subunit



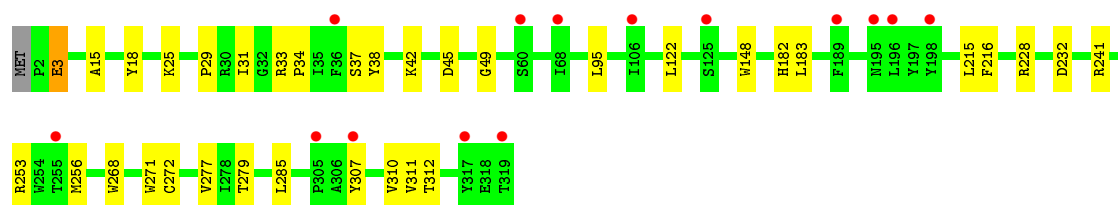
• Molecule 3: Photosynthetic reaction center M subunit



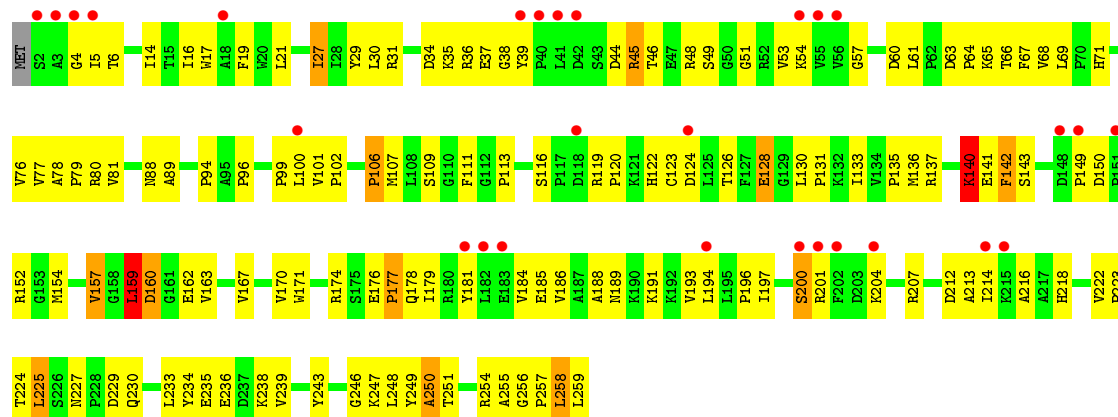
• Molecule 3: Photosynthetic reaction center M subunit



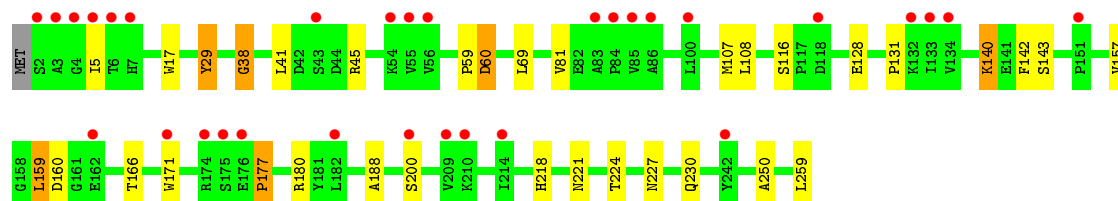
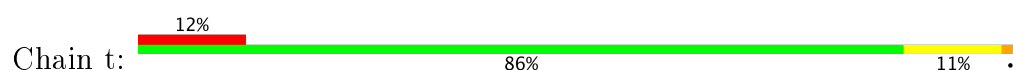




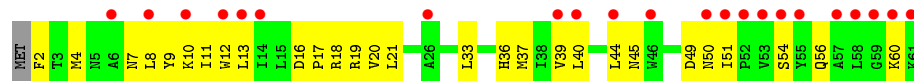
• Molecule 4: Photosynthetic reaction center H subunit



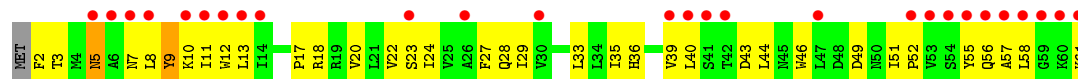
• Molecule 4: Photosynthetic reaction center H subunit



• Molecule 5: LH1 alpha polypeptide

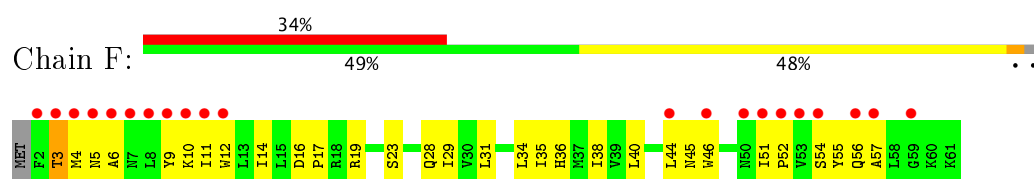


• Molecule 5: LH1 alpha polypeptide

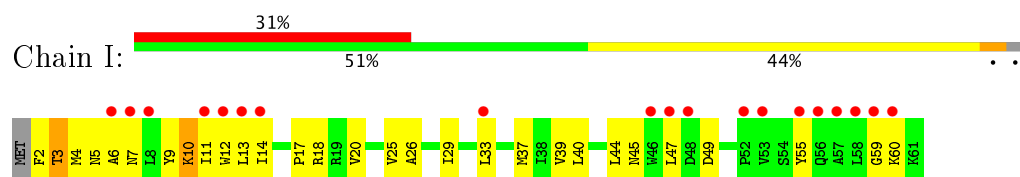


• Molecule 5: LH1 alpha polypeptide

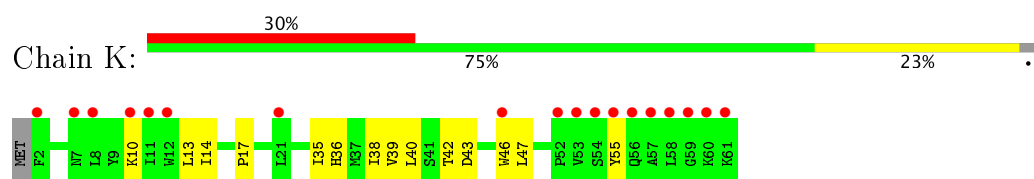




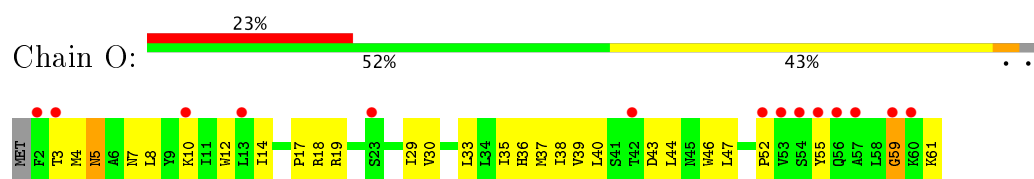
- Molecule 5: LH1 alpha polypeptide



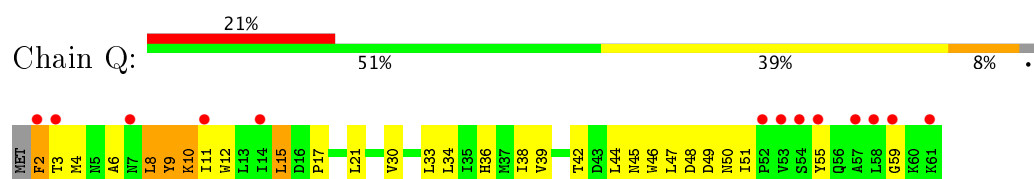
- Molecule 5: LH1 alpha polypeptide



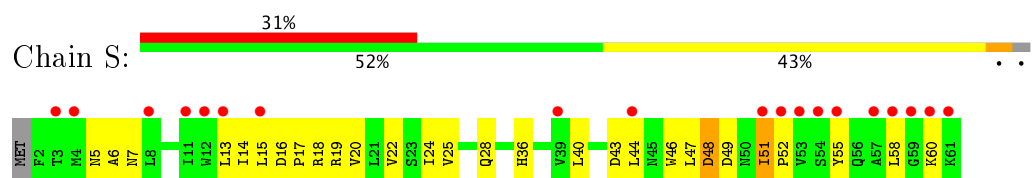
- Molecule 5: LH1 alpha polypeptide



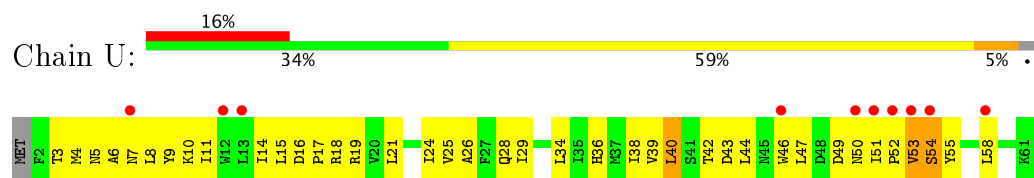
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

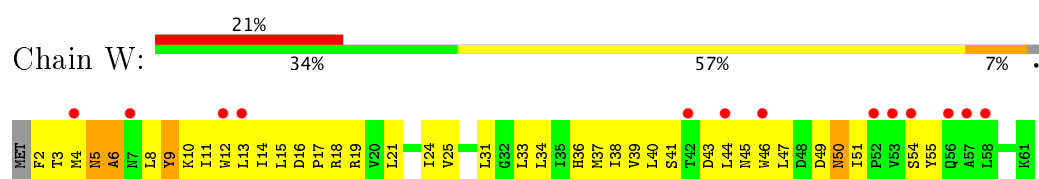


- Molecule 5: LH1 alpha polypeptide

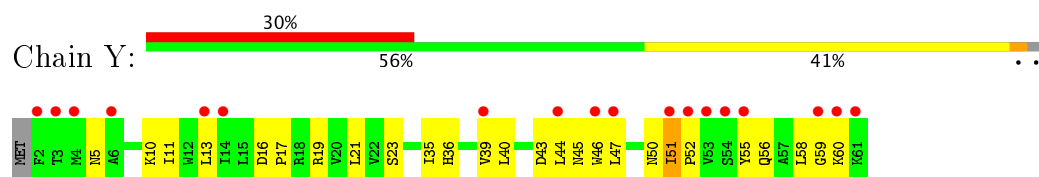


- Molecule 5: LH1 alpha polypeptide

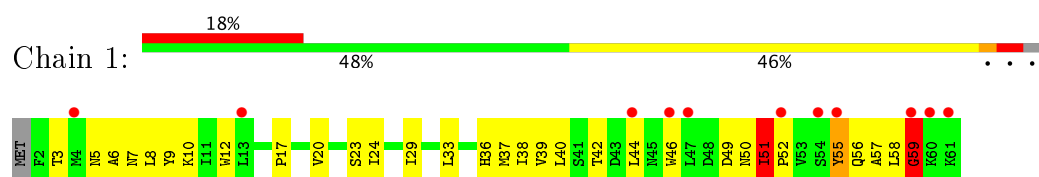




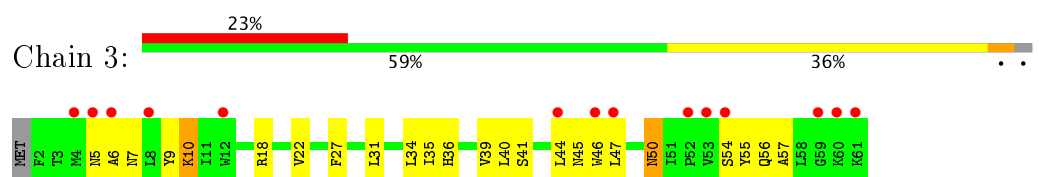
- Molecule 5: LH1 alpha polypeptide



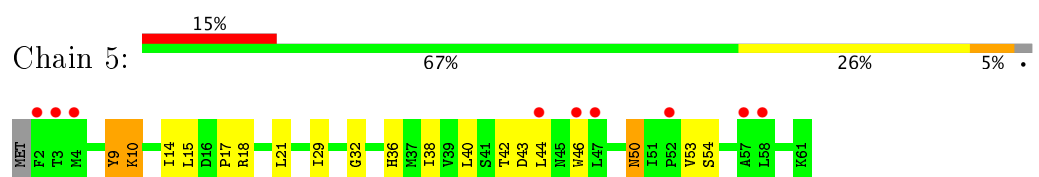
- Molecule 5: LH1 alpha polypeptide



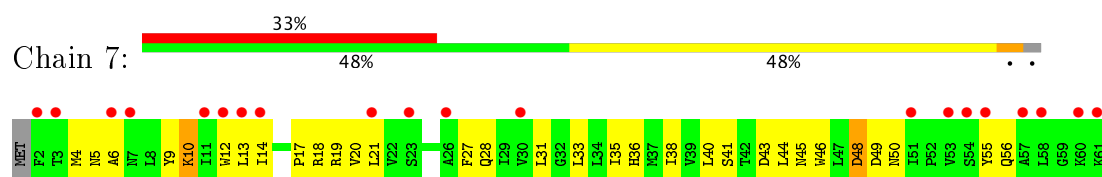
- Molecule 5: LH1 alpha polypeptide



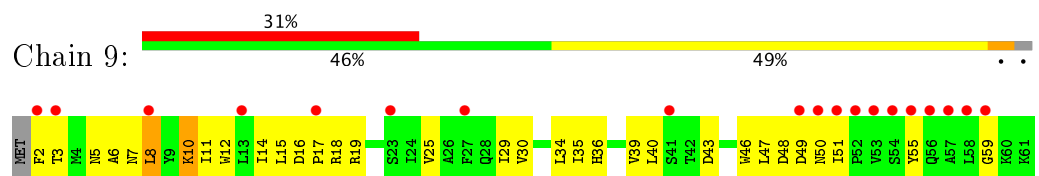
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

