



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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.

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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

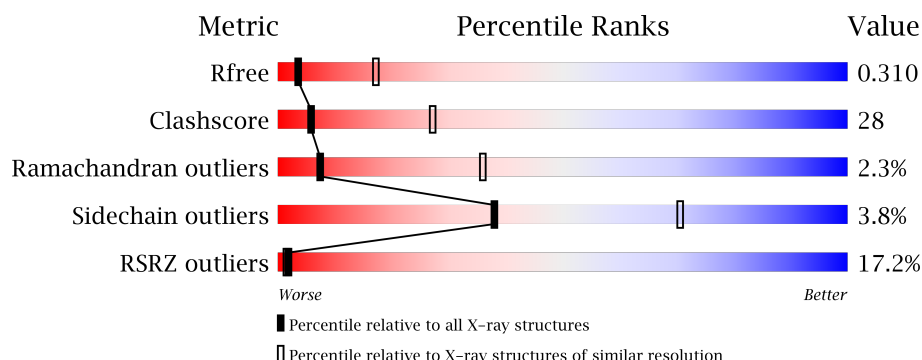
# 1 Overall quality at a glance

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>

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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	

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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>
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>
5	w	61	<div> <div>36%</div> <div>95%</div> <div>..</div> </div>
6	0	47	<div> <div>19%</div> <div>53%</div> <div>30%</div> <div>15%</div> </div>
6	2	47	<div> <div>13%</div> <div>49%</div> <div>36%</div> <div>15%</div> </div>
6	4	47	<div> <div>4%</div> <div>66%</div> <div>19%</div> <div>15%</div> </div>
6	6	47	<div> <div>11%</div> <div>60%</div> <div>26%</div> <div>15%</div> </div>
6	8	47	<div> <div>26%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
6	AB	47	<div> <div>11%</div> <div>53%</div> <div>32%</div> <div>15%</div> </div>
6	AD	47	<div> <div>9%</div> <div>60%</div> <div>26%</div> <div>15%</div> </div>
6	AF	47	<div> <div>17%</div> <div>60%</div> <div>26%</div> <div>15%</div> </div>
6	AH	47	<div> <div>15%</div> <div>53%</div> <div>32%</div> <div>15%</div> </div>
6	AJ	47	<div> <div>17%</div> <div>47%</div> <div>34%</div> <div>15%</div> </div>
6	AL	47	<div> <div>17%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
6	B	47	<div> <div>21%</div> <div>45%</div> <div>36%</div> <div>15%</div> </div>
6	E	47	<div> <div>9%</div> <div>45%</div> <div>40%</div> <div>15%</div> </div>
6	G	47	<div> <div>11%</div> <div>34%</div> <div>51%</div> <div>15%</div> </div>
6	J	47	<div> <div>19%</div> <div>43%</div> <div>43%</div> <div>15%</div> </div>

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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

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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

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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

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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			

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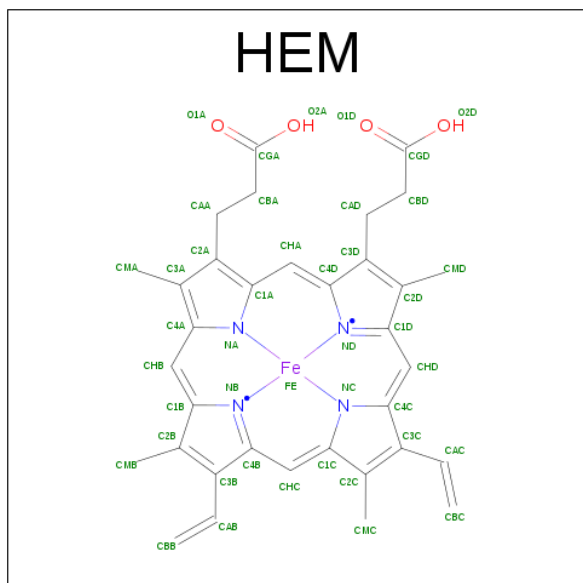
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	Z	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	8	40	Total 337	C 228	N 52	O 55	S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

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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:  $C_{34}H_{32}FeN_4O_4$ ).



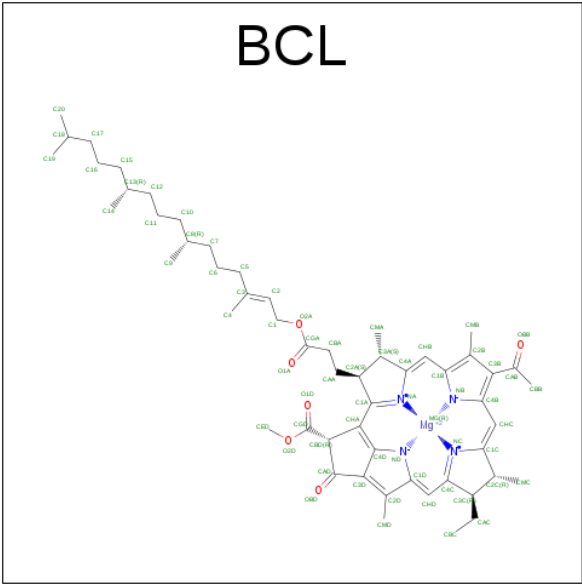
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	1	Total 1	Sr 1	0	0
8	h	1	Total 1	Sr 1	0	0
8	AC	1	Total 1	Sr 1	0	0
8	W	1	Total 1	Sr 1	0	0
8	o	1	Total 1	Sr 1	0	0
8	S	1	Total 1	Sr 1	0	0
8	f	1	Total 1	Sr 1	0	0
8	AK	1	Total 1	Sr 1	0	0
8	p	1	Total 1	Sr 1	0	0
8	AE	1	Total 1	Sr 1	0	0
8	w	2	Total 2	Sr 2	0	0
8	A	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

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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

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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

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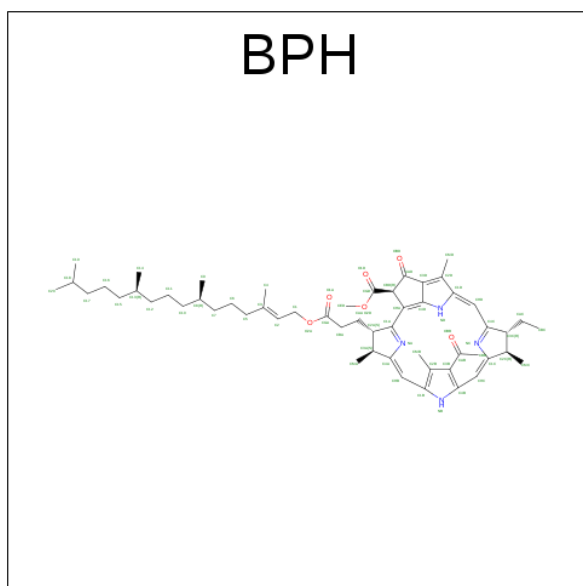
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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9	r	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	s	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	v	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	w	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	z	1	Total 66	C 55	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

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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:  $C_{55}H_{76}N_4O_6$ ).



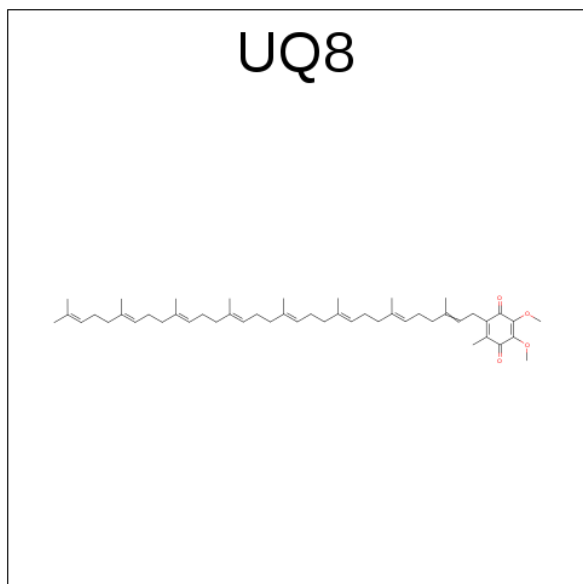
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		
10	x	1	Total	C	N	O	0	0
			65	55	4	6		

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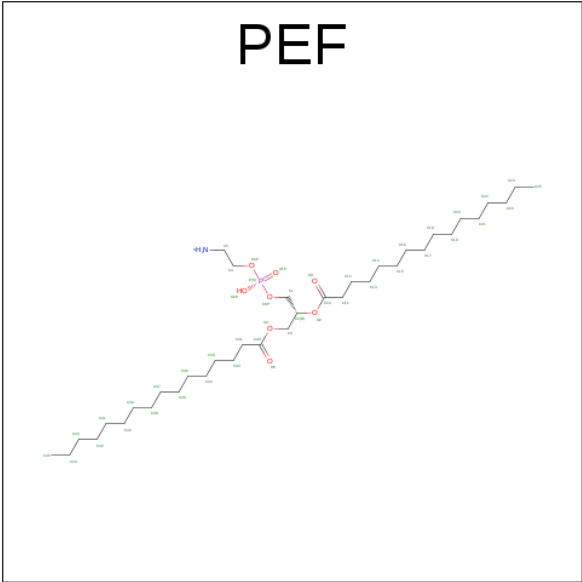
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	y	1	Total	C	N	O	0	0
			65	55	4	6		

- 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		

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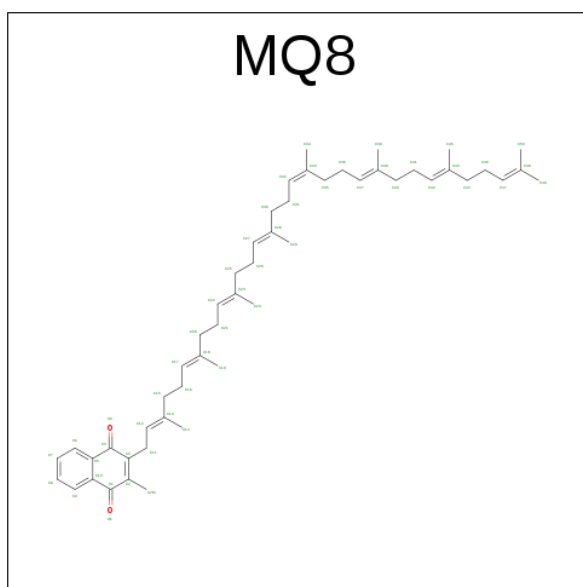
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	m	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	p	1	Total	C	N	O	P	0	0
			16	7	1	7	1		

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

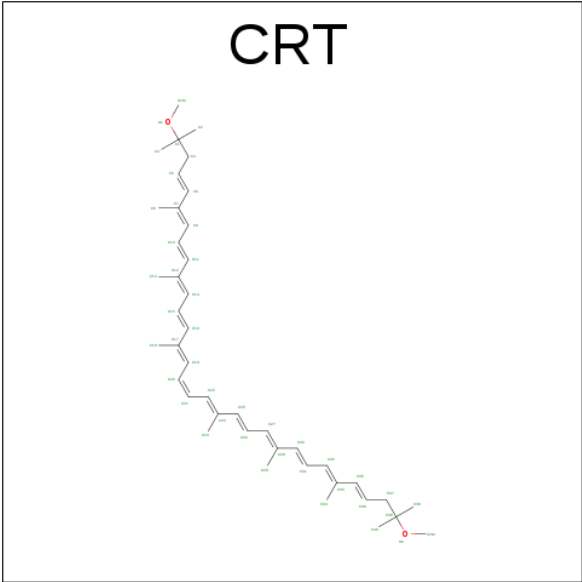
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	x	1	Total	Fe	0	0
			1	1		
13	L	1	Total	Fe	0	0
			1	1		

- 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>).