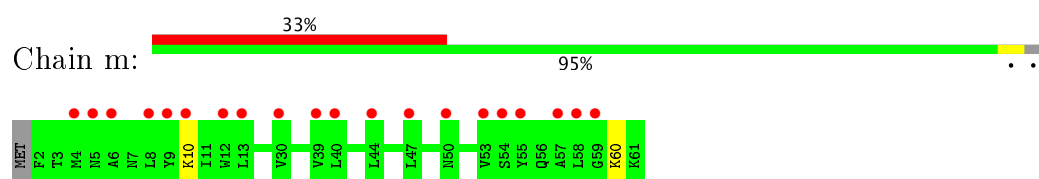


- Molecule 5: LH1 alpha polypeptide

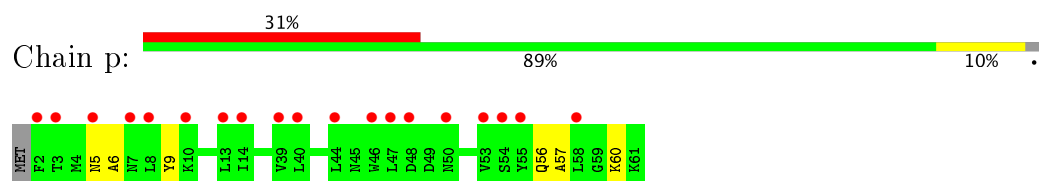


- Molecule 5: LH1 alpha polypeptide

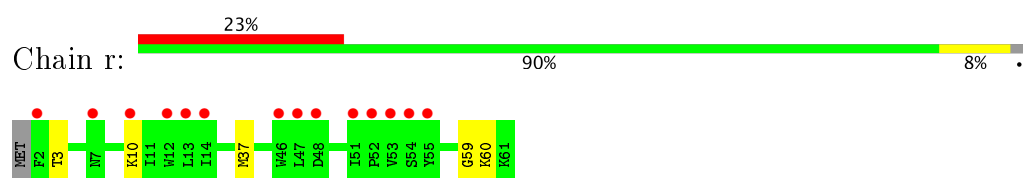




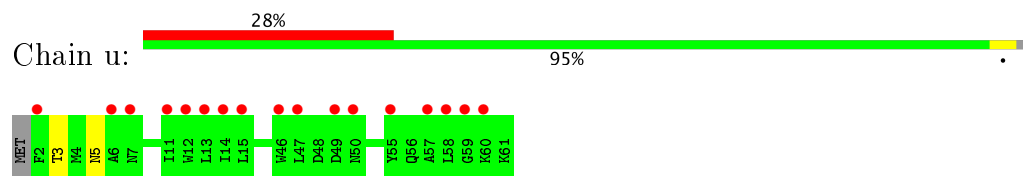
- Molecule 5: LH1 alpha polypeptide



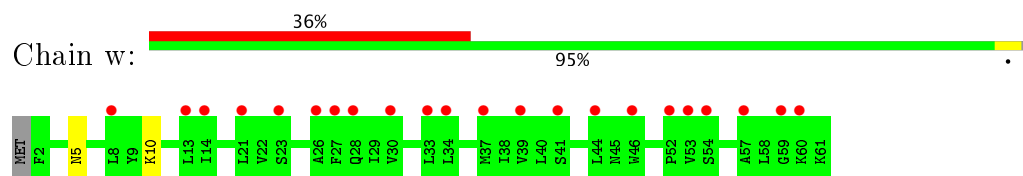
- Molecule 5: LH1 alpha polypeptide



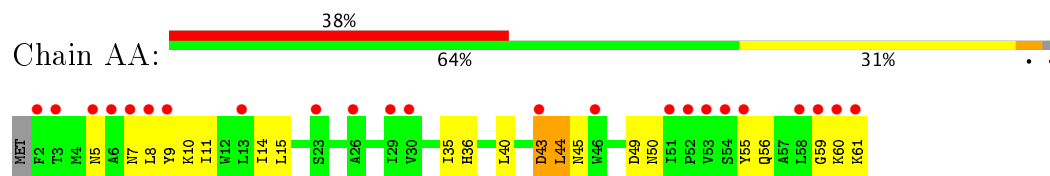
- Molecule 5: LH1 alpha polypeptide



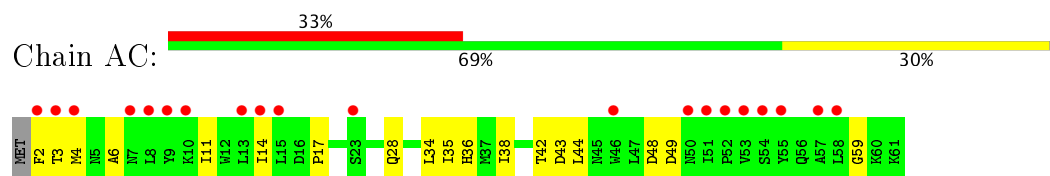
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

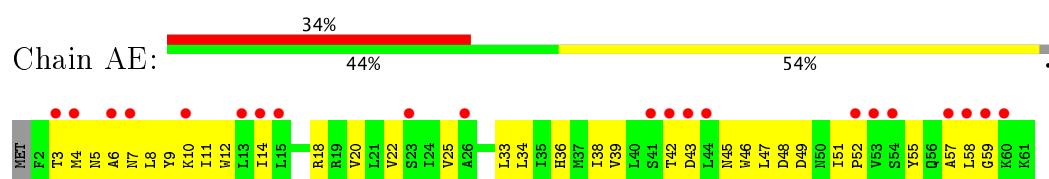


- Molecule 5: LH1 alpha polypeptide

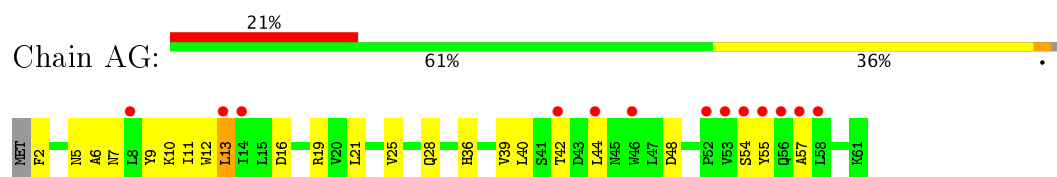


- Molecule 5: LH1 alpha polypeptide

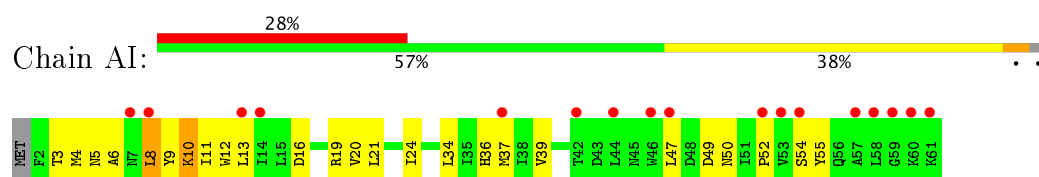




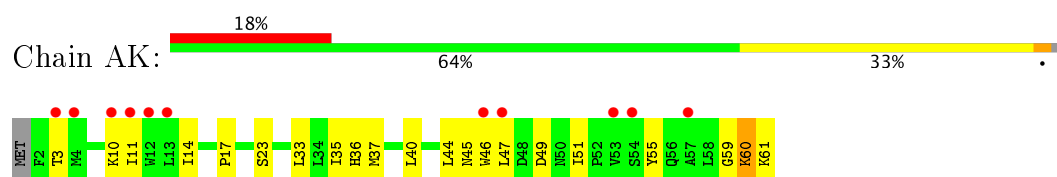
- Molecule 5: LH1 alpha polypeptide



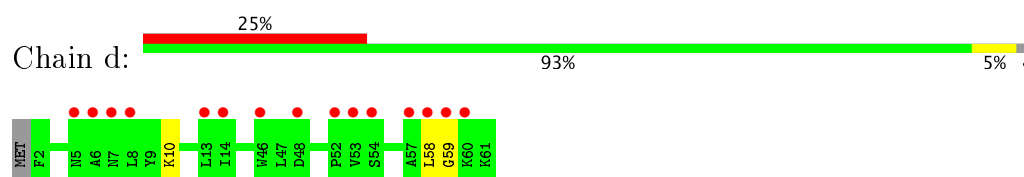
- Molecule 5: LH1 alpha polypeptide



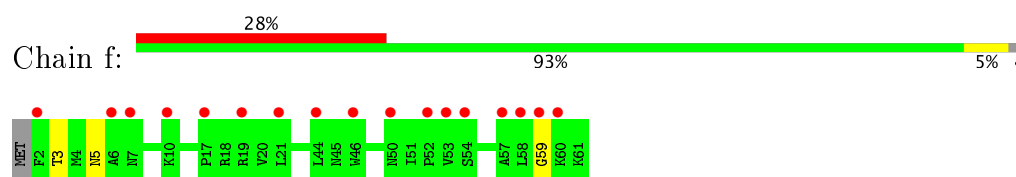
- Molecule 5: LH1 alpha polypeptide



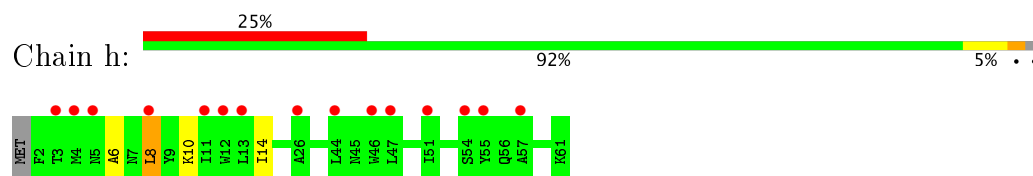
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

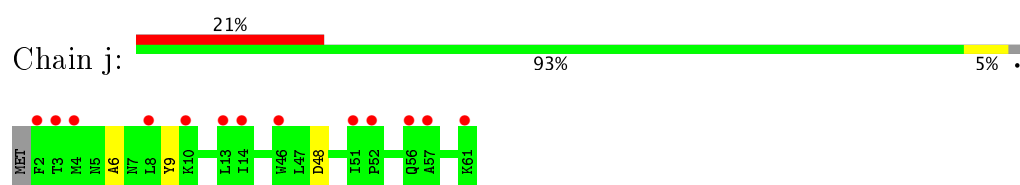


- Molecule 5: LH1 alpha polypeptide

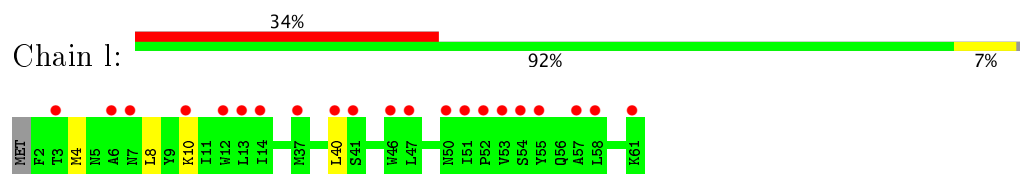


- Molecule 5: LH1 alpha polypeptide

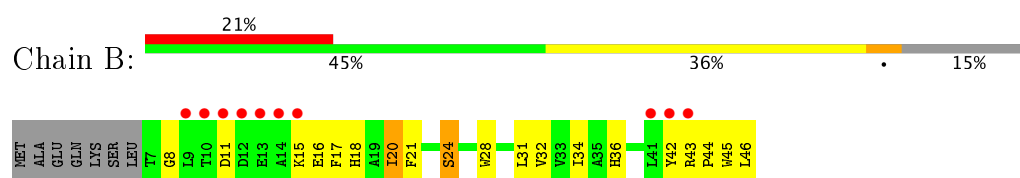




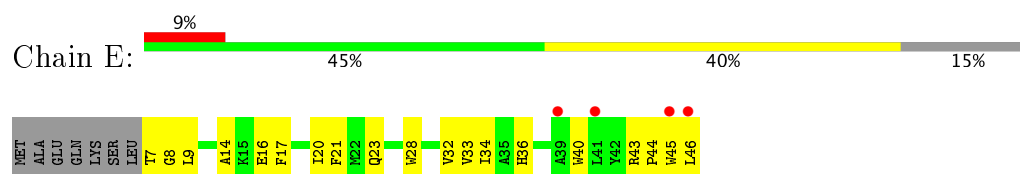
- Molecule 5: LH1 alpha polypeptide



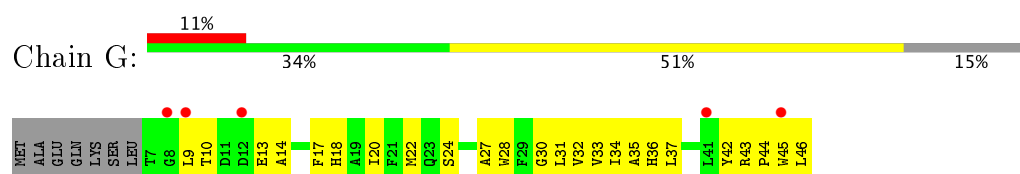
- Molecule 6: LH1 beta polypeptide



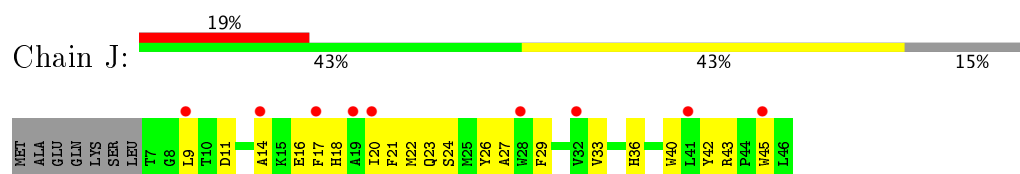
- Molecule 6: LH1 beta polypeptide



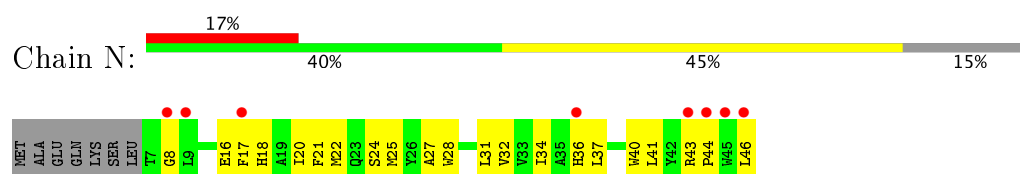
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide