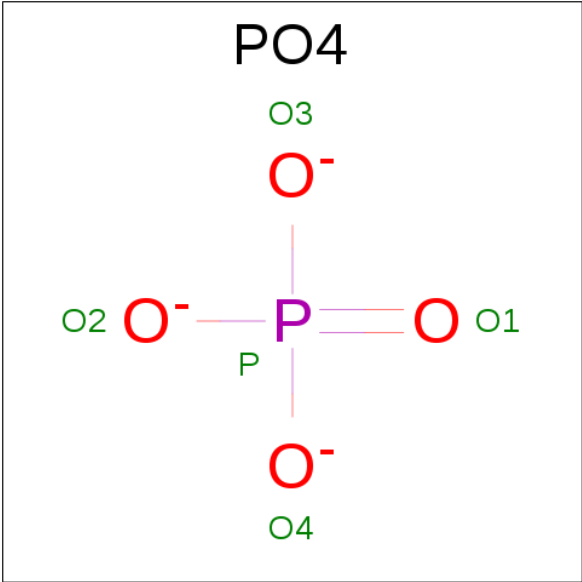
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			44	42	2		
15	A	1	Total	C	O	0	0
			44	42	2		
15	E	1	Total	C	O	0	0
			44	42	2		
15	G	1	Total	C	O	0	0
			44	42	2		
15	J	1	Total	C	O	0	0
			44	42	2		
15	N	1	Total	C	O	0	0
			44	42	2		
15	P	1	Total	C	O	0	0
			44	42	2		
15	R	1	Total	C	O	0	0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

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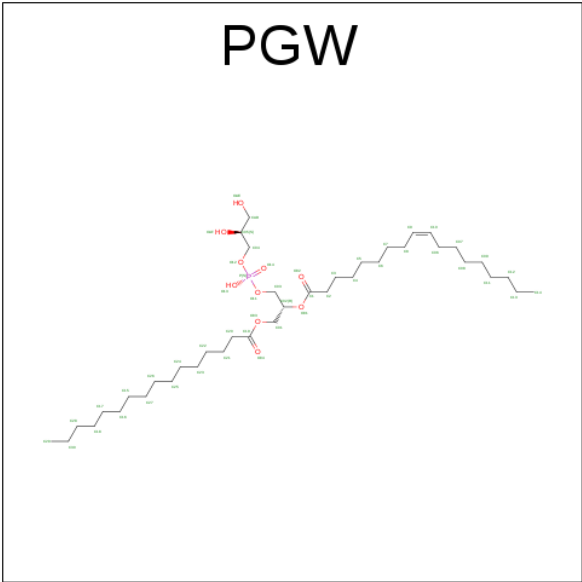
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	6	1	Total	C	O	0	0
			44	42	2		
15	8	1	Total	C	O	0	0
			44	42	2		
15	9	1	Total	C	O	0	0
			44	42	2		
15	y	1	Total	C	O	0	0
			44	42	2		
15	n	1	Total	C	O	0	0
			44	42	2		
15	p	1	Total	C	O	0	0
			44	42	2		
15	s	1	Total	C	O	0	0
			44	42	2		
15	v	1	Total	C	O	0	0
			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		

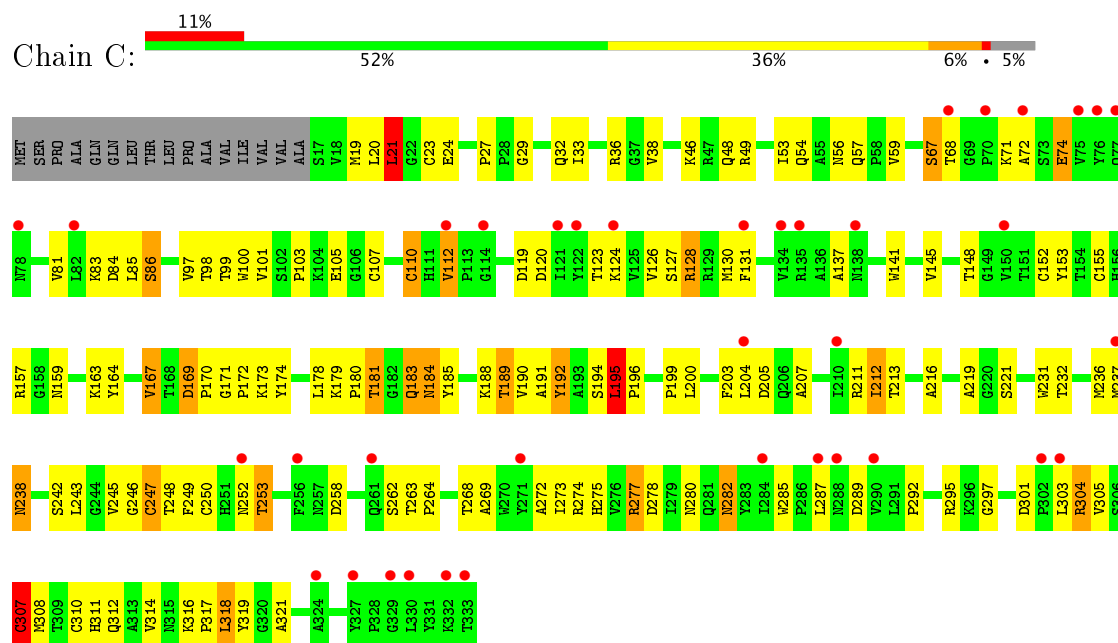
- Molecule 18 is water.

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		

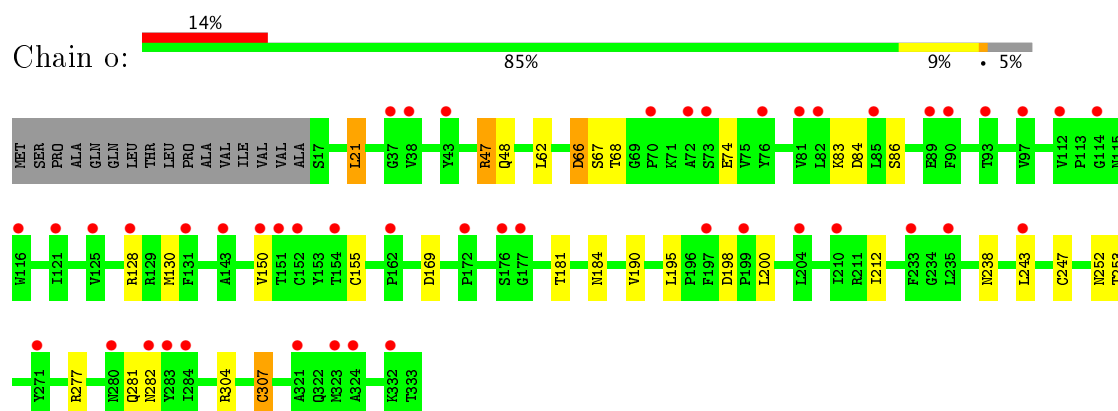
### 3 Residue-property plots

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

- Molecule 1: Photosynthetic reaction center cytochrome c subunit

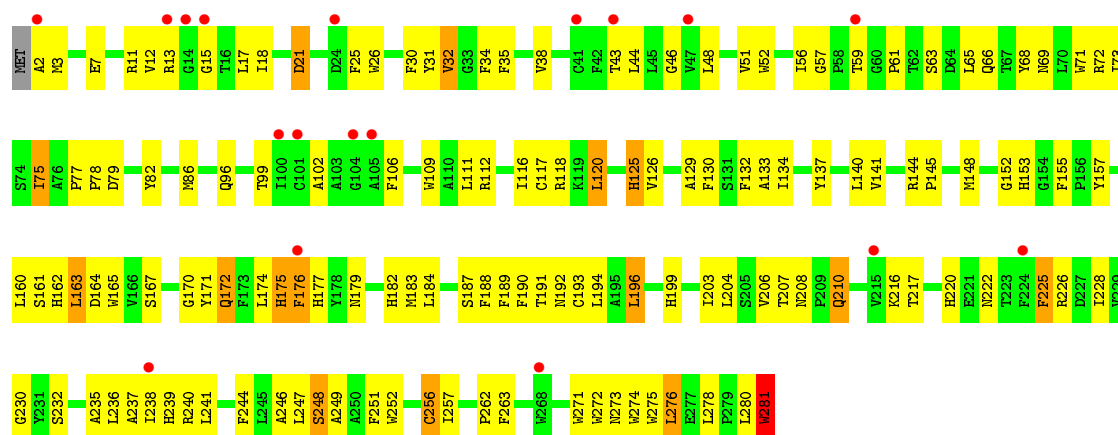


- Molecule 1: Photosynthetic reaction center cytochrome c subunit

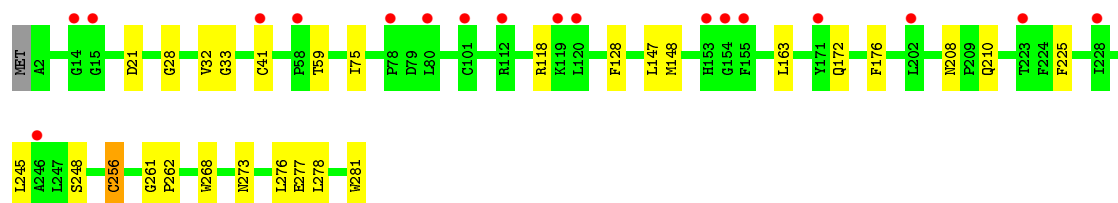


- Molecule 2: Photosynthetic reaction center L subunit

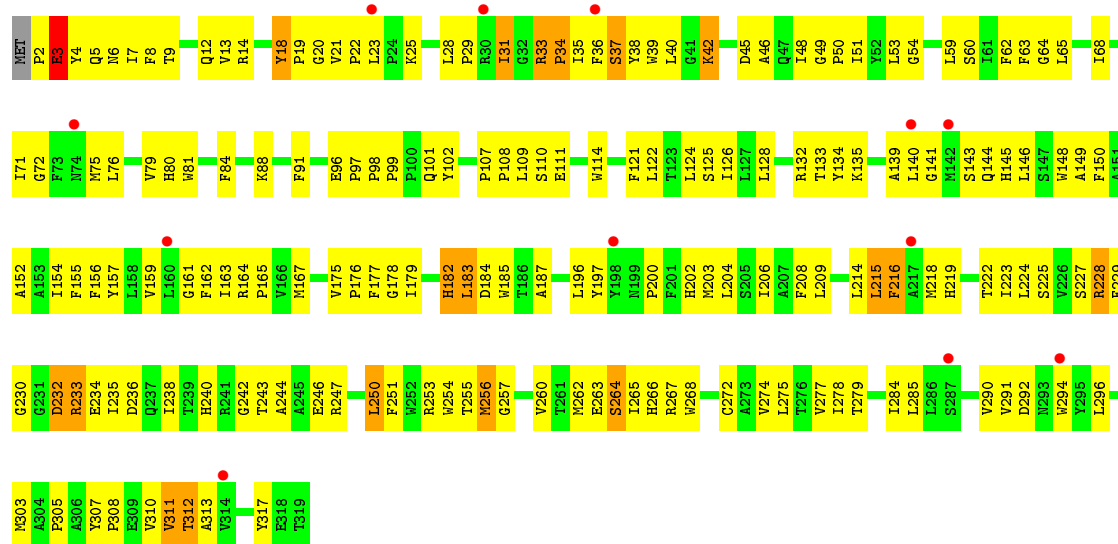
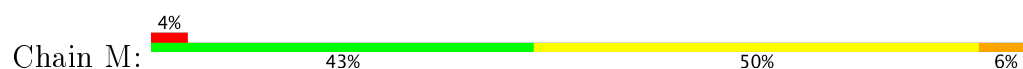




• Molecule 2: Photosynthetic reaction center L subunit

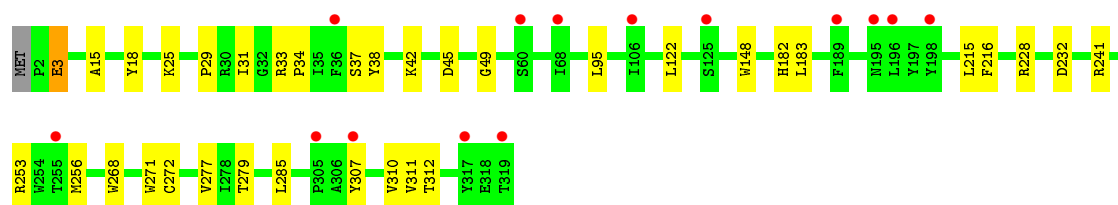


• Molecule 3: Photosynthetic reaction center M subunit

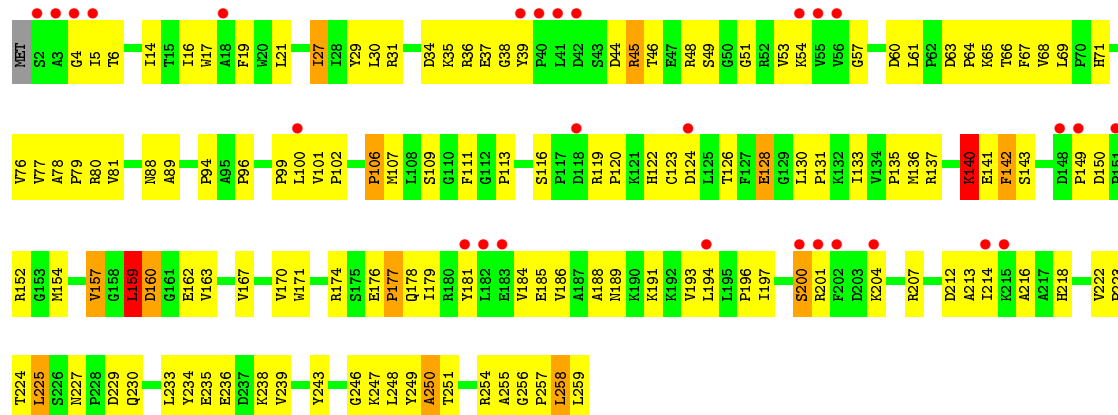


• Molecule 3: Photosynthetic reaction center M subunit

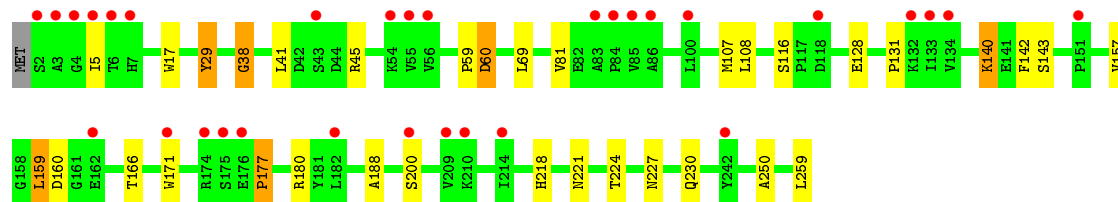
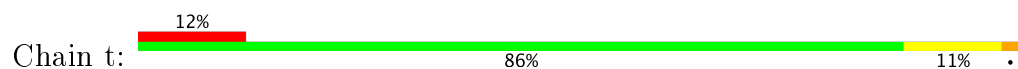




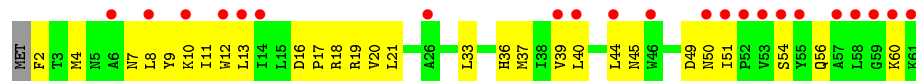
• Molecule 4: Photosynthetic reaction center H subunit



• Molecule 4: Photosynthetic reaction center H subunit



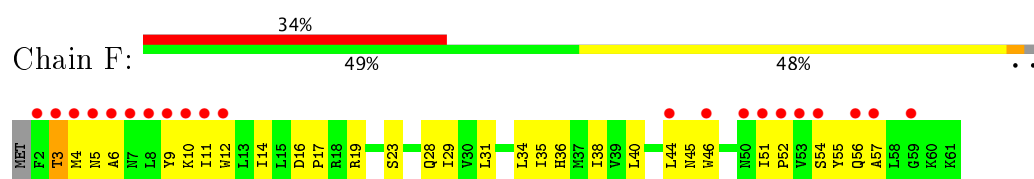
• Molecule 5: LH1 alpha polypeptide



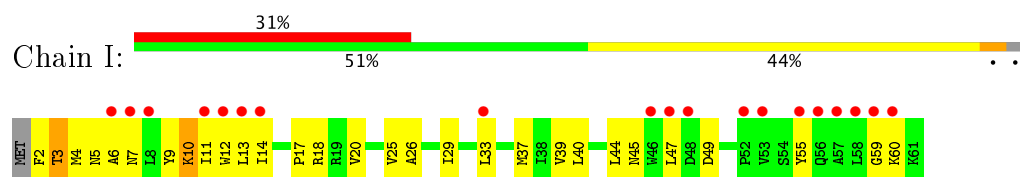
• Molecule 5: LH1 alpha polypeptide



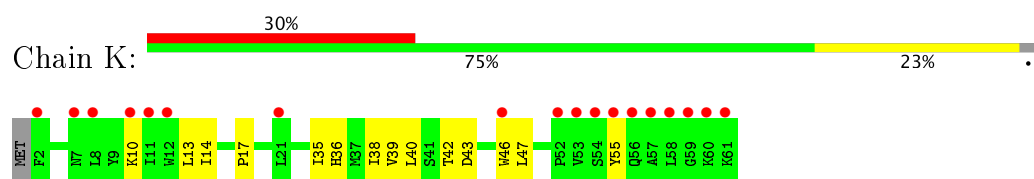
• Molecule 5: LH1 alpha polypeptide



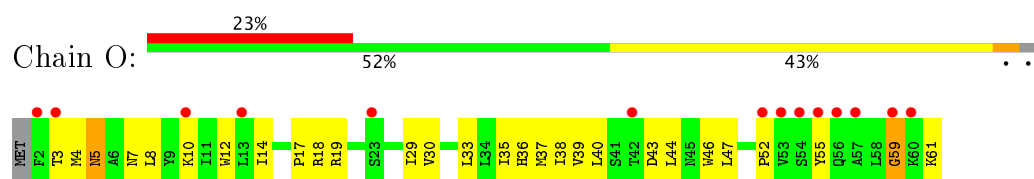
- Molecule 5: LH1 alpha polypeptide



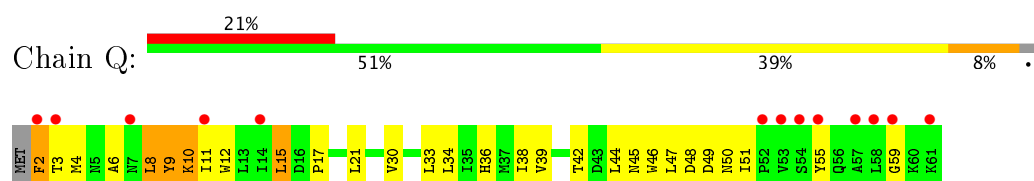
- Molecule 5: LH1 alpha polypeptide



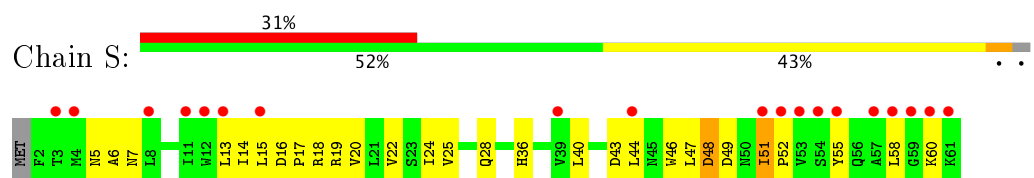
- Molecule 5: LH1 alpha polypeptide



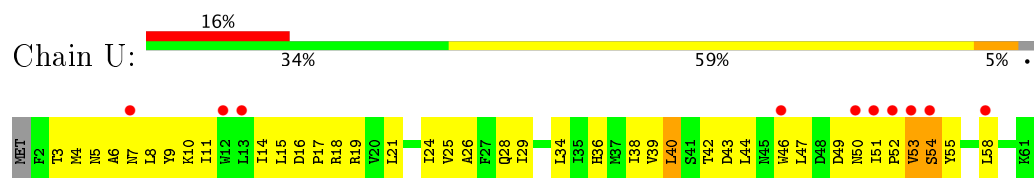
- Molecule 5: LH1 alpha polypeptide



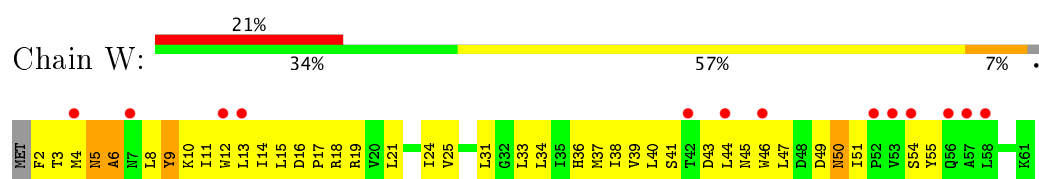
- Molecule 5: LH1 alpha polypeptide



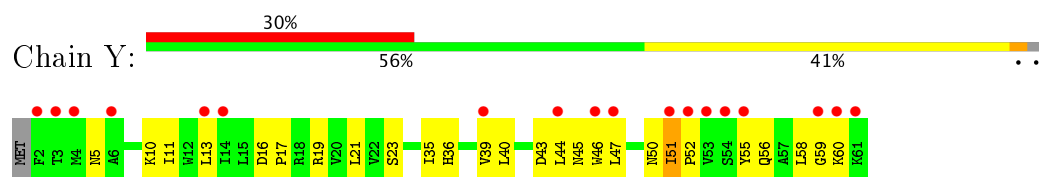
- Molecule 5: LH1 alpha polypeptide



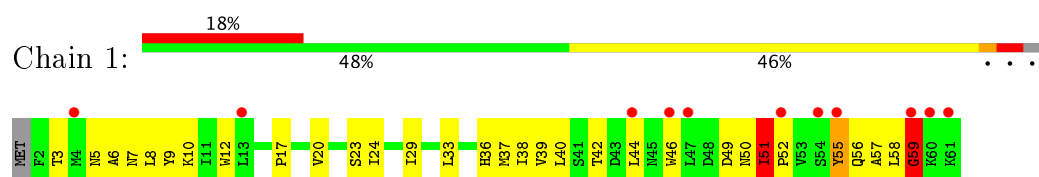
- Molecule 5: LH1 alpha polypeptide



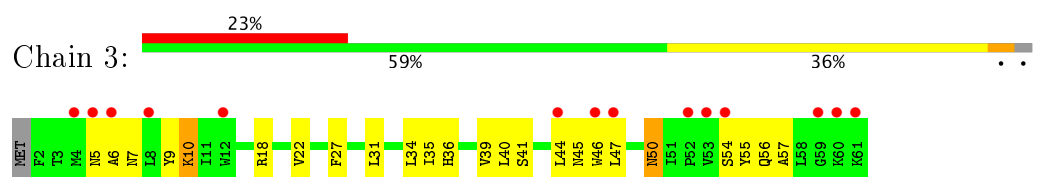
- Molecule 5: LH1 alpha polypeptide



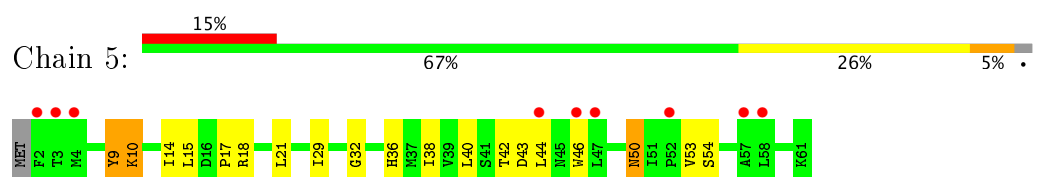
- Molecule 5: LH1 alpha polypeptide



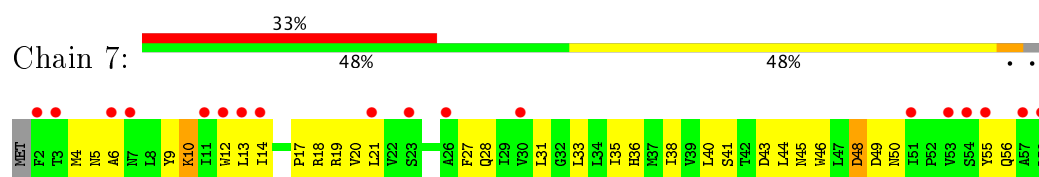
- Molecule 5: LH1 alpha polypeptide



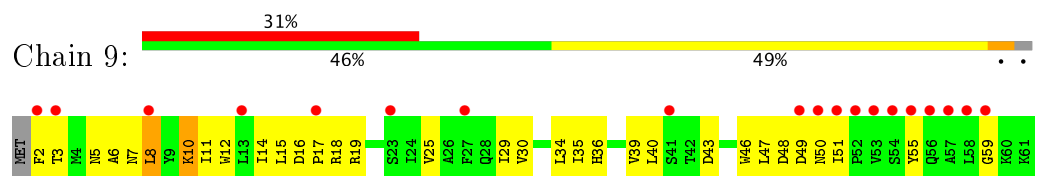
- Molecule 5: LH1 alpha polypeptide



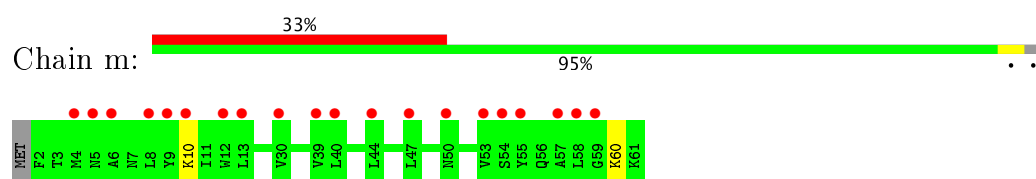
- Molecule 5: LH1 alpha polypeptide



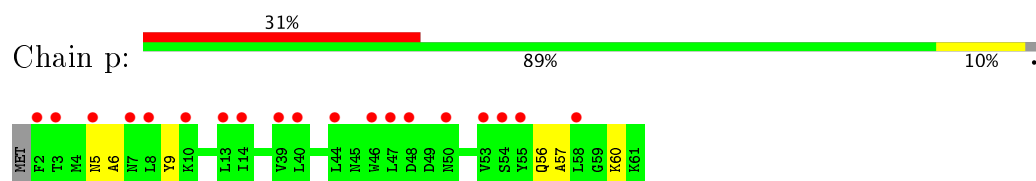
- Molecule 5: LH1 alpha polypeptide