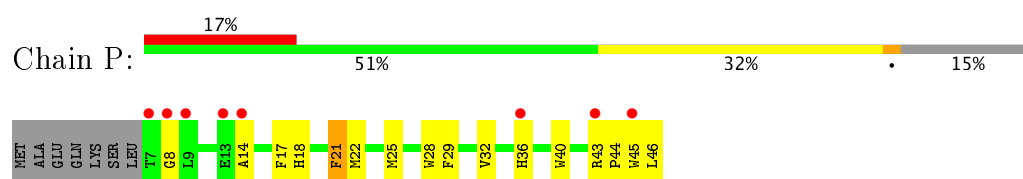


- Molecule 6: LH1 beta polypeptide

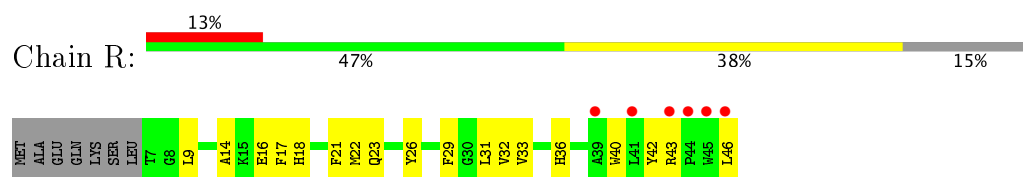


- Molecule 6: LH1 beta polypeptide

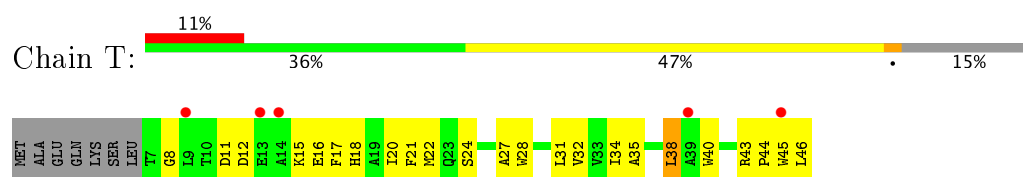




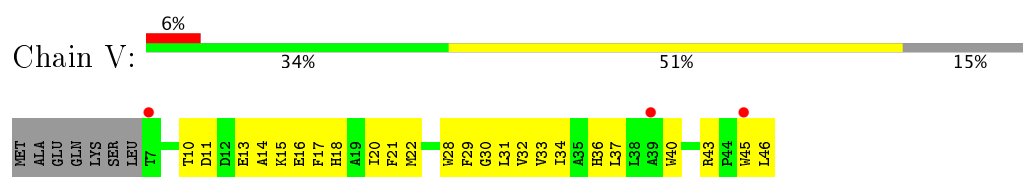
- Molecule 6: LH1 beta polypeptide



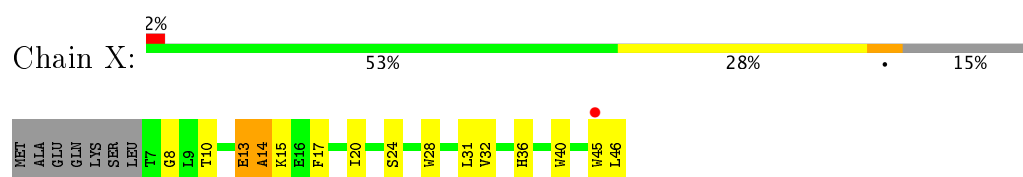
- Molecule 6: LH1 beta polypeptide



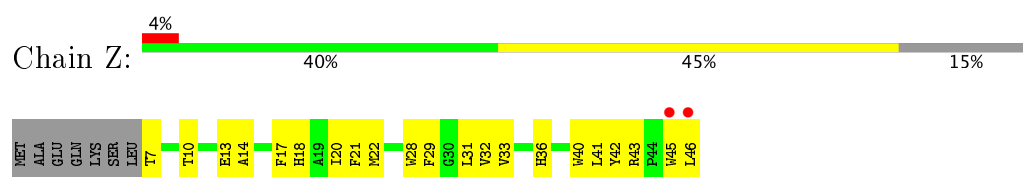
- Molecule 6: LH1 beta polypeptide



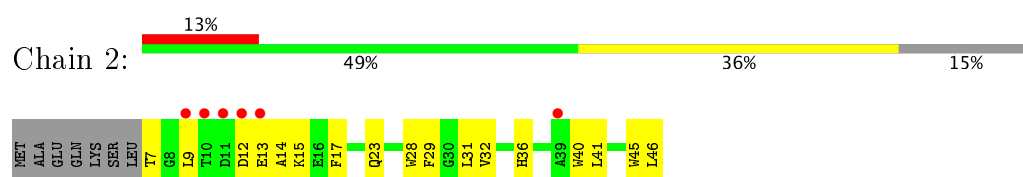
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide

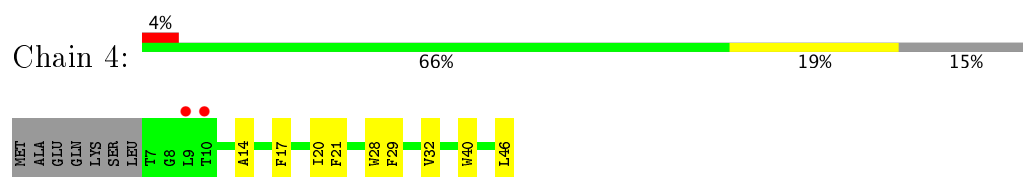


- Molecule 6: LH1 beta polypeptide

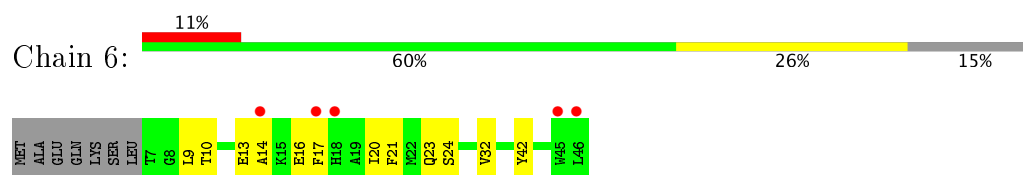


- Molecule 6: LH1 beta polypeptide

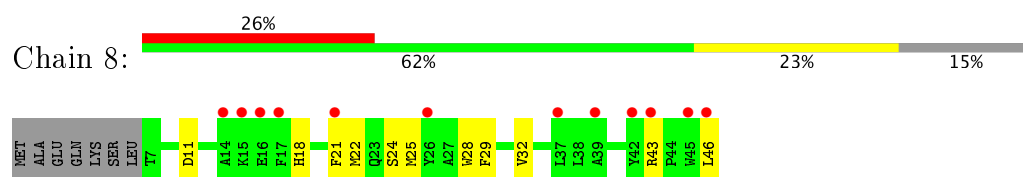




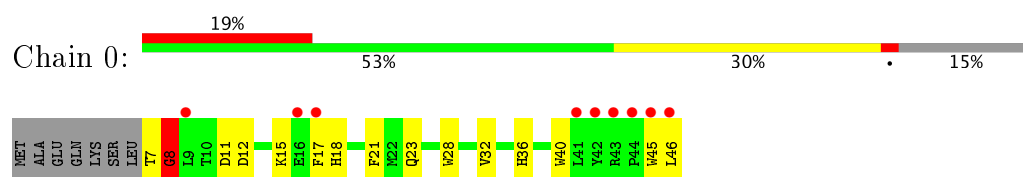
- Molecule 6: LH1 beta polypeptide



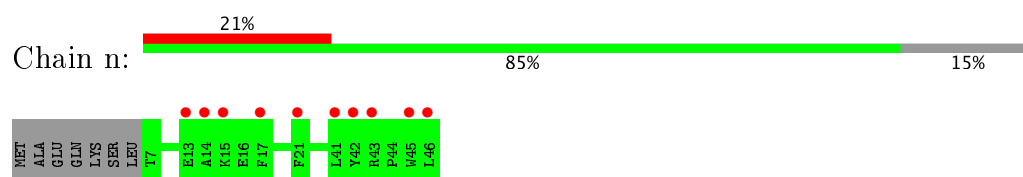
- Molecule 6: LH1 beta polypeptide



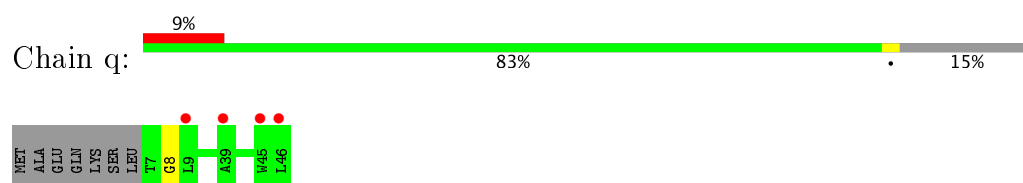
- Molecule 6: LH1 beta polypeptide



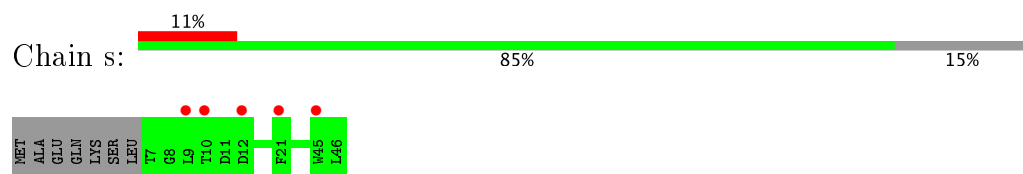
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide

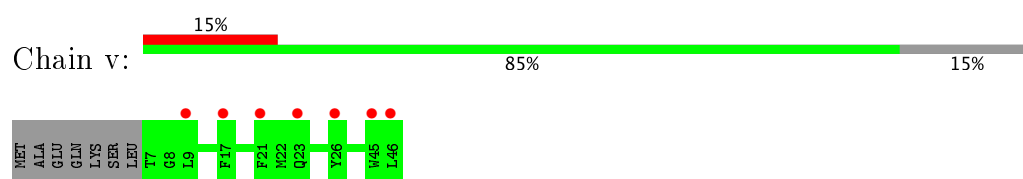


- Molecule 6: LH1 beta polypeptide

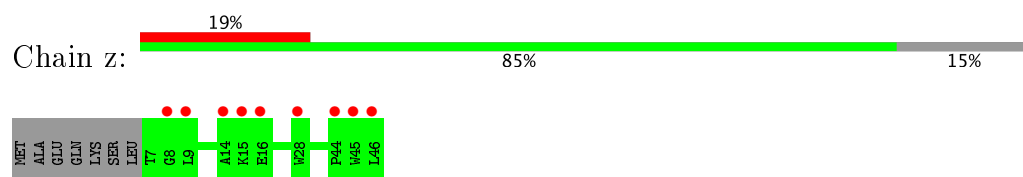


- Molecule 6: LH1 beta polypeptide

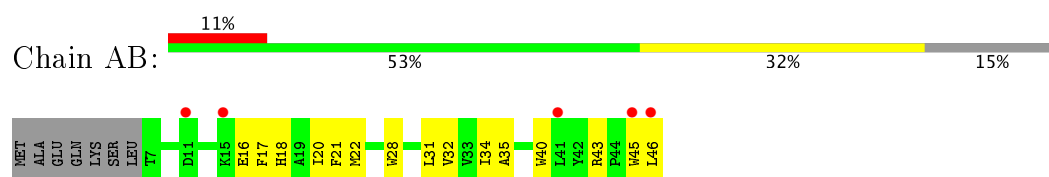




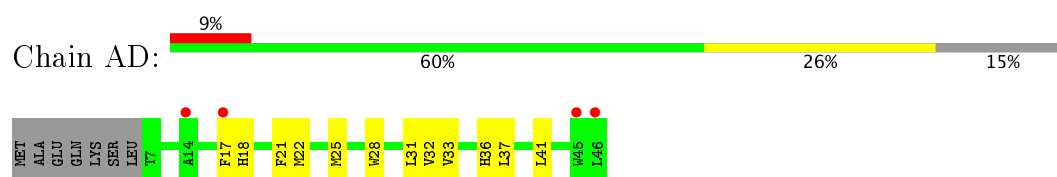
- Molecule 6: LH1 beta polypeptide



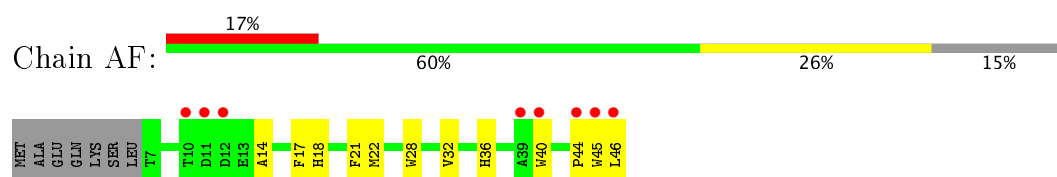
- Molecule 6: LH1 beta polypeptide



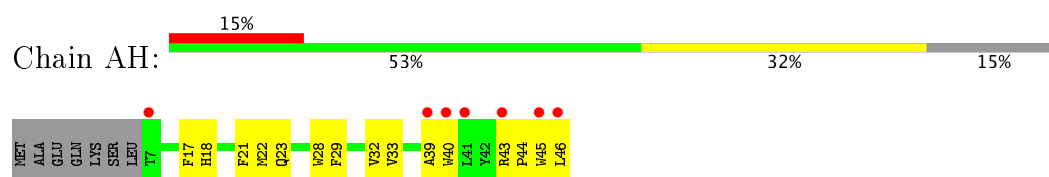
- Molecule 6: LH1 beta polypeptide



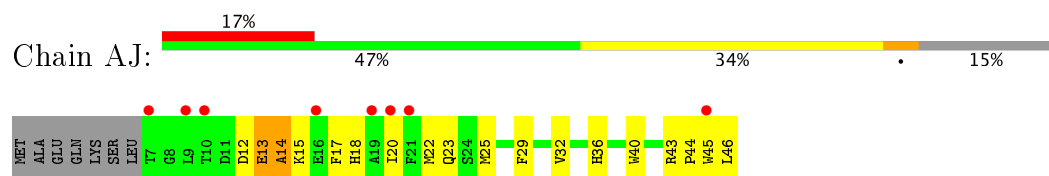
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide

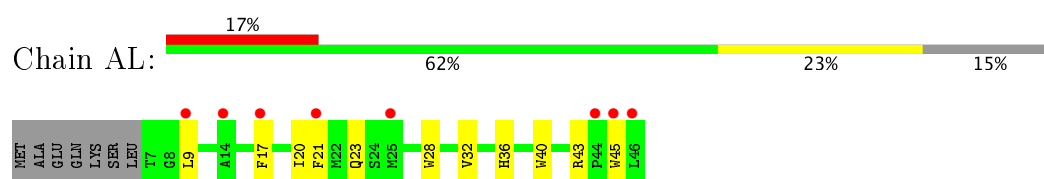


- Molecule 6: LH1 beta polypeptide

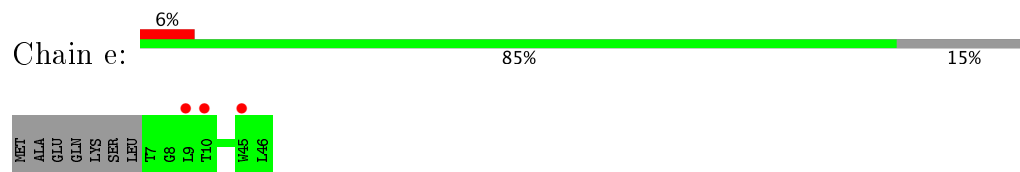


- Molecule 6: LH1 beta polypeptide

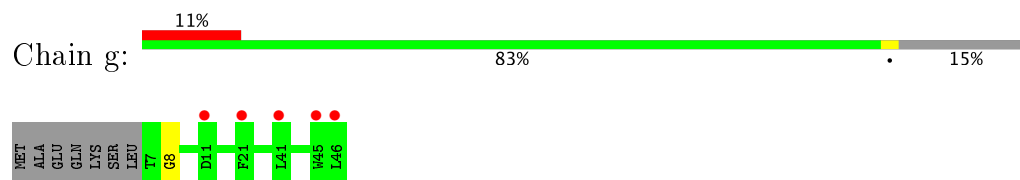




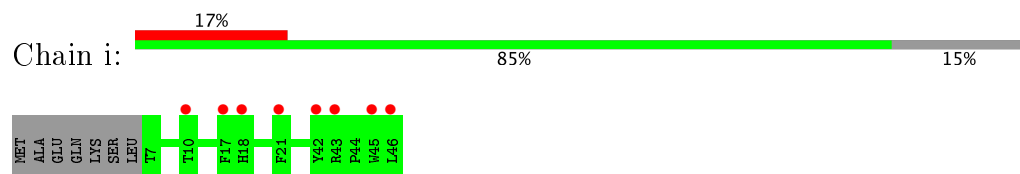
- Molecule 6: LH1 beta polypeptide



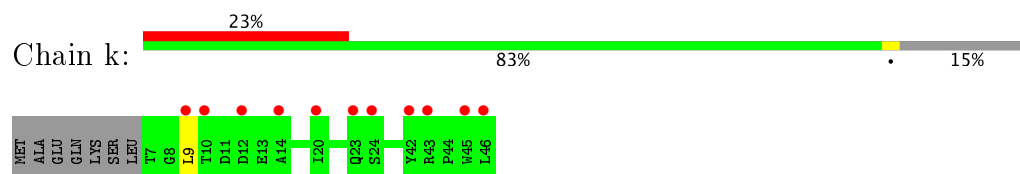
- Molecule 6: LH1 beta polypeptide



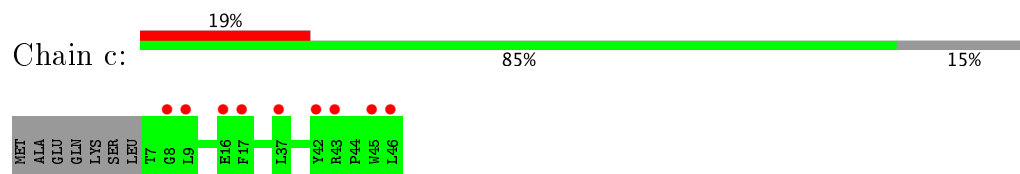
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.89Å 148.95Å 210.23Å 90.00° 108.18° 90.00°	Depositor
Resolution (Å)	48.18 – 3.30 48.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.18-3.30) 98.3 (48.18-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 3.33Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.271 , 0.309 0.272 , 0.310	Depositor DCC
$R_{free}$ test set	7020 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	107.8	Xtrriage
Anisotropy	0.339	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BCL, CRT, PGW, BPH, PO4, UQ8, FE, HEM, MQ8, PEF, SR

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	C	0.86	2/2528 (0.1%)	1.17	10/3451 (0.3%)
1	o	0.83	2/2528 (0.1%)	1.14	10/3451 (0.3%)
2	L	0.90	3/2318 (0.1%)	1.16	7/3167 (0.2%)
2	x	0.89	4/2318 (0.2%)	1.13	8/3167 (0.3%)
3	M	0.83	1/2646 (0.0%)	1.11	10/3621 (0.3%)
3	y	0.83	1/2646 (0.0%)	1.08	10/3621 (0.3%)
4	H	0.83	2/2037 (0.1%)	1.13	7/2776 (0.3%)
4	t	0.91	2/2037 (0.1%)	1.22	10/2776 (0.4%)
5	1	0.58	0/485	0.91	0/664
5	3	0.53	0/485	0.82	0/664
5	5	0.53	0/485	0.77	0/664
5	7	0.47	0/485	0.69	0/664
5	9	0.46	0/485	0.76	0/664
5	A	0.45	0/485	0.76	0/664
5	AA	0.43	0/485	0.75	1/664 (0.2%)
5	AC	0.43	0/485	0.68	0/664
5	AE	0.38	0/491	0.65	0/672
5	AG	0.43	0/485	0.71	1/664 (0.2%)
5	AI	0.49	0/485	0.81	1/664 (0.2%)
5	AK	0.53	0/485	0.80	0/664
5	D	0.46	0/485	0.79	0/664
5	F	0.46	0/485	0.74	0/664
5	I	0.48	0/485	0.73	0/664
5	K	0.42	0/485	0.72	0/664
5	O	0.47	0/485	0.77	0/664
5	Q	0.49	0/485	0.81	1/664 (0.2%)
5	S	0.50	0/491	0.74	1/672 (0.1%)
5	U	0.53	0/485	0.84	1/664 (0.2%)
5	W	0.56	0/485	0.84	0/664
5	Y	0.68	0/485	0.84	1/664 (0.2%)
5	d	0.47	0/485	0.81	1/664 (0.2%)
5	f	0.52	0/485	0.77	0/664



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	h	0.51	0/485	0.76	1/664 (0.2%)
5	j	0.46	0/485	0.68	0/664
5	l	0.48	0/485	0.75	0/664
5	m	0.46	0/485	0.77	0/664
5	p	0.51	0/485	0.81	1/664 (0.2%)
5	r	0.57	0/485	0.75	0/664
5	u	0.49	0/485	0.80	0/664
5	w	0.43	0/485	0.76	0/664
6	0	0.41	0/350	0.70	1/476 (0.2%)
6	2	0.56	0/350	0.70	0/476
6	4	0.53	0/350	0.73	0/476
6	6	0.45	0/350	0.65	0/476
6	8	0.43	0/350	0.68	0/476
6	AB	0.39	0/350	0.67	0/476
6	AD	0.42	0/350	0.60	0/476
6	AF	0.42	0/350	0.62	0/476
6	AH	0.43	0/350	0.64	0/476
6	AJ	0.50	0/350	0.67	0/476
6	AL	0.47	0/350	0.68	0/476
6	B	0.43	0/350	0.65	0/476
6	E	0.47	0/350	0.75	0/476
6	G	0.48	0/350	0.67	0/476
6	J	0.48	0/350	0.71	1/476 (0.2%)
6	N	0.44	0/350	0.73	0/476
6	P	0.45	0/350	0.71	0/476
6	R	0.43	0/350	0.73	0/476
6	T	0.48	0/350	0.73	2/476 (0.4%)
6	V	0.43	0/350	0.64	0/476
6	X	0.56	0/350	0.81	0/476
6	Z	0.51	0/350	0.74	0/476
6	c	0.36	0/350	0.61	0/476
6	e	0.45	0/350	0.66	0/476
6	g	0.44	0/350	0.62	1/476 (0.2%)
6	i	0.50	0/350	0.70	0/476
6	k	0.38	0/350	0.63	1/476 (0.2%)
6	n	0.43	0/350	0.60	0/476
6	q	0.46	0/350	0.75	1/476 (0.2%)
6	s	0.51	0/350	0.79	0/476
6	v	0.46	0/350	0.75	0/476
6	z	0.41	0/350	0.67	0/476
All	All	0.66	17/45790 (0.0%)	0.93	89/62526 (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	C	0	3
2	x	0	1
3	M	0	2
3	y	0	3
4	t	0	1
5	1	0	2
6	AJ	0	2
6	X	0	1
All	All	0	15

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	CYS	CB-SG	-7.73	1.69	1.82
2	L	256	CYS	CB-SG	-7.49	1.69	1.82
3	y	268	TRP	CB-CG	-7.36	1.36	1.50
2	x	41	CYS	CB-SG	-7.27	1.69	1.82
1	C	100	TRP	CB-CG	-6.91	1.37	1.50

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	247	CYS	CA-CB-SG	-10.24	95.56	114.00
1	C	247	CYS	CA-CB-SG	-8.96	97.86	114.00
1	C	195	LEU	CB-CG-CD2	-8.93	95.81	111.00
4	t	29	TYR	CA-CB-CG	8.57	129.69	113.40
1	o	47	ARG	NE-CZ-NH1	8.44	124.52	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	189	THR	Mainchain
1	C	246	GLY	Mainchain
1	C	57	GLN	Sidechain
3	M	272	CYS	Mainchain
3	M	9	THR	Mainchain



## 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	C	2458	0	2385	136	0
1	o	2458	0	2385	0	0
2	L	2231	0	2192	172	0
2	x	2231	0	2192	0	0
3	M	2546	0	2521	219	0
3	y	2546	0	2521	0	0
4	H	1982	0	1981	121	0
4	t	1982	0	1981	0	0
5	1	475	0	486	42	0
5	3	475	0	486	21	0
5	5	475	0	486	22	0
5	7	475	0	486	32	0
5	9	475	0	486	40	0
5	A	475	0	486	30	0
5	AA	475	0	486	17	0
5	AC	475	0	486	19	0
5	AE	481	0	490	36	0
5	AG	475	0	486	24	0
5	AI	475	0	486	24	0
5	AK	475	0	486	22	0
5	D	475	0	486	59	0
5	F	475	0	486	39	0
5	I	475	0	486	41	0
5	K	475	0	486	12	0
5	O	475	0	486	32	0
5	Q	475	0	486	35	0
5	S	481	0	490	34	0
5	U	475	0	486	53	0
5	W	475	0	486	55	0
5	Y	475	0	486	38	0
5	d	475	0	486	0	0
5	f	475	0	486	0	0
5	h	475	0	486	0	0
5	j	475	0	486	0	0
5	l	475	0	486	0	0
5	m	475	0	486	0	0
5	p	475	0	486	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	r	475	0	486	0	0
5	u	475	0	486	0	0
5	w	475	0	486	0	0
6	0	337	0	323	22	0
6	2	337	0	323	20	0
6	4	337	0	323	12	0
6	6	337	0	323	11	0
6	8	337	0	323	15	0
6	AB	337	0	323	13	0
6	AD	337	0	323	18	0
6	AF	337	0	323	15	0
6	AH	337	0	323	20	0
6	AJ	337	0	323	21	0
6	AL	337	0	323	19	0
6	B	337	0	323	31	0
6	E	337	0	323	47	0
6	G	337	0	323	35	0
6	J	337	0	323	27	0
6	N	337	0	323	27	0
6	P	337	0	323	23	0
6	R	337	0	323	25	0
6	T	337	0	323	24	0
6	V	337	0	323	29	0
6	X	337	0	323	24	0
6	Z	337	0	323	31	0
6	c	337	0	323	0	0
6	e	337	0	323	0	0
6	g	337	0	323	0	0
6	i	337	0	323	0	0
6	k	337	0	323	0	0
6	n	337	0	323	0	0
6	q	337	0	323	0	0
6	s	337	0	323	0	0
6	v	337	0	323	0	0
6	z	337	0	323	0	0
7	C	172	0	120	34	0
7	o	172	0	120	0	0
8	1	1	0	0	0	0
8	5	2	0	0	0	0
8	7	1	0	0	0	0
8	9	1	0	0	0	0
8	A	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AA	1	0	0	0	0
8	AC	1	0	0	0	0
8	AE	1	0	0	0	0
8	AI	2	0	0	0	0
8	AK	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	L	2	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	S	1	0	0	0	0
8	U	1	0	0	0	0
8	W	1	0	0	0	0
8	Y	1	0	0	0	0
8	d	1	0	0	0	0
8	f	1	0	0	0	0
8	h	1	0	0	0	0
8	j	1	0	0	0	0
8	l	1	0	0	0	0
8	m	1	0	0	0	0
8	o	1	0	0	0	0
8	p	1	0	0	0	0
8	r	1	0	0	0	0
8	w	2	0	0	0	0
8	x	2	0	0	0	0
9	0	66	0	74	8	0
9	1	132	0	148	16	0
9	3	66	0	74	10	0
9	4	66	0	74	14	0
9	5	132	0	148	14	0
9	7	66	0	74	10	0
9	8	66	0	74	15	0
9	9	66	0	74	10	0
9	A	66	0	74	10	0
9	AA	66	0	74	10	0
9	AB	66	0	74	13	0
9	AC	66	0	74	10	0
9	AD	66	0	74	12	0
9	AE	132	0	148	16	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AH	132	0	148	26	0
9	AI	66	0	74	17	0
9	AJ	66	0	74	7	0
9	AK	66	0	74	12	0
9	AL	66	0	74	16	0
9	B	66	0	74	10	0
9	D	132	0	148	33	0
9	F	66	0	74	18	0
9	G	66	0	74	12	0
9	I	66	0	74	12	0
9	J	66	0	74	13	0
9	K	66	0	74	9	0
9	L	198	0	222	36	0
9	M	66	0	74	13	0
9	N	66	0	74	10	0
9	O	66	0	74	11	0
9	P	66	0	74	9	0
9	Q	66	0	74	7	0
9	R	66	0	74	8	0
9	S	66	0	74	14	0
9	T	66	0	74	14	0
9	U	66	0	74	21	0
9	V	66	0	74	14	0
9	W	66	0	74	31	0
9	X	66	0	74	16	0
9	Y	66	0	74	14	0
9	Z	66	0	74	20	0
9	c	66	0	74	0	0
9	d	66	0	74	0	0
9	e	66	0	74	0	0
9	f	66	0	74	0	0
9	g	66	0	74	0	0
9	h	66	0	74	0	0
9	i	66	0	74	0	0
9	j	66	0	74	0	0
9	k	66	0	74	0	0
9	l	66	0	74	0	0
9	m	132	0	148	0	0
9	p	132	0	148	0	0
9	r	66	0	74	0	0
9	s	66	0	74	0	0
9	u	66	0	74	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	v	66	0	74	0	0
9	w	66	0	74	0	0
9	x	198	0	222	0	0
9	y	66	0	74	0	0
9	z	66	0	74	0	0
10	L	65	0	76	12	0
10	M	65	0	76	15	0
10	x	65	0	76	0	0
10	y	65	0	76	0	0
11	L	53	0	74	17	0
11	x	53	0	74	0	0
12	A	19	0	11	3	0
12	H	57	0	33	13	0
12	L	12	0	9	1	0
12	M	54	0	33	10	0
12	m	19	0	11	0	0
12	p	16	0	11	0	0
12	t	38	0	22	0	0
12	x	19	0	11	0	0
12	y	57	0	33	0	0
13	L	1	0	0	0	0
13	x	1	0	0	0	0
14	M	53	0	72	8	0
14	y	53	0	72	0	0
15	2	44	0	60	13	0
15	4	44	0	60	11	0
15	6	44	0	60	5	0
15	8	44	0	60	14	0
15	9	44	0	60	14	0
15	A	44	0	60	8	0
15	AC	44	0	60	7	0
15	AD	44	0	60	10	0
15	AE	44	0	60	13	0
15	AH	44	0	60	8	0
15	AJ	44	0	60	10	0
15	AL	44	0	60	12	0
15	E	44	0	60	19	0
15	G	44	0	60	10	0
15	J	44	0	60	12	0
15	M	44	0	60	11	0
15	N	44	0	60	26	0
15	P	44	0	60	9	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	R	44	0	60	8	0
15	T	44	0	60	13	0
15	U	44	0	60	5	0
15	X	44	0	60	12	0
15	Z	44	0	60	12	0
15	c	44	0	60	0	0
15	e	44	0	60	0	0
15	f	44	0	60	0	0
15	i	44	0	60	0	0
15	k	44	0	60	0	0
15	n	44	0	60	0	0
15	p	44	0	60	0	0
15	s	44	0	60	0	0
15	v	44	0	60	0	0
15	y	44	0	60	0	0
15	z	44	0	60	0	0
16	H	5	0	0	0	0
16	M	5	0	0	0	0
16	t	5	0	0	0	0
16	y	5	0	0	0	0
17	AE	21	0	12	1	0
17	S	21	0	12	3	0
18	AI	1	0	0	0	0
18	C	1	0	0	0	0
18	L	1	0	0	0	0
18	W	1	0	0	1	0
18	o	1	0	0	0	0
18	x	1	0	0	0	0
All	All	51893	0	52456	1900	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 1900 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)
5:AA:45:ASN:O	5:AA:49:ASP:OD2	1.63	1.16
1:C:307:CYS:SG	7:C:504:HEM:HAB	1.94	1.07
5:Y:5:ASN:OD1	6:2:23:GLN:NE2	1.94	1.00
2:L:46:GLY:HA3	10:L:302:BPH:H9C3	1.46	0.98
4:H:150:ASP:O	4:H:207:ARG:NH2	1.98	0.97



There are no symmetry-related clashes.