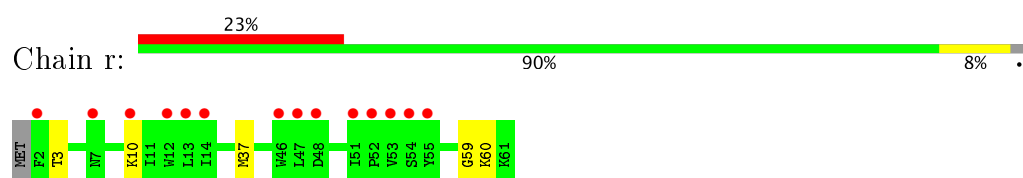
- Molecule 5: LH1 alpha polypeptide



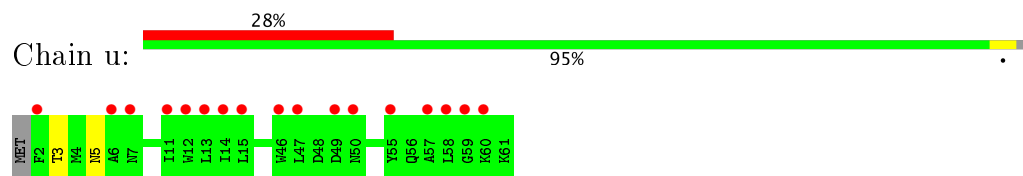
- Molecule 5: LH1 alpha polypeptide



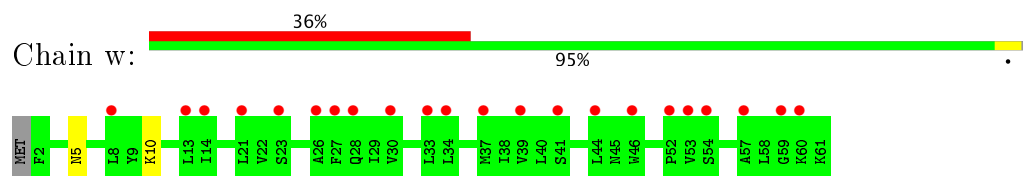
- Molecule 5: LH1 alpha polypeptide



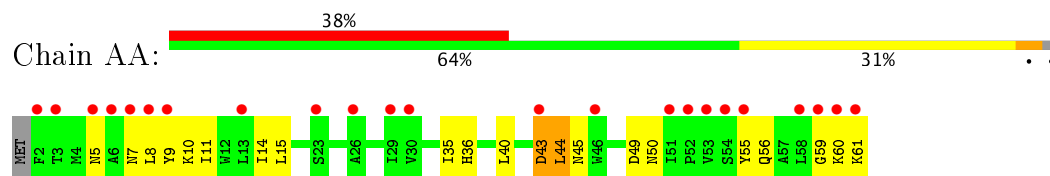
- Molecule 5: LH1 alpha polypeptide



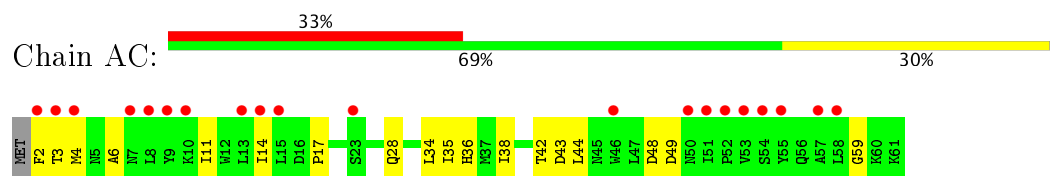
- Molecule 5: LH1 alpha polypeptide



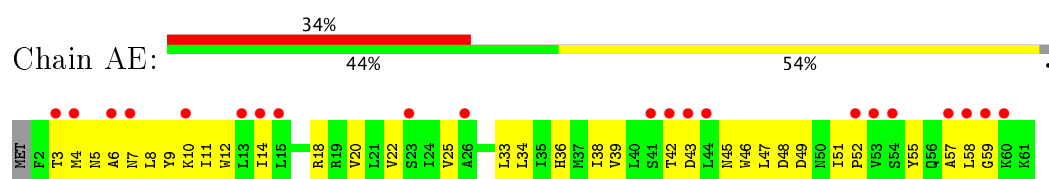
- Molecule 5: LH1 alpha polypeptide



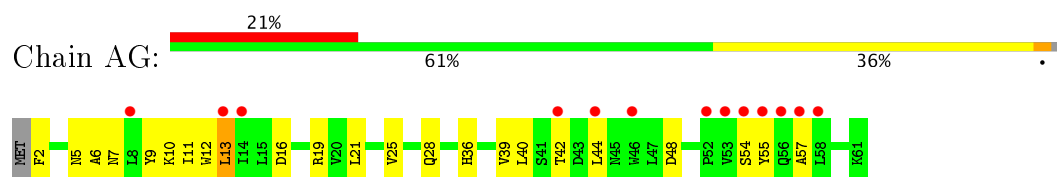
- Molecule 5: LH1 alpha polypeptide



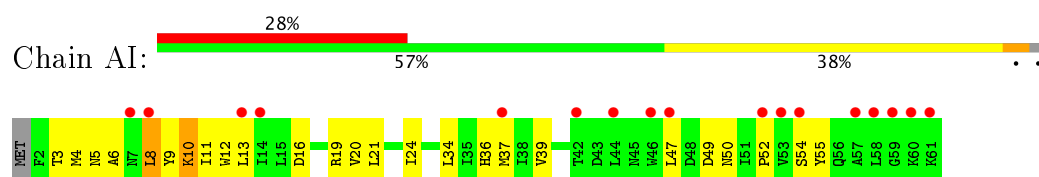
- Molecule 5: LH1 alpha polypeptide



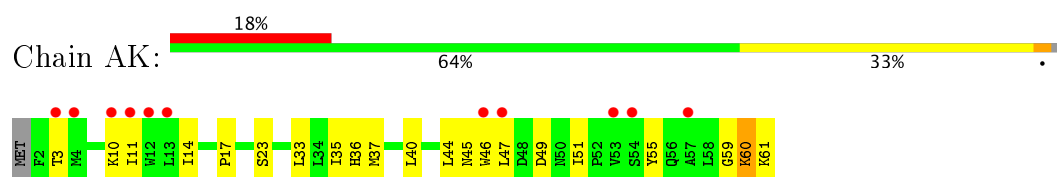
- Molecule 5: LH1 alpha polypeptide



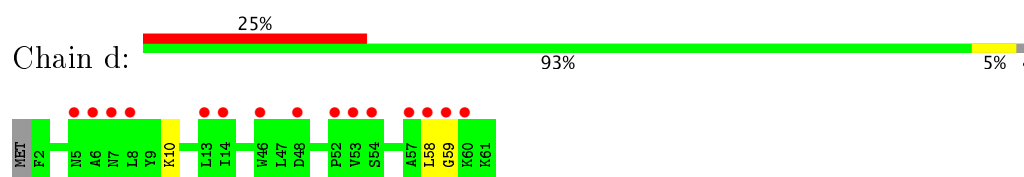
- Molecule 5: LH1 alpha polypeptide



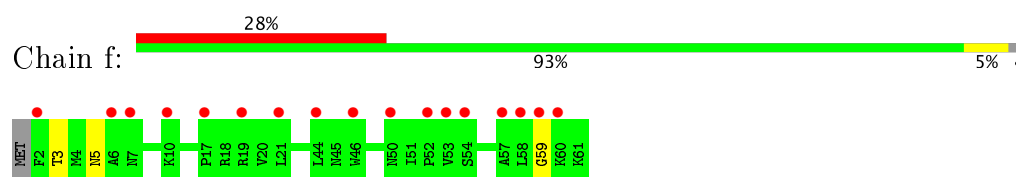
- Molecule 5: LH1 alpha polypeptide



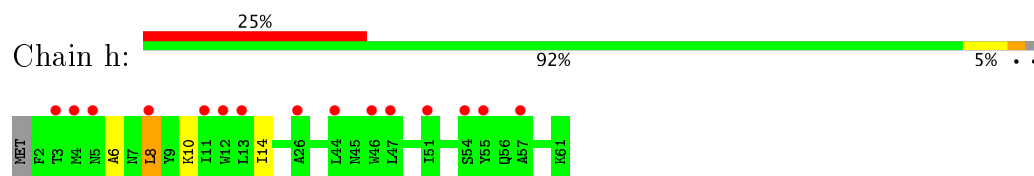
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

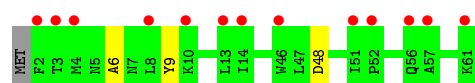
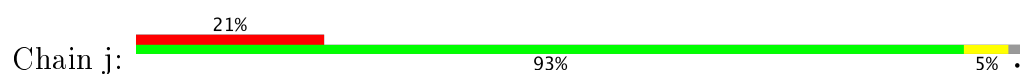


- Molecule 5: LH1 alpha polypeptide

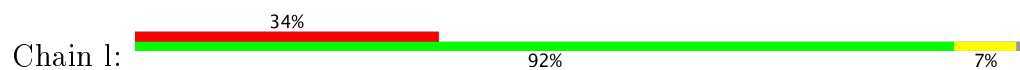


- Molecule 5: LH1 alpha polypeptide

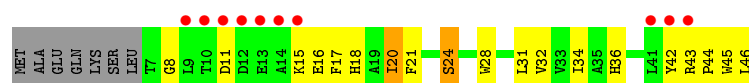




- Molecule 5: LH1 alpha polypeptide



- Molecule 6: LH1 beta polypeptide



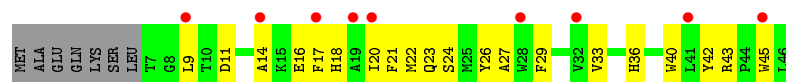
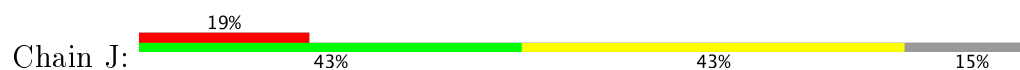
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