## 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	C	315/333 (95%)	276 (88%)	32 (10%)	7 (2%)	8	37
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	6	34
2	L	278/281 (99%)	247 (89%)	27 (10%)	4 (1%)	13	46
2	x	278/281 (99%)	248 (89%)	27 (10%)	3 (1%)	17	52
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	14	48
3	y	316/319 (99%)	284 (90%)	28 (9%)	4 (1%)	14	48
4	H	256/259 (99%)	213 (83%)	34 (13%)	9 (4%)	4	26
4	t	256/259 (99%)	214 (84%)	33 (13%)	9 (4%)	4	26
5	1	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	4	27
5	3	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	10
5	5	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	4	27
5	7	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	4	27
5	9	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	1	10
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	4	27
5	AA	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	11	42
5	AC	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	4	27
5	AE	59/61 (97%)	50 (85%)	6 (10%)	3 (5%)	2	17
5	AG	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	11	42
5	AI	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	11	42
5	AK	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	4	27
5	D	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	4	27
5	F	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	4	27

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	10
5	K	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
5	O	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	11	42
5	Q	58/61 (95%)	47 (81%)	6 (10%)	5 (9%)	1	6
5	S	59/61 (97%)	48 (81%)	8 (14%)	3 (5%)	2	17
5	U	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	11	42
5	W	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	4	27
5	Y	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	4	27
5	d	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	4	27
5	f	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	4	27
5	h	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	16
5	j	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	11	42
5	l	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	4	27
5	m	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	4	27
5	p	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	6
5	r	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1	10
5	u	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	11	42
5	w	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	11	42
6	0	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	6	33
6	2	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	4	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	6	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	8	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AB	38/47 (81%)	38 (100%)	0	0	100	100
6	AD	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AF	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AH	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	AJ	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	AL	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	6	33
6	E	38/47 (81%)	38 (100%)	0	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	38/47 (81%)	38 (100%)	0	0	100	100
6	J	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	6	33
6	P	38/47 (81%)	37 (97%)	0	1 (3%)	6	33
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	0	1 (3%)	6	33
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	6	33
6	Z	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	g	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	i	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	k	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	n	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	q	38/47 (81%)	38 (100%)	0	0	100	100
6	s	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	v	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4736 (88%)	543 (10%)	125 (2%)	7	36

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	SER
1	C	84	ASP
1	C	195	LEU
4	H	38	GLY
4	H	142	PHE

### 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	C	265/278 (95%)	245 (92%)	20 (8%)	16	48
1	o	265/278 (95%)	246 (93%)	19 (7%)	17	50
2	L	228/229 (100%)	215 (94%)	13 (6%)	24	60
2	x	228/229 (100%)	215 (94%)	13 (6%)	24	60
3	M	256/257 (100%)	238 (93%)	18 (7%)	18	52
3	y	256/257 (100%)	238 (93%)	18 (7%)	18	52
4	H	210/211 (100%)	194 (92%)	16 (8%)	15	47
4	t	210/211 (100%)	191 (91%)	19 (9%)	11	39
5	1	52/56 (93%)	50 (96%)	2 (4%)	38	70
5	3	52/56 (93%)	50 (96%)	2 (4%)	38	70
5	5	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	7	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	9	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	A	52/56 (93%)	52 (100%)	0	100	100
5	AA	52/56 (93%)	49 (94%)	3 (6%)	23	59
5	AC	52/56 (93%)	50 (96%)	2 (4%)	38	70
5	AE	53/56 (95%)	52 (98%)	1 (2%)	62	81
5	AG	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	AI	52/56 (93%)	52 (100%)	0	100	100
5	AK	52/56 (93%)	52 (100%)	0	100	100
5	D	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	F	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	I	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	K	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	O	52/56 (93%)	50 (96%)	2 (4%)	38	70
5	Q	52/56 (93%)	49 (94%)	3 (6%)	23	59
5	S	53/56 (95%)	51 (96%)	2 (4%)	38	70
5	U	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	W	52/56 (93%)	50 (96%)	2 (4%)	38	70
5	Y	52/56 (93%)	52 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	d	52/56 (93%)	52 (100%)	0	100	100
5	f	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	h	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	j	52/56 (93%)	50 (96%)	2 (4%)	38	70
5	l	52/56 (93%)	50 (96%)	2 (4%)	38	70
5	m	52/56 (93%)	52 (100%)	0	100	100
5	p	52/56 (93%)	52 (100%)	0	100	100
5	r	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	u	52/56 (93%)	51 (98%)	1 (2%)	62	81
5	w	52/56 (93%)	51 (98%)	1 (2%)	62	81
6	0	33/39 (85%)	33 (100%)	0	100	100
6	2	33/39 (85%)	33 (100%)	0	100	100
6	4	33/39 (85%)	33 (100%)	0	100	100
6	6	33/39 (85%)	33 (100%)	0	100	100
6	8	33/39 (85%)	33 (100%)	0	100	100
6	AB	33/39 (85%)	33 (100%)	0	100	100
6	AD	33/39 (85%)	33 (100%)	0	100	100
6	AF	33/39 (85%)	33 (100%)	0	100	100
6	AH	33/39 (85%)	33 (100%)	0	100	100
6	AJ	33/39 (85%)	32 (97%)	1 (3%)	46	75
6	AL	33/39 (85%)	33 (100%)	0	100	100
6	B	33/39 (85%)	31 (94%)	2 (6%)	22	57
6	E	33/39 (85%)	33 (100%)	0	100	100
6	G	33/39 (85%)	33 (100%)	0	100	100
6	J	33/39 (85%)	33 (100%)	0	100	100
6	N	33/39 (85%)	33 (100%)	0	100	100
6	P	33/39 (85%)	32 (97%)	1 (3%)	46	75
6	R	33/39 (85%)	33 (100%)	0	100	100
6	T	33/39 (85%)	33 (100%)	0	100	100
6	V	33/39 (85%)	33 (100%)	0	100	100
6	X	33/39 (85%)	32 (97%)	1 (3%)	46	75

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Z	33/39 (85%)	33 (100%)	0	100	100
6	c	33/39 (85%)	33 (100%)	0	100	100
6	e	33/39 (85%)	33 (100%)	0	100	100
6	g	33/39 (85%)	33 (100%)	0	100	100
6	i	33/39 (85%)	33 (100%)	0	100	100
6	k	33/39 (85%)	33 (100%)	0	100	100
6	n	33/39 (85%)	33 (100%)	0	100	100
6	q	33/39 (85%)	33 (100%)	0	100	100
6	s	33/39 (85%)	33 (100%)	0	100	100
6	v	33/39 (85%)	33 (100%)	0	100	100
6	z	33/39 (85%)	33 (100%)	0	100	100
All	All	4640/4990 (93%)	4462 (96%)	178 (4%)	38	70

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	S	51	ILE
1	o	128	ARG
5	AA	5	ASN
5	W	9	TYR
5	7	48	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
5	Y	56	GLN
2	x	182	HIS
6	e	23	GLN
6	Z	23	GLN
6	2	23	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 40 are monoatomic - leaving 144 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	$\# Z  > 2$
9	BCL	0	101	-	55,74,74	1.81	11 (20%)	65,115,115	2.17	21 (32%)
9	BCL	1	101	-	55,74,74	1.87	11 (20%)	65,115,115	2.20	20 (30%)
9	BCL	1	102	-	55,74,74	1.82	12 (21%)	65,115,115	2.08	15 (23%)
15	CRT	2	101	-	41,43,43	0.74	0	54,54,54	1.83	18 (33%)
9	BCL	3	101	-	55,74,74	1.78	12 (21%)	65,115,115	2.24	22 (33%)
15	CRT	4	101	-	41,43,43	0.72	0	54,54,54	3.78	24 (44%)
9	BCL	4	102	-	55,74,74	1.82	12 (21%)	65,115,115	2.30	26 (40%)
9	BCL	5	101	-	55,74,74	1.79	10 (18%)	65,115,115	2.21	23 (35%)
9	BCL	5	102	-	55,74,74	1.90	12 (21%)	65,115,115	2.48	29 (44%)
15	CRT	6	101	-	41,43,43	0.80	0	54,54,54	3.50	21 (38%)
9	BCL	7	101	-	55,74,74	1.87	11 (20%)	65,115,115	2.03	23 (35%)
15	CRT	8	101	-	41,43,43	0.84	0	54,54,54	3.32	11 (20%)
9	BCL	8	102	-	55,74,74	1.85	9 (16%)	65,115,115	2.23	21 (32%)
15	CRT	9	102	-	41,43,43	0.75	0	54,54,54	3.56	19 (35%)
9	BCL	9	103	-	55,74,74	1.78	10 (18%)	65,115,115	2.09	20 (30%)
12	PEF	A	101	-	18,18,46	1.53	2 (11%)	20,23,51	1.75	3 (15%)
9	BCL	A	102	-	55,74,74	1.89	9 (16%)	65,115,115	2.10	21 (32%)
15	CRT	A	103	-	41,43,43	0.78	0	54,54,54	3.37	19 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	BCL	AA	101	-	55,74,74	1.85	10 (18%)	65,115,115	2.12	22 (33%)
9	BCL	AB	101	-	55,74,74	1.84	9 (16%)	65,115,115	2.31	25 (38%)
15	CRT	AC	101	-	41,43,43	0.73	0	54,54,54	2.03	13 (24%)
9	BCL	AC	102	-	55,74,74	1.84	10 (18%)	65,115,115	2.09	21 (32%)
9	BCL	AD	101	-	55,74,74	1.85	9 (16%)	65,115,115	2.04	21 (32%)
15	CRT	AD	102	-	41,43,43	0.77	0	54,54,54	3.42	17 (31%)
17	PGW	AE	101	-	20,20,50	1.03	1 (5%)	21,26,56	1.36	2 (9%)
9	BCL	AE	102	-	55,74,74	1.83	10 (18%)	65,115,115	2.10	24 (36%)
15	CRT	AE	103	-	41,43,43	0.73	0	54,54,54	3.54	18 (33%)
9	BCL	AE	104	-	55,74,74	1.81	10 (18%)	65,115,115	2.21	23 (35%)
9	BCL	AH	101	-	55,74,74	1.84	11 (20%)	65,115,115	2.27	22 (33%)
15	CRT	AH	102	-	41,43,43	0.74	0	54,54,54	3.37	18 (33%)
9	BCL	AH	103	-	55,74,74	1.98	11 (20%)	65,115,115	2.17	26 (40%)
9	BCL	AI	101	-	55,74,74	1.81	9 (16%)	65,115,115	2.20	21 (32%)
15	CRT	AJ	101	-	41,43,43	0.74	0	54,54,54	2.21	17 (31%)
9	BCL	AJ	102	-	55,74,74	1.84	10 (18%)	65,115,115	2.26	18 (27%)
9	BCL	AK	101	-	55,74,74	1.86	10 (18%)	65,115,115	2.23	24 (36%)
15	CRT	AL	101	-	41,43,43	0.75	0	54,54,54	1.73	15 (27%)
9	BCL	AL	102	-	55,74,74	1.93	11 (20%)	65,115,115	2.17	21 (32%)
9	BCL	B	101	-	55,74,74	1.78	10 (18%)	65,115,115	2.04	21 (32%)
7	HEM	C	501	1	28,50,50	1.79	7 (25%)	17,82,82	3.16	9 (52%)
7	HEM	C	502	1	28,50,50	1.71	5 (17%)	17,82,82	2.24	7 (41%)
7	HEM	C	503	1	28,50,50	1.09	1 (3%)	17,82,82	2.13	4 (23%)
7	HEM	C	504	1	28,50,50	1.26	3 (10%)	17,82,82	1.83	5 (29%)
9	BCL	D	101	-	55,74,74	1.84	10 (18%)	65,115,115	2.20	23 (35%)
9	BCL	D	102	-	55,74,74	1.83	9 (16%)	65,115,115	2.32	26 (40%)
15	CRT	E	101	-	41,43,43	0.79	0	54,54,54	3.37	19 (35%)
9	BCL	F	101	-	55,74,74	1.81	10 (18%)	65,115,115	2.22	26 (40%)
15	CRT	G	101	-	41,43,43	0.72	0	54,54,54	3.60	20 (37%)
9	BCL	G	102	-	55,74,74	1.84	9 (16%)	65,115,115	2.20	29 (44%)
12	PEF	H	301	-	18,18,46	1.55	2 (11%)	20,23,51	1.80	3 (15%)
16	PO4	H	302	-	4,4,4	0.70	0	6,6,6	0.49	0
12	PEF	H	303	-	18,18,46	1.50	2 (11%)	20,23,51	1.35	2 (10%)
12	PEF	H	304	-	18,18,46	1.58	3 (16%)	20,23,51	1.83	5 (25%)
9	BCL	I	101	-	55,74,74	1.80	10 (18%)	65,115,115	2.18	22 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CRT	J	101	-	41,43,43	0.75	0	54,54,54	3.72	22 (40%)
9	BCL	J	102	-	55,74,74	1.84	10 (18%)	65,115,115	2.08	22 (33%)
9	BCL	K	101	-	55,74,74	1.81	11 (20%)	65,115,115	2.15	25 (38%)
9	BCL	L	301	-	55,74,74	2.05	13 (23%)	65,115,115	2.38	24 (36%)
10	BPH	L	302	-	65,70,70	0.84	4 (6%)	75,101,101	1.77	17 (22%)
9	BCL	L	303	-	55,74,74	1.93	11 (20%)	65,115,115	2.38	22 (33%)
11	UQ8	L	304	-	53,53,53	1.35	7 (13%)	64,67,67	1.73	19 (29%)
9	BCL	L	305	-	55,74,74	1.79	11 (20%)	65,115,115	2.26	26 (40%)
12	PEF	L	306	-	11,11,46	0.77	0	10,14,51	1.47	1 (10%)
9	BCL	M	401	-	55,74,74	2.05	13 (23%)	65,115,115	2.65	26 (40%)
10	BPH	M	402	-	65,70,70	0.98	4 (6%)	75,101,101	1.94	19 (25%)
14	MQ8	M	403	-	54,54,54	1.07	2 (3%)	67,69,69	1.56	13 (19%)
15	CRT	M	404	-	41,43,43	0.83	0	54,54,54	3.57	15 (27%)
16	PO4	M	405	-	4,4,4	0.51	0	6,6,6	0.93	0
12	PEF	M	406	-	18,18,46	1.42	2 (11%)	20,23,51	2.24	4 (20%)
12	PEF	M	407	-	15,15,46	1.03	1 (6%)	16,19,51	1.22	1 (6%)
12	PEF	M	408	-	18,18,46	1.63	2 (11%)	20,23,51	1.92	3 (15%)
15	CRT	N	101	-	41,43,43	0.80	0	54,54,54	3.90	22 (40%)
9	BCL	N	102	-	55,74,74	1.84	10 (18%)	65,115,115	2.11	18 (27%)
9	BCL	O	101	-	55,74,74	1.77	9 (16%)	65,115,115	2.31	26 (40%)
9	BCL	P	101	-	55,74,74	1.84	11 (20%)	65,115,115	2.23	24 (36%)
15	CRT	P	102	-	41,43,43	0.77	0	54,54,54	2.03	17 (31%)
9	BCL	Q	101	-	55,74,74	1.87	11 (20%)	65,115,115	2.13	26 (40%)
15	CRT	R	101	-	41,43,43	0.74	0	54,54,54	3.37	21 (38%)
9	BCL	R	102	-	55,74,74	1.84	10 (18%)	65,115,115	2.09	22 (33%)
17	PGW	S	101	-	20,20,50	1.06	1 (5%)	21,26,56	1.29	3 (14%)
9	BCL	S	102	-	55,74,74	1.80	11 (20%)	65,115,115	2.19	24 (36%)
15	CRT	T	101	-	41,43,43	0.82	0	54,54,54	3.94	26 (48%)
9	BCL	T	102	-	55,74,74	1.89	10 (18%)	65,115,115	2.17	25 (38%)
9	BCL	U	101	-	55,74,74	1.92	9 (16%)	65,115,115	2.14	21 (32%)
15	CRT	U	102	-	41,43,43	0.72	0	54,54,54	3.40	21 (38%)
9	BCL	V	101	-	55,74,74	1.94	12 (21%)	65,115,115	2.17	23 (35%)
9	BCL	W	101	-	55,74,74	1.92	12 (21%)	65,115,115	2.14	22 (33%)
15	CRT	X	101	-	41,43,43	0.85	0	54,54,54	1.88	11 (20%)
9	BCL	X	102	-	55,74,74	1.94	10 (18%)	65,115,115	2.12	25 (38%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	BCL	Y	101	-	55,74,74	1.91	11 (20%)	65,115,115	2.43	23 (35%)
15	CRT	Z	101	-	41,43,43	0.86	0	54,54,54	1.95	15 (27%)
9	BCL	Z	102	-	55,74,74	1.90	11 (20%)	65,115,115	2.21	23 (35%)
15	CRT	c	101	-	41,43,43	0.76	0	54,54,54	3.41	21 (38%)
9	BCL	c	102	-	55,74,74	1.83	9 (16%)	65,115,115	2.15	25 (38%)
9	BCL	d	101	-	55,74,74	1.82	10 (18%)	65,115,115	2.17	23 (35%)
15	CRT	e	101	-	41,43,43	0.76	0	54,54,54	1.87	14 (25%)
9	BCL	e	102	-	55,74,74	1.83	11 (20%)	65,115,115	2.19	24 (36%)
9	BCL	f	101	-	55,74,74	1.79	11 (20%)	65,115,115	2.26	20 (30%)
15	CRT	f	102	-	41,43,43	0.87	0	54,54,54	3.70	24 (44%)
9	BCL	g	101	-	55,74,74	1.86	10 (18%)	65,115,115	2.21	25 (38%)
9	BCL	h	101	-	55,74,74	1.95	12 (21%)	65,115,115	2.11	24 (36%)
15	CRT	i	101	-	41,43,43	0.80	0	54,54,54	3.36	16 (29%)
9	BCL	i	102	-	55,74,74	1.87	12 (21%)	65,115,115	2.06	20 (30%)
9	BCL	j	101	-	55,74,74	1.83	9 (16%)	65,115,115	2.16	20 (30%)
15	CRT	k	101	-	41,43,43	0.77	1 (2%)	54,54,54	3.45	18 (33%)
9	BCL	k	102	-	55,74,74	1.87	10 (18%)	65,115,115	2.22	24 (36%)
9	BCL	l	101	-	55,74,74	1.83	10 (18%)	65,115,115	2.21	24 (36%)
12	PEF	m	101	-	18,18,46	1.63	2 (11%)	20,23,51	1.59	3 (15%)
9	BCL	m	102	-	55,74,74	1.91	13 (23%)	65,115,115	2.13	20 (30%)
9	BCL	m	103	-	55,74,74	1.90	11 (20%)	65,115,115	2.31	24 (36%)
15	CRT	n	101	-	41,43,43	0.79	0	54,54,54	3.65	18 (33%)
7	HEM	o	501	1	28,50,50	1.29	5 (17%)	17,82,82	2.24	4 (23%)
7	HEM	o	502	1	28,50,50	1.68	6 (21%)	17,82,82	2.24	8 (47%)
7	HEM	o	503	1	28,50,50	1.04	1 (3%)	17,82,82	2.05	6 (35%)
7	HEM	o	504	1	28,50,50	1.20	2 (7%)	17,82,82	1.73	5 (29%)
12	PEF	p	101	-	15,15,46	0.91	1 (6%)	16,19,51	0.83	1 (6%)
9	BCL	p	102	-	55,74,74	1.76	9 (16%)	65,115,115	2.09	18 (27%)
15	CRT	p	103	-	41,43,43	0.70	0	54,54,54	3.67	19 (35%)
9	BCL	p	104	-	55,74,74	1.88	12 (21%)	65,115,115	2.38	29 (44%)
9	BCL	r	101	-	55,74,74	1.86	12 (21%)	65,115,115	2.07	19 (29%)
15	CRT	s	101	-	41,43,43	0.70	0	54,54,54	3.55	18 (33%)
9	BCL	s	102	-	55,74,74	1.84	12 (21%)	65,115,115	2.26	20 (30%)
12	PEF	t	301	-	18,18,46	1.48	2 (11%)	20,23,51	1.33	4 (20%)
16	PO4	t	302	-	4,4,4	0.40	0	6,6,6	1.70	2 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	PEF	t	303	-	18,18,46	1.48	3 (16%)	20,23,51	2.39	9 (45%)
9	BCL	u	101	-	55,74,74	1.90	12 (21%)	65,115,115	2.07	24 (36%)
15	CRT	v	101	-	41,43,43	0.76	0	54,54,54	3.82	22 (40%)
9	BCL	v	102	-	55,74,74	1.81	11 (20%)	65,115,115	2.18	26 (40%)
9	BCL	w	101	-	55,74,74	1.89	11 (20%)	65,115,115	2.16	23 (35%)
9	BCL	x	301	-	55,74,74	2.08	13 (23%)	65,115,115	2.31	25 (38%)
10	BPH	x	302	-	65,70,70	1.01	5 (7%)	75,101,101	1.83	16 (21%)
9	BCL	x	303	-	55,74,74	1.85	11 (20%)	65,115,115	2.37	21 (32%)
11	UQ8	x	304	-	53,53,53	1.37	3 (5%)	64,67,67	2.16	26 (40%)
9	BCL	x	305	-	55,74,74	1.91	12 (21%)	65,115,115	2.27	28 (43%)
12	PEF	x	306	-	18,18,46	1.70	2 (11%)	20,23,51	1.41	3 (15%)
9	BCL	y	401	-	55,74,74	1.88	11 (20%)	65,115,115	2.46	27 (41%)
10	BPH	y	402	-	65,70,70	1.01	6 (9%)	75,101,101	1.83	15 (20%)
14	MQ8	y	403	-	54,54,54	1.17	6 (11%)	67,69,69	1.64	13 (19%)
15	CRT	y	404	-	41,43,43	0.93	1 (2%)	54,54,54	3.51	19 (35%)
16	PO4	y	405	-	4,4,4	0.71	0	6,6,6	0.46	0
12	PEF	y	406	-	18,18,46	1.54	2 (11%)	20,23,51	1.73	3 (15%)
12	PEF	y	407	-	18,18,46	1.80	2 (11%)	20,23,51	1.59	2 (10%)
12	PEF	y	408	-	18,18,46	1.75	3 (16%)	20,23,51	2.03	5 (25%)
15	CRT	z	101	-	41,43,43	0.71	0	54,54,54	3.55	18 (33%)
9	BCL	z	102	-	55,74,74	1.85	10 (18%)	65,115,115	2.17	22 (33%)

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
9	BCL	0	101	-	-	0/37/137/137	0/0/9/9
9	BCL	1	101	-	-	0/37/137/137	0/0/9/9
9	BCL	1	102	-	-	0/37/137/137	0/0/9/9
15	CRT	2	101	-	-	0/51/51/51	0/0/0/0
9	BCL	3	101	-	-	0/37/137/137	0/0/9/9
15	CRT	4	101	-	-	0/51/51/51	0/0/0/0
9	BCL	4	102	-	-	0/37/137/137	0/0/9/9
9	BCL	5	101	-	-	0/37/137/137	0/0/9/9
9	BCL	5	102	-	-	1/37/137/137	0/0/9/9
15	CRT	6	101	-	-	0/51/51/51	0/0/0/0

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	7	101	-	-	0/37/137/137	0/0/9/9
15	CRT	8	101	-	-	0/51/51/51	0/0/0/0
9	BCL	8	102	-	-	1/37/137/137	0/0/9/9
15	CRT	9	102	-	-	0/51/51/51	0/0/0/0
9	BCL	9	103	-	-	0/37/137/137	0/0/9/9
12	PEF	A	101	-	-	0/20/20/50	0/0/0/0
9	BCL	A	102	-	-	0/37/137/137	0/0/9/9
15	CRT	A	103	-	-	0/51/51/51	0/0/0/0
9	BCL	AA	101	-	-	0/37/137/137	0/0/9/9
9	BCL	AB	101	-	-	1/37/137/137	0/0/9/9
15	CRT	AC	101	-	-	0/51/51/51	0/0/0/0
9	BCL	AC	102	-	-	0/37/137/137	0/0/9/9
9	BCL	AD	101	-	-	0/37/137/137	0/0/9/9
15	CRT	AD	102	-	-	0/51/51/51	0/0/0/0
17	PGW	AE	101	-	-	0/23/23/55	0/0/0/0
9	BCL	AE	102	-	-	0/37/137/137	0/0/9/9
15	CRT	AE	103	-	-	0/51/51/51	0/0/0/0
9	BCL	AE	104	-	-	1/37/137/137	0/0/9/9
9	BCL	AH	101	-	-	0/37/137/137	0/0/9/9
15	CRT	AH	102	-	-	0/51/51/51	0/0/0/0
9	BCL	AH	103	-	-	0/37/137/137	0/0/9/9
9	BCL	AI	101	-	-	0/37/137/137	0/0/9/9
15	CRT	AJ	101	-	-	0/51/51/51	0/0/0/0
9	BCL	AJ	102	-	-	0/37/137/137	0/0/9/9
9	BCL	AK	101	-	-	0/37/137/137	0/0/9/9
15	CRT	AL	101	-	-	0/51/51/51	0/0/0/0
9	BCL	AL	102	-	-	0/37/137/137	0/0/9/9
9	BCL	B	101	-	-	0/37/137/137	0/0/9/9
7	HEM	C	501	1	-	0/6/54/54	0/0/8/8
7	HEM	C	502	1	-	0/6/54/54	0/0/8/8
7	HEM	C	503	1	-	0/6/54/54	0/0/8/8
7	HEM	C	504	1	-	0/6/54/54	0/0/8/8
9	BCL	D	101	-	-	0/37/137/137	0/0/9/9
9	BCL	D	102	-	-	1/37/137/137	0/0/9/9
15	CRT	E	101	-	-	0/51/51/51	0/0/0/0
9	BCL	F	101	-	-	0/37/137/137	0/0/9/9
15	CRT	G	101	-	-	0/51/51/51	0/0/0/0
9	BCL	G	102	-	-	0/37/137/137	0/0/9/9
12	PEF	H	301	-	-	0/20/20/50	0/0/0/0
16	PO4	H	302	-	-	0/0/0/0	0/0/0/0
12	PEF	H	303	-	-	0/20/20/50	0/0/0/0
12	PEF	H	304	-	-	0/20/20/50	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	I	101	-	-	0/37/137/137	0/0/9/9
15	CRT	J	101	-	-	0/51/51/51	0/0/0/0
9	BCL	J	102	-	-	1/37/137/137	0/0/9/9
9	BCL	K	101	-	-	0/37/137/137	0/0/9/9
9	BCL	L	301	-	-	0/37/137/137	0/0/9/9
10	BPH	L	302	-	-	0/54/105/105	0/1/6/6
9	BCL	L	303	-	-	0/37/137/137	0/0/9/9
11	UQ8	L	304	-	-	0/51/75/75	0/1/1/1
9	BCL	L	305	-	-	0/37/137/137	0/0/9/9
12	PEF	L	306	-	-	0/11/11/50	0/0/0/0
9	BCL	M	401	-	-	0/37/137/137	0/0/9/9
10	BPH	M	402	-	-	0/54/105/105	0/1/6/6
14	MQ8	M	403	-	-	0/47/67/67	0/2/2/2
15	CRT	M	404	-	-	0/51/51/51	0/0/0/0
16	PO4	M	405	-	-	0/0/0/0	0/0/0/0
12	PEF	M	406	-	-	0/20/20/50	0/0/0/0
12	PEF	M	407	-	-	0/16/16/50	0/0/0/0
12	PEF	M	408	-	-	0/20/20/50	0/0/0/0
15	CRT	N	101	-	-	0/51/51/51	0/0/0/0
9	BCL	N	102	-	-	1/37/137/137	0/0/9/9
9	BCL	O	101	-	-	1/37/137/137	0/0/9/9
9	BCL	P	101	-	-	0/37/137/137	0/0/9/9
15	CRT	P	102	-	-	0/51/51/51	0/0/0/0
9	BCL	Q	101	-	-	0/37/137/137	0/0/9/9
15	CRT	R	101	-	-	0/51/51/51	0/0/0/0
9	BCL	R	102	-	-	0/37/137/137	0/0/9/9
17	PGW	S	101	-	-	0/23/23/55	0/0/0/0
9	BCL	S	102	-	-	0/37/137/137	0/0/9/9
15	CRT	T	101	-	-	0/51/51/51	0/0/0/0
9	BCL	T	102	-	-	1/37/137/137	0/0/9/9
9	BCL	U	101	-	-	0/37/137/137	0/0/9/9
15	CRT	U	102	-	-	0/51/51/51	0/0/0/0
9	BCL	V	101	-	-	0/37/137/137	0/0/9/9
9	BCL	W	101	-	-	0/37/137/137	0/0/9/9
15	CRT	X	101	-	-	0/51/51/51	0/0/0/0
9	BCL	X	102	-	-	1/37/137/137	0/0/9/9
9	BCL	Y	101	-	-	0/37/137/137	0/0/9/9
15	CRT	Z	101	-	-	0/51/51/51	0/0/0/0
9	BCL	Z	102	-	-	0/37/137/137	0/0/9/9
15	CRT	c	101	-	-	0/51/51/51	0/0/0/0
9	BCL	c	102	-	-	0/37/137/137	0/0/9/9
9	BCL	d	101	-	-	0/37/137/137	0/0/9/9