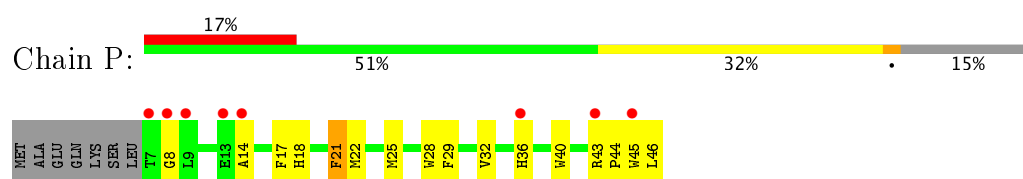
- Molecule 6: LH1 beta polypeptide



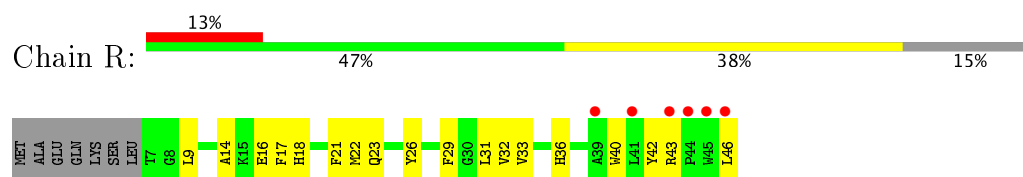
- Molecule 6: LH1 beta polypeptide



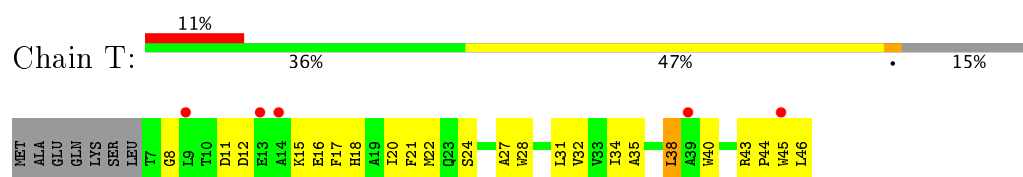
- Molecule 6: LH1 beta polypeptide



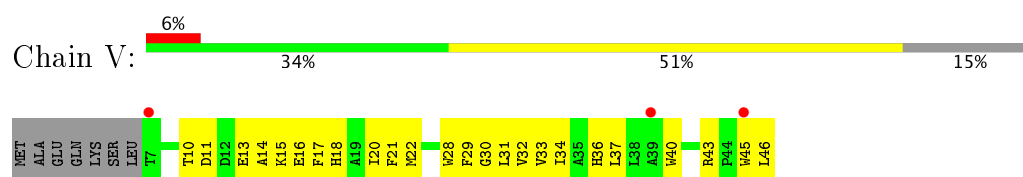
- Molecule 6: LH1 beta polypeptide



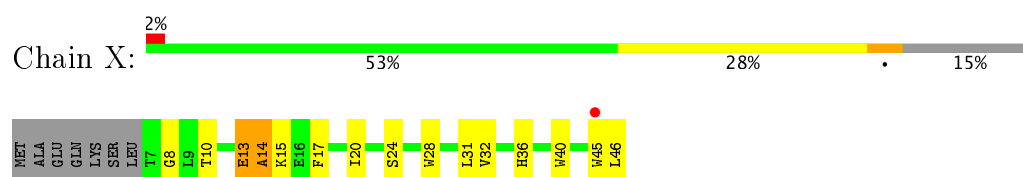
- Molecule 6: LH1 beta polypeptide



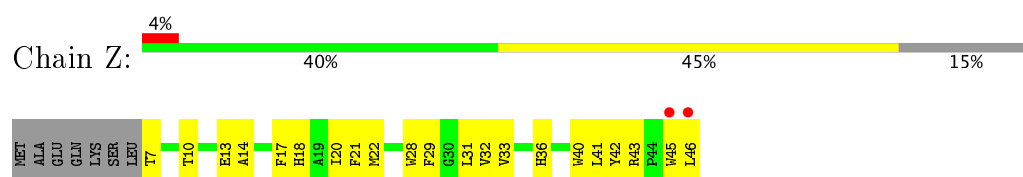
- Molecule 6: LH1 beta polypeptide



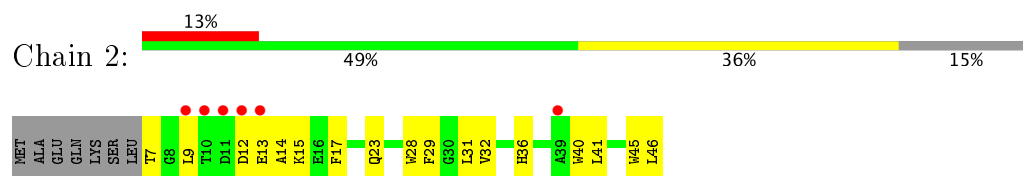
- Molecule 6: LH1 beta polypeptide



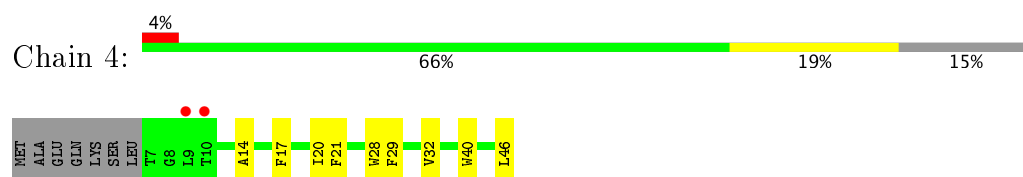
- Molecule 6: LH1 beta polypeptide



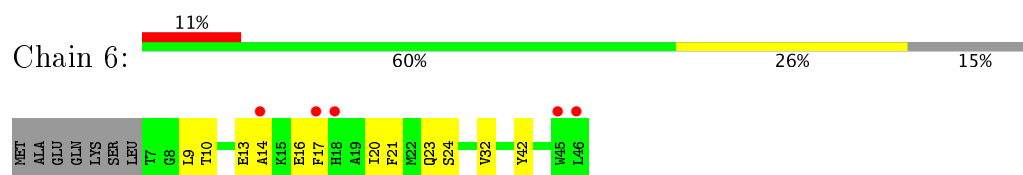
- Molecule 6: LH1 beta polypeptide



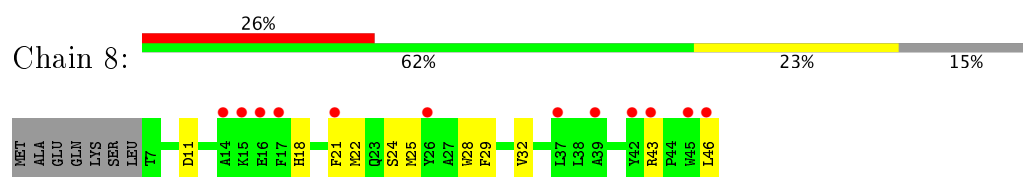
- Molecule 6: LH1 beta polypeptide



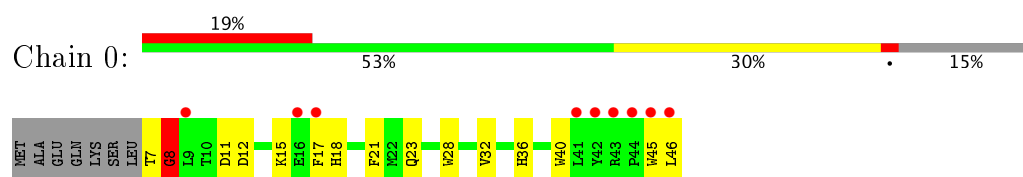
- Molecule 6: LH1 beta polypeptide



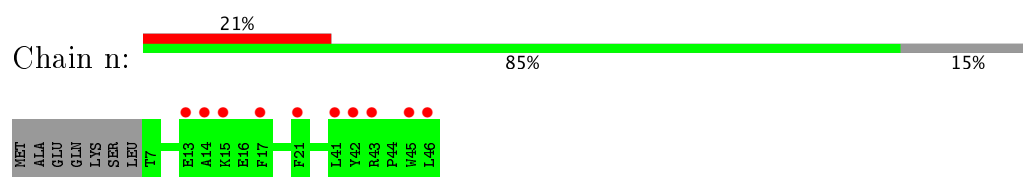
- Molecule 6: LH1 beta polypeptide



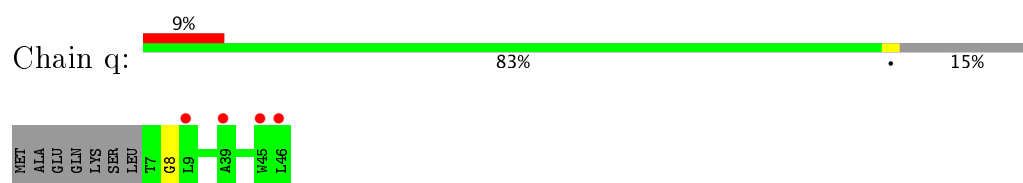
- Molecule 6: LH1 beta polypeptide



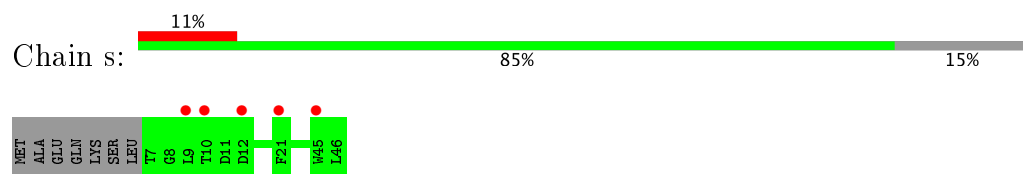
- Molecule 6: LH1 beta polypeptide



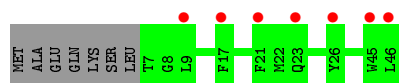
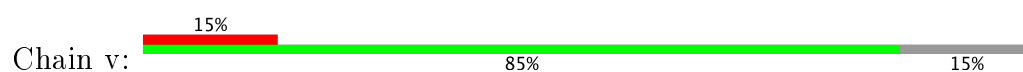
- Molecule 6: LH1 beta polypeptide



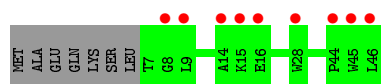
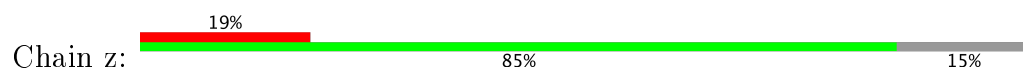
- Molecule 6: LH1 beta polypeptide



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- Molecule 6: LH1 beta polypeptide



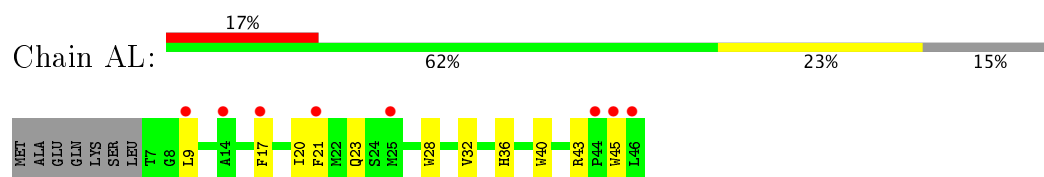
- Molecule 6: LH1 beta polypeptide



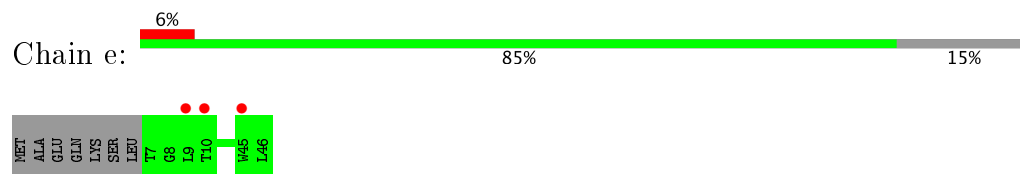
- Molecule 6: LH1 beta polypeptide



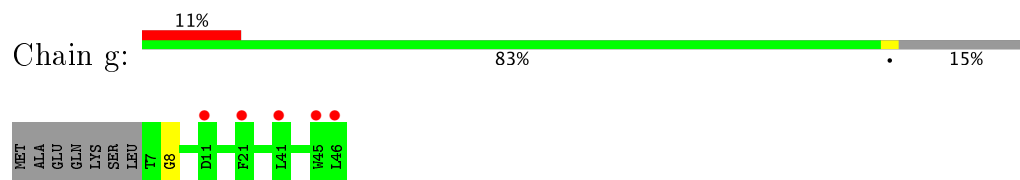
- Molecule 6: LH1 beta polypeptide



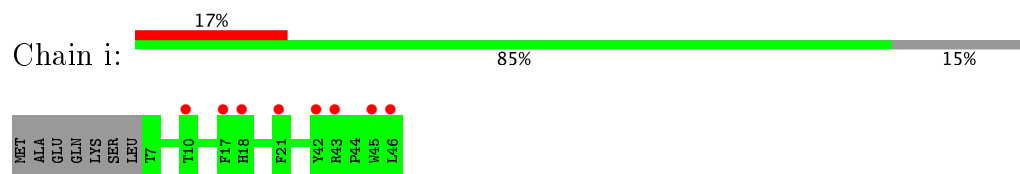
- Molecule 6: LH1 beta polypeptide



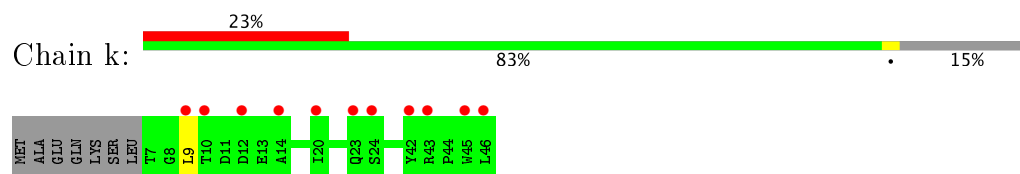
- Molecule 6: LH1 beta polypeptide



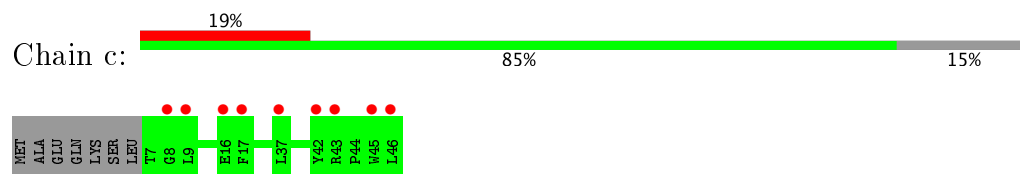
- Molecule 6: LH1 beta polypeptide



- 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)	Xtriage
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	Xtriage
Anisotropy	0.339	Xtriage
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>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	168.0	wwPDB-VP

Xtriage'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

All (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
2	x	256	CYS	CB-SG	-6.50	1.71	1.82
1	o	155	CYS	CB-SG	-6.37	1.71	1.82
4	H	123	CYS	CB-SG	-6.13	1.71	1.82
4	H	128	GLU	CG-CD	6.00	1.60	1.51
1	o	247	CYS	CB-SG	-5.99	1.72	1.81
3	M	3	GLU	CB-CG	5.99	1.63	1.52
4	t	171	TRP	CB-CG	5.73	1.60	1.50
4	t	60	ASP	CB-CG	5.51	1.63	1.51
2	L	117	CYS	CB-SG	-5.33	1.73	1.81
2	x	273	ASN	CB-CG	5.33	1.63	1.51
2	L	281	TRP	C-O	5.28	1.33	1.23
2	x	277	GLU	CG-CD	5.06	1.59	1.51