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	e	101	-	-	0/51/51/51	0/0/0/0
9	BCL	e	102	-	-	0/37/137/137	0/0/9/9
9	BCL	f	101	-	-	0/37/137/137	0/0/9/9
15	CRT	f	102	-	-	0/51/51/51	0/0/0/0
9	BCL	g	101	-	-	1/37/137/137	0/0/9/9
9	BCL	h	101	-	-	0/37/137/137	0/0/9/9
15	CRT	i	101	-	-	0/51/51/51	0/0/0/0
9	BCL	i	102	-	-	0/37/137/137	0/0/9/9
9	BCL	j	101	-	-	0/37/137/137	0/0/9/9
15	CRT	k	101	-	-	0/51/51/51	0/0/0/0
9	BCL	k	102	-	-	0/37/137/137	0/0/9/9
9	BCL	l	101	-	-	0/37/137/137	0/0/9/9
12	PEF	m	101	-	-	0/20/20/50	0/0/0/0
9	BCL	m	102	-	-	0/37/137/137	0/0/9/9
9	BCL	m	103	-	-	0/37/137/137	0/0/9/9
15	CRT	n	101	-	-	0/51/51/51	0/0/0/0
7	HEM	o	501	1	-	0/6/54/54	0/0/8/8
7	HEM	o	502	1	-	0/6/54/54	0/0/8/8
7	HEM	o	503	1	-	0/6/54/54	0/0/8/8
7	HEM	o	504	1	-	0/6/54/54	0/0/8/8
12	PEF	p	101	-	-	0/16/16/50	0/0/0/0
9	BCL	p	102	-	-	0/37/137/137	0/0/9/9
15	CRT	p	103	-	-	0/51/51/51	0/0/0/0
9	BCL	p	104	-	-	0/37/137/137	0/0/9/9
9	BCL	r	101	-	-	0/37/137/137	0/0/9/9
15	CRT	s	101	-	-	0/51/51/51	0/0/0/0
9	BCL	s	102	-	-	0/37/137/137	0/0/9/9
12	PEF	t	301	-	-	0/20/20/50	0/0/0/0
16	PO4	t	302	-	-	0/0/0/0	0/0/0/0
12	PEF	t	303	-	-	0/20/20/50	0/0/0/0
9	BCL	u	101	-	-	0/37/137/137	0/0/9/9
15	CRT	v	101	-	-	0/51/51/51	0/0/0/0
9	BCL	v	102	-	-	0/37/137/137	0/0/9/9
9	BCL	w	101	-	-	0/37/137/137	0/0/9/9
9	BCL	x	301	-	-	0/37/137/137	0/0/9/9
10	BPH	x	302	-	-	0/54/105/105	0/1/6/6
9	BCL	x	303	-	-	0/37/137/137	0/0/9/9
11	UQ8	x	304	-	-	0/51/75/75	0/1/1/1
9	BCL	x	305	-	-	0/37/137/137	0/0/9/9
12	PEF	x	306	-	-	0/20/20/50	0/0/0/0
9	BCL	y	401	-	-	0/37/137/137	0/0/9/9
10	BPH	y	402	-	-	0/54/105/105	0/1/6/6

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MQ8	y	403	-	-	0/47/67/67	0/2/2/2
15	CRT	y	404	-	-	0/51/51/51	0/0/0/0
16	PO4	y	405	-	-	0/0/0/0	0/0/0/0
12	PEF	y	406	-	-	0/20/20/50	0/0/0/0
12	PEF	y	407	-	-	0/20/20/50	0/0/0/0
12	PEF	y	408	-	-	0/20/20/50	0/0/0/0
15	CRT	z	101	-	-	0/51/51/51	0/0/0/0
9	BCL	z	102	-	-	1/37/137/137	0/0/9/9

The worst 5 of 869 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	502	HEM	C3B-C2B	-4.92	1.33	1.40
7	C	501	HEM	C4D-ND	-4.90	1.31	1.36
9	x	305	BCL	O1D-CGD	-4.37	1.10	1.21
10	x	302	BPH	C1C-NC	-4.31	1.28	1.37
9	L	303	BCL	O1D-CGD	-4.30	1.10	1.21

The worst 5 of 2529 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	404	CRT	C2-C1-C4	-17.57	81.03	110.90
15	T	101	CRT	C3-C1-C4	-17.33	81.43	110.90
15	4	101	CRT	C3-C1-C4	-16.46	82.92	110.90
15	s	101	CRT	C2-C1-C4	-16.35	83.10	110.90
15	A	103	CRT	C2-C1-C4	-15.45	84.63	110.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	8	102	BCL	O2A-C1-C2-C3
9	T	102	BCL	CED-O2D-CGD-CBD
9	J	102	BCL	CED-O2D-CGD-CBD
9	5	102	BCL	CED-O2D-CGD-CBD
9	D	102	BCL	CED-O2D-CGD-CBD

There are no ring outliers.

89 monomers are involved in 868 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	0	101	BCL	8	0
9	1	101	BCL	8	0
9	1	102	BCL	8	0
15	2	101	CRT	13	0
9	3	101	BCL	10	0
15	4	101	CRT	11	0
9	4	102	BCL	14	0
9	5	101	BCL	9	0
9	5	102	BCL	5	0
15	6	101	CRT	5	0
9	7	101	BCL	10	0
15	8	101	CRT	14	0
9	8	102	BCL	15	0
15	9	102	CRT	14	0
9	9	103	BCL	10	0
12	A	101	PEF	3	0
9	A	102	BCL	10	0
15	A	103	CRT	8	0
9	AA	101	BCL	10	0
9	AB	101	BCL	13	0
15	AC	101	CRT	7	0
9	AC	102	BCL	10	0
9	AD	101	BCL	12	0
15	AD	102	CRT	10	0
17	AE	101	PGW	1	0
9	AE	102	BCL	7	0
15	AE	103	CRT	13	0
9	AE	104	BCL	9	0
9	AH	101	BCL	13	0
15	AH	102	CRT	8	0
9	AH	103	BCL	13	0
9	AI	101	BCL	17	0
15	AJ	101	CRT	10	0
9	AJ	102	BCL	7	0
9	AK	101	BCL	12	0
15	AL	101	CRT	12	0
9	AL	102	BCL	16	0
9	B	101	BCL	10	0
7	C	501	HEM	10	0
7	C	502	HEM	5	0
7	C	503	HEM	8	0
7	C	504	HEM	11	0
9	D	101	BCL	25	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	102	BCL	9	0
15	E	101	CRT	19	0
9	F	101	BCL	18	0
15	G	101	CRT	10	0
9	G	102	BCL	12	0
12	H	301	PEF	4	0
12	H	303	PEF	3	0
12	H	304	PEF	6	0
9	I	101	BCL	12	0
15	J	101	CRT	12	0
9	J	102	BCL	13	0
9	K	101	BCL	9	0
9	L	301	BCL	15	0
10	L	302	BPH	12	0
9	L	303	BCL	14	0
11	L	304	UQ8	17	0
9	L	305	BCL	9	0
12	L	306	PEF	1	0
9	M	401	BCL	13	0
10	M	402	BPH	15	0
14	M	403	MQ8	8	0
15	M	404	CRT	11	0
12	M	406	PEF	2	0
12	M	407	PEF	5	0
12	M	408	PEF	4	0
15	N	101	CRT	26	0
9	N	102	BCL	10	0
9	O	101	BCL	11	0
9	P	101	BCL	9	0
15	P	102	CRT	9	0
9	Q	101	BCL	7	0
15	R	101	CRT	8	0
9	R	102	BCL	8	0
17	S	101	PGW	3	0
9	S	102	BCL	14	0
15	T	101	CRT	13	0
9	T	102	BCL	14	0
9	U	101	BCL	21	0
15	U	102	CRT	5	0
9	V	101	BCL	14	0
9	W	101	BCL	31	0
15	X	101	CRT	12	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	102	BCL	16	0
9	Y	101	BCL	14	0
15	Z	101	CRT	12	0
9	Z	102	BCL	20	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	317/333 (95%)	0.50	37 (11%) 5 4	79, 112, 143, 161	0
1	o	317/333 (95%)	0.63	46 (14%) 3 2	96, 133, 172, 190	0
2	L	280/281 (99%)	0.35	18 (6%) 20 20	60, 95, 154, 189	0
2	x	280/281 (99%)	0.36	18 (6%) 20 20	63, 97, 147, 181	0
3	M	318/319 (99%)	0.28	12 (3%) 41 37	65, 100, 140, 160	0
3	y	318/319 (99%)	0.30	14 (4%) 35 33	61, 111, 158, 187	0
4	H	258/259 (99%)	0.41	28 (10%) 6 5	77, 105, 171, 274	0
4	t	258/259 (99%)	0.55	31 (12%) 5 4	77, 106, 143, 251	0
5	1	60/61 (98%)	0.88	11 (18%) 1 1	130, 158, 212, 237	0
5	3	60/61 (98%)	1.29	14 (23%) 1 1	129, 157, 225, 232	0
5	5	60/61 (98%)	0.89	9 (15%) 3 2	137, 174, 239, 244	0
5	7	60/61 (98%)	2.00	20 (33%) 0 1	159, 188, 259, 272	0
5	9	60/61 (98%)	1.87	19 (31%) 0 1	163, 204, 239, 243	0
5	A	60/61 (98%)	2.48	22 (36%) 0 1	170, 210, 257, 260	0
5	AA	60/61 (98%)	2.08	23 (38%) 0 0	165, 216, 280, 292	0
5	AC	60/61 (98%)	1.97	20 (33%) 0 1	176, 225, 276, 279	0
5	AE	60/61 (98%)	1.91	21 (35%) 0 1	191, 230, 263, 270	0
5	AG	60/61 (98%)	1.16	13 (21%) 1 1	177, 216, 274, 278	0
5	AI	60/61 (98%)	1.42	17 (28%) 1 1	159, 194, 255, 261	0
5	AK	60/61 (98%)	0.88	11 (18%) 1 1	151, 180, 247, 264	0
5	D	60/61 (98%)	2.24	27 (45%) 0 0	170, 217, 266, 269	0
5	F	60/61 (98%)	1.86	21 (35%) 0 1	174, 215, 261, 264	0
5	I	60/61 (98%)	1.79	19 (31%) 0 1	179, 222, 268, 269	0
5	K	60/61 (98%)	2.23	18 (30%) 1 1	164, 214, 288, 303	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )		Q<0.9
5	O	60/61 (98%)	1.70	14 (23%)	1	1	143, 195, 279, 284
5	Q	60/61 (98%)	1.24	13 (21%)	1	1	139, 185, 264, 270
5	S	60/61 (98%)	2.29	19 (31%)	0	1	153, 193, 256, 260
5	U	60/61 (98%)	1.03	10 (16%)	2	2	138, 179, 250, 256
5	W	60/61 (98%)	1.04	13 (21%)	1	1	126, 164, 228, 235
5	Y	60/61 (98%)	1.93	18 (30%)	1	1	123, 153, 233, 264
5	d	60/61 (98%)	1.21	15 (25%)	1	1	147, 181, 240, 252
5	f	60/61 (98%)	1.26	17 (28%)	1	1	157, 180, 247, 253
5	h	60/61 (98%)	1.56	15 (25%)	1	1	154, 189, 257, 267
5	j	60/61 (98%)	1.27	13 (21%)	1	1	157, 191, 243, 257
5	l	60/61 (98%)	1.82	21 (35%)	0	1	147, 187, 241, 251
5	m	60/61 (98%)	1.89	20 (33%)	0	1	146, 186, 255, 259
5	p	60/61 (98%)	1.56	19 (31%)	0	1	135, 189, 258, 262
5	r	60/61 (98%)	1.42	14 (23%)	1	1	139, 186, 274, 280
5	u	60/61 (98%)	1.69	17 (28%)	1	1	156, 202, 257, 263
5	w	60/61 (98%)	1.54	22 (36%)	0	1	168, 218, 271, 277
6	0	40/47 (85%)	0.73	9 (22%)	1	1	178, 236, 246, 250
6	2	40/47 (85%)	0.56	6 (15%)	3	2	164, 177, 210, 219
6	4	40/47 (85%)	-0.14	2 (5%)	30	27	166, 181, 200, 210
6	6	40/47 (85%)	0.41	5 (12%)	4	4	178, 203, 222, 224
6	8	40/47 (85%)	0.89	12 (30%)	1	1	194, 230, 240, 241
6	AB	40/47 (85%)	0.44	5 (12%)	4	4	198, 237, 255, 258
6	AD	40/47 (85%)	0.56	4 (10%)	8	7	210, 245, 256, 257
6	AF	40/47 (85%)	0.64	8 (20%)	1	1	230, 249, 257, 257
6	AH	40/47 (85%)	0.63	7 (17%)	2	1	224, 241, 251, 254
6	AJ	40/47 (85%)	0.46	8 (20%)	1	1	199, 230, 241, 243
6	AL	40/47 (85%)	0.70	8 (20%)	1	1	190, 211, 236, 238
6	B	40/47 (85%)	0.69	10 (25%)	1	1	189, 239, 250, 254
6	E	40/47 (85%)	0.35	4 (10%)	8	7	193, 239, 251, 252
6	G	40/47 (85%)	0.42	5 (12%)	4	4	187, 239, 252, 255
6	J	40/47 (85%)	0.74	9 (22%)	1	1	191, 243, 258, 262

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
6	N	40/47 (85%)	0.83	8 (20%) 1 1	175, 225, 247, 254	0
6	P	40/47 (85%)	0.81	8 (20%) 1 1	170, 220, 241, 245	0
6	R	40/47 (85%)	0.50	6 (15%) 3 2	170, 223, 236, 236	0
6	T	40/47 (85%)	0.43	5 (12%) 4 4	184, 218, 236, 237	0
6	V	40/47 (85%)	0.12	3 (7%) 15 14	171, 205, 226, 234	0
6	X	40/47 (85%)	-0.40	1 (2%) 58 54	160, 186, 205, 209	0
6	Z	40/47 (85%)	0.03	2 (5%) 30 27	159, 173, 197, 202	0
6	c	40/47 (85%)	0.72	9 (22%) 1 1	160, 217, 245, 247	0
6	e	40/47 (85%)	0.47	3 (7%) 15 14	189, 204, 236, 240	0
6	g	40/47 (85%)	0.21	5 (12%) 4 4	195, 213, 235, 239	0
6	i	40/47 (85%)	0.71	8 (20%) 1 1	199, 223, 240, 241	0
6	k	40/47 (85%)	0.81	11 (27%) 1 1	195, 233, 251, 255	0
6	n	40/47 (85%)	0.91	10 (25%) 1 1	153, 214, 249, 253	0
6	q	40/47 (85%)	0.29	4 (10%) 8 7	156, 199, 239, 246	0
6	s	40/47 (85%)	0.44	5 (12%) 4 4	151, 198, 236, 238	0
6	v	40/47 (85%)	0.73	7 (17%) 2 1	182, 205, 244, 247	0
6	z	40/47 (85%)	1.05	9 (22%) 1 1	184, 224, 266, 271	0
All	All	5546/5840 (94%)	0.86	955 (17%) 2 1	60, 169, 252, 303	0

The worst 5 of 955 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	59	GLY	26.8
5	AC	54	SER	22.0
5	7	2	PHE	19.7
5	AA	52	PRO	17.8
5	S	60	LYS	15.6