All (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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	183	LEU	CB-CG-CD2	-8.42	96.68	111.00
3	y	253	ARG	NE-CZ-NH2	-8.12	116.24	120.30
4	t	29	TYR	CB-CG-CD2	-7.93	116.24	121.00
4	t	159	LEU	CB-CG-CD1	7.90	124.43	111.00
2	L	276	LEU	CB-CG-CD2	-7.53	98.20	111.00
2	L	75	ILE	CG1-CB-CG2	-7.53	94.84	111.40
1	o	252	ASN	N-CA-C	-7.18	91.62	111.00
2	x	75	ILE	CG1-CB-CG2	-7.16	95.64	111.40
1	o	200	LEU	CB-CG-CD2	-7.09	98.95	111.00
2	x	276	LEU	CB-CG-CD2	-6.95	99.19	111.00
5	h	8	LEU	CA-CB-CG	6.82	130.99	115.30
1	o	307	CYS	CA-CB-SG	-6.72	101.90	114.00
1	o	243	LEU	CA-CB-CG	6.62	130.52	115.30
6	0	8	GLY	N-CA-C	6.52	129.41	113.10
3	y	183	LEU	CB-CG-CD2	-6.26	100.36	111.00
3	M	49	GLY	C-N-CD	-6.24	106.86	120.60
4	t	180	ARG	NE-CZ-NH2	-6.24	117.18	120.30
4	H	71	HIS	N-CA-C	6.20	127.75	111.00
3	y	49	GLY	C-N-CD	-5.96	107.48	120.60
1	C	252	ASN	N-CA-C	-5.95	94.94	111.00
4	t	108	LEU	CA-CB-CG	-5.95	101.62	115.30
4	t	41	LEU	CB-CG-CD1	-5.94	100.90	111.00
5	p	9	TYR	N-CA-C	-5.94	94.97	111.00
2	L	196	LEU	CB-CG-CD1	-5.91	100.96	111.00
3	y	122	LEU	CB-CG-CD2	5.85	120.95	111.00
4	H	225	LEU	CA-CB-CG	5.84	128.73	115.30
1	C	307	CYS	CA-CB-SG	-5.84	103.49	114.00
3	y	95	LEU	CA-CB-CG	5.82	128.69	115.30
5	AI	8	LEU	CA-CB-CG	5.82	128.69	115.30
1	o	155	CYS	CA-CB-SG	-5.80	103.56	114.00
6	q	8	GLY	N-CA-C	-5.79	98.62	113.10
3	M	18	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	C	29	GLY	N-CA-C	-5.78	98.65	113.10
1	C	192	TYR	CB-CG-CD1	-5.73	117.56	121.00
5	Q	15	LEU	CA-CB-CG	5.69	128.40	115.30
4	H	160	ASP	CB-CG-OD2	5.68	123.41	118.30
2	x	261	GLY	N-CA-C	-5.66	98.96	113.10
1	o	62	LEU	CA-CB-CG	5.64	128.27	115.30
2	L	280	LEU	CA-CB-CG	5.63	128.26	115.30
4	H	159	LEU	CB-CG-CD1	5.62	120.56	111.00
4	H	256	GLY	N-CA-C	-5.62	99.05	113.10
1	C	192	TYR	CB-CG-CD2	5.61	124.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	198	ASP	CB-CG-OD1	5.61	123.35	118.30
3	M	18	TYR	CB-CG-CD1	5.58	124.35	121.00
6	T	31	LEU	CA-CB-CG	5.55	128.06	115.30
6	k	9	LEU	CA-CB-CG	5.45	127.84	115.30
6	T	38	LEU	CA-CB-CG	5.43	127.79	115.30
5	d	59	GLY	N-CA-C	-5.43	99.53	113.10
3	M	154	ILE	CG1-CB-CG2	-5.41	99.50	111.40
3	M	262	MET	CG-SD-CE	5.41	108.85	100.20
6	J	9	LEU	CA-CB-CG	5.40	127.72	115.30
2	x	28	GLY	N-CA-C	-5.34	99.75	113.10
1	C	243	LEU	CA-CB-CG	5.33	127.56	115.30
6	g	8	GLY	N-CA-C	5.33	126.42	113.10
2	x	118	ARG	CG-CD-NE	5.33	122.98	111.80
1	C	318	LEU	CA-CB-CG	5.32	127.53	115.30
2	L	257	ILE	CG1-CB-CG2	-5.28	99.78	111.40
4	t	38	GLY	N-CA-C	5.27	126.28	113.10
4	H	185	GLU	N-CA-C	-5.26	96.79	111.00
2	x	245	LEU	CB-CG-CD2	5.25	119.92	111.00
5	Y	51	ILE	CG1-CB-CG2	-5.23	99.89	111.40
4	t	69	LEU	CB-CG-CD2	5.19	119.82	111.00
5	S	15	LEU	CA-CB-CG	5.16	127.16	115.30
3	y	148	TRP	CA-CB-CG	5.14	123.48	113.70
3	y	18	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	C	112	VAL	N-CA-C	-5.12	97.19	111.00
3	M	250	LEU	CB-CG-CD1	-5.11	102.32	111.00
5	AA	15	LEU	CA-CB-CG	5.10	127.03	115.30
1	o	150	VAL	CG1-CB-CG2	-5.08	102.77	110.90
3	y	15	ALA	N-CA-C	-5.07	97.30	111.00
3	y	241	ARG	NE-CZ-NH1	-5.06	117.77	120.30
3	M	196	LEU	CB-CG-CD2	-5.05	102.42	111.00
3	M	215	LEU	CA-CB-CG	-5.05	103.69	115.30
3	M	233	ARG	NE-CZ-NH2	-5.05	117.78	120.30
5	U	40	LEU	CA-CB-CG	5.05	126.91	115.30
4	H	27	ILE	CG1-CB-CG2	-5.04	100.31	111.40
2	L	280	LEU	CB-CG-CD2	-5.03	102.45	111.00
2	x	278	LEU	CB-CG-CD1	-5.03	102.45	111.00
3	y	307	TYR	CA-CB-CG	5.03	122.95	113.40
4	t	107	MET	CB-CG-SD	-5.02	97.33	112.40
4	t	17	TRP	CA-CB-CG	5.02	123.23	113.70
5	AG	13	LEU	CA-CB-CG	5.01	126.83	115.30
2	L	278	LEU	CA-CB-CG	5.01	126.81	115.30
2	x	33	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	1	51	ILE	Peptide
5	1	59	GLY	Peptide
6	AJ	13	GLU	Peptide
6	AJ	14	ALA	Peptide
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
6	X	14	ALA	Peptide
4	t	29	TYR	Sidechain
2	x	268	TRP	Mainchain
3	y	215	LEU	Mainchain
3	y	271	TRP	Mainchain
3	y	272	CYS	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:L:177:HIS:HB3	3:M:183:LEU:HD13	1.49	0.94
1:C:189:THR:O	1:C:238:ASN:ND2	1.99	0.93
9:G:102:BCL:H3A	9:G:102:BCL:H12	1.52	0.92
2:L:244:PHE:HD1	11:L:304:UQ8:H43	1.36	0.90
5:9:3:THR:HB	5:9:8:LEU:HB2	1.54	0.89
2:L:239:HIS:CD2	3:M:223:ILE:HG13	2.08	0.88
5:A:2:PHE:HB3	5:A:4:MET:HB2	1.55	0.87
5:AI:10:LYS:HA	5:AI:13:LEU:HD13	1.55	0.87
5:3:5:ASN:O	5:3:7:ASN:N	2.07	0.87
1:C:32:GLN:NE2	2:L:79:ASP:OD1	2.08	0.87
6:AF:44:PRO:O	5:AG:55:TYR:OH	1.93	0.86
9:R:102:BCL:H3A	9:R:102:BCL:H2	1.55	0.86
9:X:102:BCL:HMA1	9:Y:101:BCL:HMA1	1.57	0.86
5:1:36:HIS:CE1	9:1:102:BCL:HMD1	2.11	0.86
2:L:189:PHE:CD1	2:L:249:ALA:HB1	2.12	0.85
6:T:17:PHE:HA	15:T:101:CRT:H6	1.58	0.85
3:M:18:TYR:CE2	3:M:20:GLY:HA2	2.12	0.85
9:B:101:BCL:H122	5:9:2:PHE:HA	1.55	0.85
2:L:188:PHE:CD2	2:L:248:SER:HB3	2.12	0.85
4:H:137:ARG:NH1	4:H:229:ASP:OD1	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:176:PHE:HE1	2:L:179:ASN:HD22	1.25	0.84
4:H:94:PRO:HG2	6:O:8:GLY:HA2	1.60	0.83
5:A:49:ASP:OD2	6:B:43:ARG:NH1	2.11	0.83
3:M:12:GLN:OE1	3:M:14:ARG:NH2	2.11	0.83
5:5:50:ASN:HB2	5:5:54:SER:HA	1.59	0.83
5:I:11:ILE:HG12	9:K:101:BCL:H161	1.61	0.83
4:H:113:PRO:HG3	4:H:248:LEU:HB3	1.60	0.81
2:L:44:LEU:HD23	5:9:30:VAL:HG11	1.62	0.81
3:M:214:LEU:O	3:M:218:MET:HG3	1.80	0.81
1:C:278:ASP:OD1	1:C:282:ASN:ND2	2.14	0.81
6:E:16:GLU:HB3	15:E:101:CRT:H21A	2.53	0.80
10:L:302:BPH:H18	9:L:305:BCL:HMB3	1.62	0.80
5:AI:4:MET:O	5:AI:5:ASN:ND2	2.15	0.80
6:B:20:ILE:O	6:B:24:SER:OG	1.99	0.80
15:2:101:CRT:H35	9:3:101:BCL:HMB2	1.62	0.80
5:9:11:ILE:HD13	15:9:102:CRT:H10	1.63	0.80
6:J:17:PHE:HA	15:J:101:CRT:H6	1.64	0.80
3:M:99:PRO:HD2	3:M:102:TYR:HD2	1.47	0.79
1:C:20:LEU:HA	1:C:21:LEU:HB2	1.62	0.79
3:M:145:HIS:HA	3:M:148:TRP:CE3	2.17	0.79
6:P:17:PHE:HA	15:P:102:CRT:H6	1.63	0.79
5:A:50:ASN:HB3	5:A:54:SER:HA	1.64	0.78
5:U:5:ASN:OD1	5:U:7:ASN:N	2.15	0.78
2:L:203:ILE:HG13	3:M:266:HIS:CD2	2.19	0.78
5:I:40:LEU:O	5:I:45:ASN:ND2	2.17	0.77
5:AI:36:HIS:CE1	9:AJ:102:BCL:HMD1	2.19	0.77
6:R:43:ARG:HG3	5:S:55:TYR:CZ	2.19	0.77
1:C:169:ASP:OD1	1:C:171:GLY:N	2.18	0.77
5:W:50:ASN:HB2	5:W:54:SER:HA	4.51	0.77
5:I:9:TYR:OH	6:J:11:ASP:OD1	2.03	0.77
2:L:179:ASN:O	2:L:183:MET:HG3	1.85	0.77
1:C:173:LYS:HB2	3:M:80:HIS:HB2	1.66	0.77
5:Y:44:LEU:HD23	5:1:55:TYR:HE2	1.48	0.77
5:AC:36:HIS:CE1	9:AC:102:BCL:HMD1	2.20	0.76
2:L:21:ASP:O	5:9:18:ARG:NH2	2.19	0.76
5:AI:49:ASP:O	5:AK:60:LYS:N	2.15	0.76
5:D:49:ASP:HB2	5:D:51:ILE:HG13	2.16	0.76
5:AE:11:ILE:HD12	5:AE:14:ILE:HD12	1.67	0.76
9:4:102:BCL:HMA1	9:5:101:BCL:HMA1	1.66	0.75
3:M:267:ARG:NH1	12:H:304:PEF:O1P	2.17	0.75
6:R:17:PHE:HA	15:R:101:CRT:H6	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:51:ILE:HG23	5:Y:52:PRO:HA	1.68	0.75
4:H:37:GLU:O	4:H:39:TYR:N	2.20	0.75
15:9:102:CRT:H81	15:9:102:CRT:H11	1.67	0.75
15:X:101:CRT:H21	15:X:101:CRT:H181	1.69	0.75
12:M:406:PEF:N	4:H:39:TYR:OH	2.20	0.75
6:AL:17:PHE:HA	15:AL:101:CRT:H6	1.69	0.75
5:5:36:HIS:CE1	9:5:102:BCL:HMD1	2.21	0.74
5:AA:50:ASN:ND2	5:AC:59:GLY:O	2.19	0.74
6:G:17:PHE:HA	15:G:101:CRT:H6	1.67	0.74
6:N:17:PHE:HD1	15:N:101:CRT:H5	4.04	0.74
5:U:25:VAL:HG13	9:U:101:BCL:H71	7.01	0.74
5:AE:43:ASP:HB2	5:AG:48:ASP:HA	1.70	0.74
6:2:17:PHE:HA	15:2:101:CRT:H6	1.68	0.74
3:M:126:ILE:HD13	9:M:401:BCL:H91	1.71	0.73
6:E:40:TRP:HZ3	6:E:46:LEU:H	1.36	0.73
4:H:249:TYR:O	4:H:251:THR:N	2.21	0.73
9:F:101:BCL:H62	9:F:101:BCL:H121	5.81	0.73
15:U:102:CRT:H14	6:V:21:PHE:HA	1.69	0.73
5:W:11:ILE:HD13	15:Z:101:CRT:H10	1.70	0.73
2:L:2:ALA:N	12:A:101:PEF:O1P	2.22	0.73
2:L:232:SER:OG	11:L:304:UQ8:O5	2.05	0.73
3:M:65:LEU:HD21	10:M:402:BPH:H102	1.70	0.73
1:C:247:CYS:SG	7:C:503:HEM:CAB	2.76	0.73
6:B:20:ILE:HG23	5:9:5:ASN:HB3	1.71	0.72
6:J:43:ARG:HG3	5:K:55:TYR:CZ	2.24	0.72
1:C:19:MET:O	1:C:21:LEU:HD22	1.89	0.72
6:X:17:PHE:HA	15:X:101:CRT:H6	1.70	0.72
3:M:229:PHE:HE2	3:M:247:ARG:HD3	1.51	0.72
2:L:72:ARG:HD2	3:M:305:PRO:HA	1.70	0.72
5:7:36:HIS:CE1	9:8:102:BCL:HMD1	2.25	0.72
5:7:45:ASN:O	5:7:49:ASP:OD2	2.06	0.72
6:AL:21:PHE:HD1	15:AL:101:CRT:H14	1.54	0.72
6:B:17:PHE:HD1	15:9:102:CRT:H5	1.53	0.72
2:L:118:ARG:NH1	12:L:306:PEF:O1P	2.22	0.72
2:L:225:PHE:CE2	11:L:304:UQ8:H1MA	2.23	0.72
3:M:177:PHE:HD1	15:M:404:CRT:H16	1.55	0.72
9:M:401:BCL:H61	10:M:402:BPH:C4B	2.19	0.72
5:3:40:LEU:HG	5:3:46:TRP:CH2	2.25	0.72
9:AK:101:BCL:H2	6:AL:28:TRP:CH2	2.25	0.72
9:R:102:BCL:HMB3	9:S:102:BCL:HMA3	1.72	0.72
1:C:152:CYS:SG	7:C:502:HEM:CAB	2.78	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:60:ASP:OD1	4:H:61:LEU:N	2.22	0.71
1:C:264:PRO:HD3	3:M:312:THR:O	1.90	0.71
1:C:153:TYR:CD1	1:C:157:ARG:HA	2.25	0.71
1:C:263:THR:HG22	3:M:311:VAL:HG11	1.71	0.71
3:M:260:VAL:HB	3:M:264:SER:OG	1.90	0.71
9:R:102:BCL:HMA1	9:S:102:BCL:HMA1	1.71	0.71
5:1:57:ALA:H	5:1:59:GLY:N	1.89	0.71
3:M:219:HIS:CE1	3:M:266:HIS:HE1	2.08	0.71
2:L:225:PHE:HE2	11:L:304:UQ8:H1MA	1.54	0.71
3:M:37:SER:HG	3:M:40:LEU:H	1.39	0.71
5:Y:36:HIS:CE1	9:Z:102:BCL:HMD1	2.26	0.71
2:L:225:PHE:CD2	11:L:304:UQ8:H7A	2.26	0.71
1:C:307:CYS:SG	7:C:504:HEM:CAB	2.77	0.70
10:L:302:BPH:H201	9:L:305:BCL:HMA1	1.72	0.70
6:N:21:PHE:HA	15:N:101:CRT:H14	2.20	0.70
5:F:34:LEU:HD21	15:G:101:CRT:H2M2	1.72	0.70
9:1:102:BCL:HMA1	9:3:101:BCL:HMA1	1.73	0.70
6:B:44:PRO:HG2	5:D:52:PRO:HD3	1.73	0.70
9:W:101:BCL:C1D	9:Z:102:BCL:HMD2	18.36	0.70
2:L:222:ASN:O	2:L:226:ARG:HG3	1.92	0.70
5:I:11:ILE:HD13	15:N:101:CRT:H10	1.73	0.70
15:A:103:CRT:H5	5:7:14:ILE:HD11	1.73	0.70
9:AK:101:BCL:H2	6:AL:28:TRP:CZ2	2.26	0.70
5:D:5:ASN:HB3	5:D:8:LEU:HB2	3.80	0.70
9:O:101:BCL:HMA1	9:Q:101:BCL:HMA1	1.72	0.70
6:AB:45:TRP:CD1	6:AB:46:LEU:HG	2.26	0.70
5:Y:39:VAL:HG11	9:Y:101:BCL:HBC1	1.73	0.70
9:A:102:BCL:HMB2	9:A:102:BCL:H122	1.74	0.70
5:S:44:LEU:HD22	6:T:43:ARG:HD3	1.73	0.70
15:AJ:101:CRT:H181	15:AJ:101:CRT:H21	1.73	0.70
6:N:32:VAL:HG21	9:N:102:BCL:HBA2	1.74	0.70
5:D:33:LEU:HD23	15:9:102:CRT:H36	1.74	0.69
5:U:16:ASP:OD2	5:U:18:ARG:NH2	2.16	0.69
9:D:102:BCL:H92	6:E:33:VAL:HG22	1.74	0.69
4:H:126:THR:HG23	4:H:130:LEU:O	1.92	0.69
3:M:134:TYR:CE1	3:M:144:GLN:HG3	2.26	0.69
5:1:57:ALA:H	5:1:58:LEU:C	1.96	0.69
5:AG:5:ASN:O	5:AG:7:ASN:N	2.24	0.69
4:H:14:ILE:HD13	5:I:37:MET:SD	2.32	0.69
6:AB:17:PHE:HA	15:AC:101:CRT:H6	1.75	0.69
9:Y:101:BCL:H2	6:Z:28:TRP:CZ2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ALA:O	1:C:273:ILE:HG13	1.92	0.69
1:C:107:CYS:SG	7:C:501:HEM:HAB	2.32	0.69
3:M:99:PRO:HD2	3:M:102:TYR:CD2	2.26	0.69
5:F:9:TYR:HB2	6:G:14:ALA:O	2.59	0.69
2:L:240:ARG:NH1	3:M:7:ILE:O	2.26	0.69
5:S:51:ILE:HG22	5:S:52:PRO:HA	1.73	0.69
5:U:39:VAL:HG11	9:U:101:BCL:HBC1	1.74	0.69
5:9:5:ASN:O	5:9:7:ASN:N	2.20	0.68
6:G:44:PRO:O	5:I:55:TYR:OH	2.11	0.68
5:A:16:ASP:OD2	5:A:19:ARG:HG3	1.93	0.68
9:Z:102:BCL:HMA1	9:AA:101:BCL:HMA1	98.71	0.68
6:AB:21:PHE:HA	15:AC:101:CRT:H14	1.75	0.68
6:AD:31:LEU:HD22	9:AD:101:BCL:H191	1.75	0.68
15:U:102:CRT:H22A	6:V:17:PHE:HB2	1.76	0.68
9:AA:101:BCL:HBD	9:AB:101:BCL:HED3	1.74	0.68
9:AH:101:BCL:HAA1	9:AH:101:BCL:HBD	1.75	0.68
15:4:101:CRT:H30	9:4:102:BCL:HMA2	1.75	0.68
1:C:292:PRO:HG2	1:C:295:ARG:HG2	1.76	0.68
1:C:71:LYS:O	1:C:74:GLU:HG2	1.93	0.68
5:AI:8:LEU:HD11	9:AK:101:BCL:H191	1.76	0.68
3:M:175:VAL:HG22	3:M:185:TRP:CE2	2.28	0.68
6:AB:32:VAL:HG21	9:AB:101:BCL:HBA2	1.76	0.68
3:M:145:HIS:HA	3:M:148:TRP:HE3	1.59	0.68
9:K:101:BCL:HED1	6:N:28:TRP:CZ2	2.29	0.68
5:O:14:ILE:HD11	15:R:101:CRT:H31A	1.75	0.68
5:3:36:HIS:CE1	9:4:102:BCL:HMD1	2.29	0.67
4:H:54:LYS:NZ	12:H:303:PEF:O1P	2.28	0.67
5:D:7:ASN:HB3	5:D:10:LYS:HD2	3.89	0.67
4:H:88:ASN:ND2	4:H:109:SER:O	2.27	0.67
9:AA:101:BCL:HBA2	9:AB:101:BCL:HED3	1.76	0.67
1:C:112:VAL:HG21	1:C:120:ASP:HB3	1.77	0.67
1:C:310:CYS:SG	7:C:504:HEM:CAC	2.82	0.67
5:AC:28:GLN:HB3	9:AD:101:BCL:H42	1.77	0.67
5:AG:5:ASN:OD1	5:AG:7:ASN:HB2	1.95	0.67
2:L:106:PHE:CE1	9:L:301:BCL:H121	2.30	0.66
3:M:208:PHE:CD2	3:M:275:LEU:HB3	2.30	0.66
9:S:102:BCL:HMA1	9:U:101:BCL:HMA1	17.71	0.66
5:AC:43:ASP:HB2	5:AE:48:ASP:HA	1.77	0.66
9:D:101:BCL:HHB	15:AL:101:CRT:H35	115.21	0.66
4:H:159:LEU:HD22	4:H:254:ARG:NH2	2.10	0.66
5:W:16:ASP:OD2	5:W:19:ARG:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:5:ASN:OD1	5:O:5:ASN:N	2.29	0.66
1:C:107:CYS:SG	7:C:501:HEM:CAB	2.83	0.66
5:U:11:ILE:HD12	5:U:14:ILE:HD12	2.30	0.66
1:C:164:TYR:HD2	1:C:312:GLN:HG2	1.59	0.66
9:AH:103:BCL:HMB2	9:AH:103:BCL:H102	1.77	0.66
2:L:160:LEU:O	2:L:163:LEU:HB2	1.96	0.66
1:C:153:TYR:CE1	1:C:157:ARG:HA	2.30	0.66
3:M:265:ILE:HD13	14:M:403:MQ8:H121	1.78	0.66
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.78	0.66
5:1:51:ILE:HG22	5:1:52:PRO:HA	1.78	0.65
5:AE:22:VAL:HG22	9:AE:102:BCL:H172	1.79	0.65
4:H:65:LYS:HE2	4:H:67:PHE:CE1	2.30	0.65
3:M:229:PHE:CE2	3:M:247:ARG:HD3	2.30	0.65
5:F:31:LEU:HD12	5:F:34:LEU:HD23	1.79	0.65
9:I:101:BCL:C1D	9:J:102:BCL:HMD2	2.26	0.65
3:M:265:ILE:HG23	3:M:266:HIS:ND1	2.11	0.65
2:L:31:TYR:HB3	2:L:116:ILE:HD11	1.77	0.65
1:C:137:ALA:HA	1:C:141:TRP:HD1	1.62	0.65
1:C:21:LEU:HG	2:L:274:TRP:CD1	2.32	0.65
9:G:102:BCL:HMA1	9:I:101:BCL:HMA1	1.78	0.65
2:L:184:LEU:HD23	2:L:252:TRP:CD2	2.32	0.65
9:8:102:BCL:H2	9:8:102:BCL:H8	1.78	0.65
4:H:31:ARG:NH1	4:H:34:ASP:OD2	2.30	0.65
1:C:21:LEU:HD23	2:L:271:TRP:CZ2	2.30	0.65
5:U:11:ILE:HG12	9:W:101:BCL:H161	6.42	0.65
6:8:32:VAL:HG21	9:8:102:BCL:HBA2	1.79	0.65
6:G:18:HIS:O	6:G:22:MET:HG2	1.97	0.65
6:G:43:ARG:HG3	5:I:55:TYR:CE1	2.32	0.65
2:L:188:PHE:CE2	2:L:248:SER:HB3	2.32	0.65
5:Q:17:PRO:HB3	6:R:17:PHE:CZ	2.32	0.65
1:C:194:SER:OG	3:M:184:ASP:OD2	2.13	0.65
1:C:307:CYS:HG	7:C:504:HEM:HAB	1.61	0.65
4:H:246:GLY:HA2	4:H:250:ALA:H	1.61	0.65
6:8:43:ARG:HG3	5:9:55:TYR:CZ	2.32	0.64
15:AH:102:CRT:H292	9:AI:101:BCL:H43	1.79	0.64
6:N:17:PHE:HA	15:N:101:CRT:H83	5.24	0.64
5:S:25:VAL:HG22	9:S:102:BCL:H8	1.80	0.64
5:K:40:LEU:HG	5:K:46:TRP:CH2	2.33	0.64
5:F:11:ILE:HD13	15:J:101:CRT:H10	1.79	0.64
2:L:239:HIS:CG	3:M:223:ILE:HG21	2.31	0.64
5:Q:38:ILE:O	5:Q:42:THR:HG23	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:24:SER:HB2	15:X:101:CRT:H14	1.77	0.64
5:U:7:ASN:HB3	5:U:10:LYS:HD2	2.33	0.64
10:L:302:BPH:H141	9:L:305:BCL:HBB3	1.80	0.64
5:Q:44:LEU:HD12	5:S:47:LEU:HD22	1.79	0.64
15:2:101:CRT:H372	5:3:36:HIS:CD2	2.33	0.64
5:7:12:TRP:HB3	5:7:17:PRO:HG3	1.80	0.64
1:C:250:CYS:SG	7:C:503:HEM:CAC	2.86	0.64
9:L:303:BCL:H203	9:L:303:BCL:H141	1.80	0.64
6:T:35:ALA:HA	6:T:38:LEU:HD12	1.78	0.64
4:H:150:ASP:OD1	4:H:152:ARG:HB2	1.97	0.64
3:M:62:PHE:HB3	5:Q:30:VAL:HG21	1.80	0.64
9:1:101:BCL:HMD1	6:2:36:HIS:CE1	2.33	0.64
5:D:36:HIS:CD2	15:AL:101:CRT:H372	117.20	0.64
4:H:186:VAL:HG23	4:H:191:LYS:O	1.96	0.64
6:R:32:VAL:HG21	9:R:102:BCL:HBA2	1.80	0.64
9:5:102:BCL:HMA1	9:7:101:BCL:HMA1	1.81	0.63
5:AI:21:LEU:HD11	15:AJ:101:CRT:H133	1.80	0.63