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

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

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	CRT	U	102	44/44	0.73	1.16	6.25	132,179,205,208	0
15	CRT	6	101	44/44	0.70	0.92	5.78	153,180,198,203	0
15	CRT	Z	101	44/44	0.82	1.17	5.59	114,157,190,195	0
15	CRT	AH	102	44/44	0.67	1.17	5.39	163,220,243,244	0
15	CRT	R	101	44/44	0.46	0.86	5.24	157,189,197,198	0
15	CRT	AJ	101	44/44	0.66	1.18	4.64	147,203,240,241	0
15	CRT	AE	103	44/44	0.69	0.91	4.28	182,236,248,249	0
15	CRT	X	101	44/44	0.78	0.84	4.25	118,164,193,198	0
15	CRT	J	101	44/44	0.05	1.33	4.18	196,214,220,222	0
15	CRT	T	101	44/44	0.70	0.89	3.81	145,187,206,207	0
15	CRT	k	101	44/44	0.44	0.77	3.72	172,200,217,220	0
15	CRT	4	101	44/44	0.80	0.74	3.64	136,169,192,198	0
15	CRT	M	404	44/44	0.57	0.61	3.56	75,96,139,150	0
15	CRT	AC	101	44/44	0.41	0.81	3.50	195,211,216,218	0
15	CRT	e	101	44/44	0.69	1.22	3.49	149,194,237,241	0
15	CRT	p	103	44/44	0.39	1.14	3.47	158,177,182,187	0
16	PO4	H	302	5/5	0.75	0.61	3.45	170,172,178,179	0
15	CRT	i	101	44/44	0.53	0.80	3.24	163,197,220,226	0
14	MQ8	M	403	53/53	0.51	0.66	3.24	75,98,159,170	0
15	CRT	c	101	44/44	0.10	1.11	3.23	179,196,203,207	0
11	UQ8	L	304	53/53	0.77	0.55	3.20	75,80,82,83	0
15	CRT	AL	101	44/44	0.77	1.16	3.17	140,190,233,236	0
15	CRT	N	101	44/44	0.28	0.99	3.01	179,199,209,214	0
15	CRT	8	101	44/44	0.33	0.84	2.95	174,203,220,223	0
15	CRT	s	101	44/44	0.67	0.98	2.82	155,177,181,183	0
12	PEF	y	408	19/47	0.87	0.44	2.72	93,103,113,116	0
15	CRT	A	103	44/44	0.40	0.84	2.62	186,214,224,225	0
15	CRT	2	101	44/44	0.78	0.95	2.61	128,165,195,200	0
15	CRT	n	101	44/44	0.40	1.16	2.39	173,188,197,201	0
15	CRT	G	101	44/44	0.63	0.91	2.38	187,217,225,228	0
15	CRT	f	102	44/44	0.68	0.93	2.38	152,190,223,230	0
11	UQ8	x	304	53/53	0.80	0.58	2.36	73,85,92,93	0
15	CRT	v	101	44/44	0.41	0.94	2.13	165,192,198,200	0
15	CRT	y	404	44/44	0.70	0.49	1.97	96,117,155,166	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CRT	9	102	44/44	0.78	0.85	1.95	188,217,226,230	0
15	CRT	E	101	44/44	0.54	0.79	1.87	182,217,225,226	0
9	BCL	AB	101	66/66	0.84	0.52	1.73	197,232,260,262	0
16	PO4	t	302	5/5	0.73	0.39	1.43	138,140,144,147	0
14	MQ8	y	403	53/53	0.75	0.40	1.39	71,88,135,144	0
17	PGW	AE	101	21/51	0.70	0.34	1.17	149,167,181,187	0
15	CRT	z	101	44/44	0.52	0.81	1.08	179,205,209,210	0
15	CRT	P	102	44/44	0.68	0.55	0.88	169,193,199,202	0
10	BPH	x	302	65/65	0.78	0.41	0.87	71,78,102,105	0
9	BCL	D	102	66/66	0.87	0.45	0.86	202,232,246,247	0
7	HEM	o	502	43/43	0.96	0.47	0.81	125,134,142,145	0
9	BCL	7	101	66/66	0.88	0.35	0.77	162,184,202,209	0
9	BCL	5	102	66/66	0.87	0.43	0.76	150,176,224,240	0
9	BCL	y	401	66/66	0.90	0.42	0.74	78,88,101,108	0
9	BCL	x	303	66/66	0.92	0.34	0.73	73,82,94,98	0
9	BCL	0	101	66/66	0.82	0.44	0.72	190,224,244,245	0
9	BCL	x	301	66/66	0.89	0.34	0.68	75,81,87,90	0
15	CRT	AD	102	44/44	0.69	0.50	0.66	192,225,232,234	0
7	HEM	o	503	43/43	0.93	0.42	0.63	94,106,122,126	0
9	BCL	W	101	66/66	0.93	0.36	0.63	146,162,172,181	0
7	HEM	C	504	43/43	0.93	0.38	0.62	97,99,104,107	0
9	BCL	d	101	66/66	0.85	0.37	0.62	138,175,187,197	0
9	BCL	e	102	66/66	0.93	0.46	0.60	166,180,213,225	0
9	BCL	F	101	66/66	0.90	0.45	0.60	184,220,238,242	0
10	BPH	y	402	65/65	0.72	0.38	0.59	80,90,143,155	0
9	BCL	M	401	66/66	0.94	0.34	0.54	74,82,88,94	0
9	BCL	AC	102	66/66	0.72	0.47	0.54	205,236,259,261	0
9	BCL	AE	104	66/66	0.85	0.45	0.52	208,235,262,264	0
9	BCL	N	102	66/66	0.89	0.50	0.52	187,219,242,244	0
7	HEM	o	501	43/43	0.82	0.46	0.51	142,155,165,169	0
9	BCL	V	101	66/66	0.86	0.35	0.50	159,175,219,232	0
8	SR	U	103	1/1	0.90	0.38	0.47	233,233,233,233	0
9	BCL	r	101	66/66	0.92	0.42	0.46	154,192,211,214	0
9	BCL	3	101	66/66	0.92	0.39	0.45	134,153,169,173	0
9	BCL	AH	101	66/66	0.88	0.41	0.44	199,218,233,243	0
9	BCL	AI	101	66/66	0.91	0.40	0.42	177,195,210,216	0
7	HEM	C	502	43/43	0.94	0.41	0.41	97,104,111,113	0
9	BCL	9	103	66/66	0.88	0.34	0.41	169,202,226,235	0
9	BCL	K	101	66/66	0.86	0.45	0.41	181,215,235,242	0
9	BCL	Z	102	66/66	0.93	0.45	0.40	141,150,181,191	0
9	BCL	4	102	66/66	0.93	0.41	0.38	138,159,198,209	0
7	HEM	C	503	43/43	0.94	0.39	0.38	85,100,116,119	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	BCL	AK	101	66/66	0.90	0.42	0.37	168,180,199,220	0
9	BCL	AD	101	66/66	0.82	0.34	0.36	193,224,242,252	0
10	BPH	L	302	65/65	0.86	0.32	0.33	68,81,108,115	0
9	BCL	O	101	66/66	0.85	0.42	0.33	179,211,234,235	0
12	PEF	A	101	19/47	0.67	0.46	0.29	141,149,161,165	0
7	HEM	o	504	43/43	0.93	0.41	0.29	112,116,123,124	0
9	BCL	c	102	66/66	0.87	0.38	0.28	177,211,249,251	0
9	BCL	f	101	66/66	0.90	0.37	0.26	157,181,196,203	0
10	BPH	M	402	65/65	0.84	0.29	0.25	72,77,113,123	0
9	BCL	g	101	66/66	0.90	0.40	0.24	169,190,234,245	0
9	BCL	L	301	66/66	0.92	0.29	0.18	67,74,92,98	0
9	BCL	Y	101	66/66	0.93	0.37	0.17	139,149,163,175	0
9	BCL	AE	102	66/66	0.89	0.36	0.17	169,228,244,254	0
9	BCL	w	101	66/66	0.91	0.42	0.13	174,206,228,234	0
9	BCL	l	102	66/66	0.93	0.36	0.12	140,153,192,205	0
9	BCL	A	102	66/66	0.93	0.38	0.11	202,230,242,244	0
9	BCL	s	102	66/66	0.93	0.43	0.11	171,202,247,248	0
9	BCL	m	102	66/66	0.84	0.40	0.10	160,202,221,229	0
9	BCL	G	102	66/66	0.93	0.40	0.10	203,233,249,251	0
9	BCL	p	102	66/66	0.88	0.39	0.09	124,199,217,224	0
9	BCL	J	102	66/66	0.92	0.41	0.09	202,233,255,257	0
12	PEF	m	101	19/47	0.76	0.32	0.08	124,130,143,146	0
9	BCL	I	101	66/66	0.88	0.38	0.08	141,226,243,247	0
9	BCL	D	101	66/66	0.90	0.35	0.07	149,221,243,245	0
9	BCL	u	101	66/66	0.88	0.37	0.07	120,199,218,223	0
9	BCL	AL	102	66/66	0.91	0.37	0.07	167,178,209,221	0
9	BCL	X	102	66/66	0.94	0.28	0.06	142,155,182,199	0
9	BCL	L	305	66/66	0.91	0.28	0.06	76,88,106,115	0
12	PEF	H	303	19/47	0.89	0.35	0.05	164,173,184,191	0
9	BCL	z	102	66/66	0.87	0.42	0.04	193,228,269,271	0
9	BCL	h	101	66/66	0.91	0.33	0.04	168,188,207,212	0
9	BCL	Q	101	66/66	0.94	0.30	0.01	165,201,216,224	0
9	BCL	S	102	66/66	0.90	0.32	0.01	129,190,203,213	0
9	BCL	i	102	66/66	0.93	0.36	-0.01	173,197,242,261	0
9	BCL	j	101	66/66	0.82	0.34	-0.02	177,199,217,223	0
9	BCL	AJ	102	66/66	0.91	0.29	-0.02	177,189,226,232	0
9	BCL	5	101	66/66	0.95	0.31	-0.02	141,165,182,188	0
9	BCL	v	102	66/66	0.92	0.34	-0.05	182,211,260,262	0
12	PEF	M	408	19/47	0.87	0.28	-0.05	87,92,97,100	0
9	BCL	P	101	66/66	0.90	0.37	-0.06	171,205,223,228	0
9	BCL	l	101	66/66	0.89	0.33	-0.06	115,148,161,169	0
9	BCL	L	303	66/66	0.91	0.28	-0.08	62,70,78,83	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	BCL	U	101	66/66	0.93	0.32	-0.08	151,179,188,195	0
9	BCL	m	103	66/66	0.88	0.36	-0.08	178,209,237,245	0
9	BCL	k	102	66/66	0.88	0.35	-0.09	181,211,246,260	0
7	HEM	C	501	43/43	0.88	0.33	-0.12	110,120,129,134	0
9	BCL	T	102	66/66	0.88	0.34	-0.13	164,188,236,238	0
9	BCL	AA	101	66/66	0.94	0.32	-0.15	177,212,237,244	0
17	PGW	S	101	21/51	0.78	0.24	-0.16	118,132,142,148	0
9	BCL	p	104	66/66	0.95	0.34	-0.17	170,202,241,242	0
9	BCL	R	102	66/66	0.90	0.34	-0.18	174,203,233,235	0
9	BCL	8	102	66/66	0.88	0.32	-0.19	177,207,239,244	0
8	SR	Y	102	1/1	0.94	0.35	-0.21	191,191,191,191	0
9	BCL	B	101	66/66	0.90	0.35	-0.25	187,218,239,241	0
12	PEF	t	301	19/47	0.89	0.22	-0.28	94,98,103,104	0
9	BCL	l	101	66/66	0.86	0.26	-0.29	161,201,221,228	0
12	PEF	M	406	19/47	0.89	0.29	-0.33	107,115,119,124	0
12	PEF	x	306	19/47	0.90	0.18	-0.37	96,102,108,108	0
8	SR	7	102	1/1	0.90	0.34	-0.38	221,221,221,221	0
8	SR	w	103	1/1	0.43	0.28	-0.40	260,260,260,260	0
8	SR	AC	103	1/1	0.94	0.22	-0.47	265,265,265,265	0
9	BCL	x	305	66/66	0.94	0.23	-0.49	72,82,91,99	0
12	PEF	p	101	16/47	0.74	0.23	-0.50	132,144,152,156	0
8	SR	A	104	1/1	0.96	0.31	-0.52	256,256,256,256	0
9	BCL	AH	103	66/66	0.83	0.29	-0.52	195,211,245,252	0
12	PEF	H	301	19/47	0.64	0.26	-0.59	140,163,175,180	0
8	SR	W	102	1/1	0.91	0.23	-0.60	205,205,205,205	0
8	SR	o	505	1/1	0.94	0.16	-0.65	111,111,111,111	0
8	SR	K	102	1/1	0.72	0.31	-0.66	270,270,270,270	0
8	SR	Q	102	1/1	0.89	0.19	-0.66	256,256,256,256	0
8	SR	F	102	1/1	0.85	0.21	-0.67	262,262,262,262	0
12	PEF	t	303	19/47	0.85	0.23	-0.68	83,87,94,95	0
12	PEF	y	406	19/47	0.81	0.23	-0.69	124,132,141,146	0
8	SR	I	102	1/1	0.70	0.17	-0.80	284,284,284,284	0
8	SR	5	104	1/1	0.84	0.16	-0.82	206,206,206,206	0
8	SR	x	308	1/1	0.88	0.15	-0.82	196,196,196,196	0
13	FE	x	309	1/1	0.99	0.15	-0.83	65,65,65,65	0
8	SR	l	102	1/1	0.83	0.15	-0.89	245,245,245,245	0
8	SR	j	102	1/1	0.98	0.17	-0.89	233,233,233,233	0
8	SR	AI	103	1/1	0.80	0.21	-0.91	228,228,228,228	0
8	SR	p	105	1/1	0.65	0.17	-0.92	265,265,265,265	0
16	PO4	y	405	5/5	0.92	0.16	-0.98	138,141,147,148	0
8	SR	h	102	1/1	0.90	0.14	-1.00	220,220,220,220	0
8	SR	O	102	1/1	0.77	0.13	-1.00	254,254,254,254	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SR	S	103	1/1	0.49	0.14	-1.02	235,235,235,235	0
12	PEF	H	304	19/47	0.89	0.17	-1.05	92,98,106,108	0
12	PEF	y	407	19/47	0.86	0.20	-1.08	91,96,102,105	0
8	SR	9	101	1/1	0.81	0.15	-1.09	236,236,236,236	0
8	SR	AA	102	1/1	0.81	0.13	-1.09	273,273,273,273	0
16	PO4	M	405	5/5	0.92	0.14	-1.10	120,126,128,129	0
8	SR	w	102	1/1	0.73	0.09	-1.15	263,263,263,263	0
8	SR	l	103	1/1	0.93	0.06	-1.16	176,176,176,176	0
8	SR	r	102	1/1	0.86	0.09	-1.19	252,252,252,252	0
8	SR	m	104	1/1	0.79	0.19	-1.21	253,253,253,253	0
8	SR	AI	102	1/1	0.48	0.07	-1.25	245,245,245,245	0
8	SR	AE	105	1/1	0.87	0.14	-1.31	257,257,257,257	0
8	SR	f	103	1/1	0.88	0.09	-1.34	208,208,208,208	0
8	SR	C	505	1/1	0.96	0.12	-1.35	113,113,113,113	0
12	PEF	M	407	16/47	0.88	0.19	-1.36	79,83,87,89	0
8	SR	L	307	1/1	0.98	0.07	-1.37	205,205,205,205	0
8	SR	D	103	1/1	0.84	0.19	-1.39	269,269,269,269	0
13	FE	L	309	1/1	0.99	0.13	-1.41	65,65,65,65	0
8	SR	5	103	1/1	0.73	0.14	-1.54	197,197,197,197	0
8	SR	d	102	1/1	0.66	0.05	-1.66	198,198,198,198	0
8	SR	AK	102	1/1	0.82	0.04	-2.55	203,203,203,203	0
8	SR	L	308	1/1	0.90	0.26	-	145,145,145,145	0
12	PEF	L	306	12/47	0.80	0.32	-	113,119,126,127	0
8	SR	x	307	1/1	0.81	0.24	-	168,168,168,168	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.