1:C:128:ARG:NE	7:C:501:HEM:O2D	2.31	0.63
5:AE:38:ILE:O	5:AE:42:THR:HG23	1.98	0.63
9:D:101:BCL:HMB2	15:AL:101:CRT:H35	116.63	0.63
4:H:57:GLY:H	12:H:301:PEF:HN2	1.46	0.63
1:C:179:LYS:HD2	3:M:111:GLU:HG3	1.80	0.63
5:AK:36:HIS:CE1	9:AL:102:BCL:HMD1	2.33	0.63
2:L:281:TRP:HB2	3:M:88:LYS:HD2	1.78	0.63
6:X:28:TRP:HZ2	9:X:102:BCL:HED1	1.62	0.63
3:M:34:PRO:HG3	3:M:50:PRO:HD3	1.78	0.63
15:8:101:CRT:H371	9:9:103:BCL:HMB2	1.80	0.63
4:H:141:GLU:HG2	4:H:142:PHE:H	1.64	0.63
4:H:234:TYR:O	4:H:238:LYS:HG2	1.99	0.63
9:W:101:BCL:HMD1	6:X:36:HIS:CE1	2.33	0.63
5:W:14:ILE:HD11	15:AC:101:CRT:H21A	58.58	0.63
4:H:45:ARG:HH11	4:H:53:VAL:HG11	1.63	0.63
1:C:159:ASN:OD1	1:C:163:LYS:HE3	1.99	0.63
1:C:97:VAL:HG21	1:C:131:PHE:CZ	2.33	0.63
5:I:39:VAL:HG11	9:I:101:BCL:HAC2	1.81	0.63
2:L:237:ALA:HA	2:L:240:ARG:HD2	1.81	0.63
3:M:175:VAL:HG13	3:M:185:TRP:CG	2.33	0.63
9:AA:101:BCL:H162	9:AA:101:BCL:H101	1.81	0.63
6:AJ:44:PRO:O	5:AK:55:TYR:OH	2.17	0.63
9:AK:101:BCL:CHD	9:AL:102:BCL:HMD2	2.29	0.63
9:A:102:BCL:HMA1	9:D:101:BCL:HMA1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:45:TRP:CD1	6:G:46:LEU:HG	2.34	0.63
15:G:101:CRT:H32	9:I:101:BCL:H3A	1.80	0.63
9:O:101:BCL:H2	9:O:101:BCL:HBA1	1.81	0.63
6:T:44:PRO:HG2	5:U:52:PRO:HG3	1.80	0.63
6:AF:45:TRP:HD1	6:AF:46:LEU:HG	1.62	0.62
3:M:219:HIS:CE1	3:M:266:HIS:CE1	2.87	0.62
6:Z:32:VAL:HG21	9:Z:102:BCL:HBA2	1.96	0.62
5:U:43:ASP:HB3	5:W:50:ASN:HD21	7.77	0.62
6:O:11:ASP:O	6:O:15:LYS:HG3	2.00	0.62
3:M:159:VAL:HA	3:M:163:ILE:HB	1.82	0.62
5:1:44:LEU:HD23	5:3:55:TYR:CE2	2.34	0.62
15:AJ:101:CRT:H36	5:AK:33:LEU:HD23	1.80	0.62
3:M:267:ARG:NH1	12:H:304:PEF:O3	2.33	0.62
2:L:68:TYR:HA	2:L:73:ILE:HD11	1.80	0.62
5:5:17:PRO:HB3	6:6:17:PHE:CZ	2.34	0.62
3:M:240:HIS:CE1	4:H:69:LEU:HD11	2.33	0.62
5:U:49:ASP:OD2	6:V:43:ARG:NH1	6.74	0.62
5:A:45:ASN:O	5:A:49:ASP:OD2	2.17	0.62
6:E:21:PHE:HA	15:E:101:CRT:H11	1.81	0.62
3:M:28:LEU:HD12	3:M:54:GLY:HA2	1.80	0.62
5:5:14:ILE:HG13	5:5:15:LEU:HG	1.82	0.62
5:D:36:HIS:CD2	15:9:102:CRT:H372	2.34	0.62
3:M:59:LEU:HB3	3:M:128:LEU:HD13	1.82	0.62
5:Y:50:ASN:OD1	5:Y:55:TYR:N	2.33	0.62
5:9:36:HIS:CE1	9:O:101:BCL:HMD1	2.35	0.61
6:AH:28:TRP:CZ2	9:AH:101:BCL:H2	2.34	0.61
6:N:40:TRP:HH2	6:N:46:LEU:OXT	1.83	0.61
3:M:135:LYS:HD3	5:O:19:ARG:HH11	1.64	0.61
6:Z:45:TRP:NE1	9:Z:102:BCL:OBB	4.12	0.61
5:AG:5:ASN:C	5:AG:7:ASN:H	2.03	0.61
1:C:152:CYS:SG	7:C:502:HEM:HAB	2.40	0.61
9:K:101:BCL:C1D	9:N:102:BCL:HMD2	2.31	0.61
2:L:69:ASN:OD1	2:L:71:TRP:N	2.30	0.61
5:1:17:PRO:HB3	6:2:17:PHE:CZ	2.36	0.61
9:AC:102:BCL:HBA2	6:AD:32:VAL:HG21	1.82	0.61
6:AJ:17:PHE:HA	15:AJ:101:CRT:H6	1.82	0.61
6:AJ:32:VAL:HG21	9:AJ:102:BCL:HBA2	1.81	0.61
6:E:43:ARG:HG3	5:F:55:TYR:CZ	2.35	0.61
9:M:401:BCL:C2	10:M:402:BPH:HBB2	2.31	0.61
3:M:76:LEU:HG	3:M:81:TRP:HA	1.82	0.61
6:AF:18:HIS:O	6:AF:22:MET:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:43:ASP:CG	5:U:50:ASN:HA	2.21	0.61
6:AB:18:HIS:O	6:AB:22:MET:HG2	2.00	0.61
3:M:150:PHE:N	10:M:402:BPH:HMD3	2.16	0.61
2:L:196:LEU:HD13	3:M:216:PHE:CG	2.36	0.61
5:W:16:ASP:OD2	5:W:19:ARG:HB2	3.36	0.61
3:M:161:GLY:HA3	15:M:404:CRT:H292	1.82	0.61
5:A:39:VAL:HG21	9:A:102:BCL:H3C	1.83	0.61
5:AK:59:GLY:O	5:AK:61:LYS:N	2.32	0.61
3:M:6:ASN:HD22	3:M:227:SER:HB2	1.65	0.61
6:Z:43:ARG:HD3	5:1:55:TYR:OH	2.01	0.61
1:C:141:TRP:O	1:C:145:VAL:HG22	2.01	0.61
5:I:2:PHE:HA	5:I:4:MET:SD	2.41	0.61
2:L:175:HIS:NE2	3:M:184:ASP:OD1	2.33	0.61
15:M:404:CRT:H2M3	5:O:38:ILE:HG12	1.81	0.61
5:O:43:ASP:OD2	5:Q:50:ASN:ND2	2.32	0.61
5:A:18:ARG:NH1	12:A:101:PEF:H51	2.16	0.61
5:AG:42:THR:HG21	5:AI:47:LEU:HD13	1.83	0.61
1:C:316:LYS:HG2	7:C:504:HEM:HAD2	1.81	0.61
3:M:146:LEU:O	3:M:149:ALA:N	2.34	0.61
5:O:43:ASP:HB2	5:Q:48:ASP:HA	1.83	0.61
15:AE:103:CRT:H372	5:AG:36:HIS:CG	2.35	0.60
6:AF:45:TRP:CD1	6:AF:46:LEU:HG	2.35	0.60
5:D:5:ASN:ND2	6:G:20:ILE:HA	6.63	0.60
5:U:5:ASN:HB3	5:U:8:LEU:HB2	1.83	0.60
6:Z:29:PHE:O	6:Z:33:VAL:HG23	2.41	0.60
6:G:13:GLU:HB3	15:G:101:CRT:H21A	1.82	0.60
2:L:77:PRO:HB2	2:L:152:GLY:HA2	1.82	0.60
9:W:101:BCL:HBD	9:W:101:BCL:HAA2	1.83	0.60
5:1:10:LYS:HB3	15:4:101:CRT:H22A	1.84	0.60
5:9:39:VAL:HG11	9:9:103:BCL:HBC1	1.83	0.60
9:AH:103:BCL:H52	9:AH:103:BCL:H3A	1.83	0.60
9:G:102:BCL:H3A	9:G:102:BCL:C1	2.30	0.60
9:A:102:BCL:HBA2	6:B:32:VAL:HG21	1.84	0.60
3:M:72:GLY:HA3	15:M:404:CRT:C6	2.31	0.60
9:Z:102:BCL:HMB1	9:Z:102:BCL:HBB2	1.83	0.60
6:Z:18:HIS:O	6:Z:22:MET:HG2	2.71	0.60
9:Y:101:BCL:H2	6:Z:28:TRP:CH2	2.36	0.60
5:W:36:HIS:CE1	9:X:102:BCL:HMD1	2.36	0.60
5:AA:50:ASN:HB2	5:AC:59:GLY:HA3	1.82	0.60
5:D:36:HIS:CE1	9:D:102:BCL:HMD1	2.36	0.60
9:D:101:BCL:H2	6:E:28:TRP:CH2	3.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:235:GLU:O	4:H:239:VAL:HG23	2.02	0.60
6:J:18:HIS:O	6:J:22:MET:HG2	2.00	0.60
15:AE:103:CRT:H6	6:AF:17:PHE:HA	1.83	0.60
9:1:102:BCL:H102	6:2:36:HIS:CD2	2.37	0.60
9:9:103:BCL:H2	6:0:28:TRP:CZ2	2.36	0.60
5:9:16:ASP:OD2	5:9:19:ARG:HG3	2.01	0.60
4:H:196:PRO:HD3	4:H:243:TYR:CE2	2.37	0.60
9:Z:102:BCL:H52	9:Z:102:BCL:HBA1	1.83	0.60
5:7:43:ASP:N	5:9:48:ASP:OD1	2.34	0.60
3:M:99:PRO:HB2	3:M:101:GLN:HG2	1.82	0.60
5:AC:14:ILE:HD11	15:AE:103:CRT:H5	1.83	0.59
5:AE:36:HIS:CE1	9:AE:104:BCL:HMD1	2.37	0.59
6:AJ:18:HIS:O	6:AJ:22:MET:HG2	2.01	0.59
6:B:24:SER:HB3	5:9:2:PHE:C	2.22	0.59
2:L:125:HIS:CD2	3:M:224:LEU:HB3	2.37	0.59
6:0:36:HIS:CG	9:0:101:BCL:H91	2.37	0.59
6:4:29:PHE:CE1	9:4:102:BCL:H11	2.37	0.59
5:AG:54:SER:HB3	5:AG:57:ALA:HB3	1.84	0.59
2:L:144:ARG:HB3	2:L:145:PRO:HD3	1.84	0.59
2:L:18:ILE:HD12	2:L:35:PHE:HZ	1.67	0.59
6:N:18:HIS:O	6:N:22:MET:HG2	2.02	0.59
6:P:28:TRP:HH2	9:P:101:BCL:HBA1	1.67	0.59
9:AA:101:BCL:HED2	6:AB:35:ALA:HB2	1.82	0.59
1:C:273:ILE:HG12	7:C:504:HEM:HBB2	1.85	0.59
5:F:4:MET:O	5:F:6:ALA:N	2.67	0.59
4:H:176:GLU:O	4:H:178:GLN:HG2	2.03	0.59
3:M:2:PRO:HB2	4:H:201:ARG:CZ	2.32	0.59
2:L:191:THR:OG1	9:L:303:BCL:H12	2.02	0.59
6:E:17:PHE:HA	15:E:101:CRT:H6	1.83	0.59
6:Z:45:TRP:CD1	6:Z:46:LEU:HG	2.78	0.59
5:D:17:PRO:HB3	6:E:17:PHE:CZ	2.37	0.59
6:Z:17:PHE:HA	15:Z:101:CRT:H6	1.85	0.59
4:H:257:PRO:HG3	5:7:19:ARG:NH1	2.17	0.59
5:I:44:LEU:HD13	9:J:102:BCL:HAC1	1.83	0.59
5:I:45:ASN:O	6:J:43:ARG:NH1	2.34	0.59
2:L:167:SER:HA	9:L:301:BCL:HBC1	1.84	0.59
2:L:188:PHE:HD2	2:L:248:SER:HB3	1.66	0.59
2:L:106:PHE:CZ	9:L:301:BCL:H121	2.37	0.59
15:Z:101:CRT:H372	5:1:36:HIS:CD2	2.38	0.59
2:L:44:LEU:HD23	5:9:30:VAL:CG1	2.32	0.59
15:AE:103:CRT:H372	5:AG:36:HIS:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:5:ASN:ND2	6:AJ:23:GLN:OE1	2.33	0.59
5:W:10:LYS:HA	5:W:13:LEU:HD13	1.83	0.59
5:W:39:VAL:HG11	9:W:101:BCL:HBC1	1.85	0.59
5:1:56:GLN:HB2	5:1:57:ALA:HA	1.84	0.59
6:AH:43:ARG:HG3	5:AI:55:TYR:CE1	2.37	0.59
1:C:59:VAL:HG23	1:C:153:TYR:CE2	2.38	0.59
5:I:17:PRO:HB3	6:J:17:PHE:CZ	2.38	0.59
9:U:101:BCL:HED3	6:V:32:VAL:HA	1.85	0.59
5:AC:36:HIS:CD2	15:AC:101:CRT:H372	2.37	0.58
9:F:101:BCL:HMD1	6:G:36:HIS:CE1	3.08	0.58
5:I:3:THR:N	5:I:4:MET:HA	2.18	0.58
6:T:43:ARG:HG3	5:U:55:TYR:OH	2.03	0.58
6:V:11:ASP:O	6:V:15:LYS:HG3	5.53	0.58
15:E:101:CRT:H82	5:AK:14:ILE:HD12	72.51	0.58
1:C:123:THR:O	1:C:127:SER:OG	2.13	0.58
2:L:244:PHE:CD1	11:L:304:UQ8:H43	2.28	0.58
6:Z:21:PHE:HA	15:Z:101:CRT:H11	1.85	0.58
9:N:102:BCL:HMA1	9:P:101:BCL:HMA1	1.84	0.58
6:N:43:ARG:HG3	5:O:55:TYR:OH	2.04	0.58
15:8:101:CRT:H27	9:8:102:BCL:H42	1.85	0.58
5:A:36:HIS:CE1	9:A:102:BCL:HMD1	2.38	0.58
5:AC:17:PRO:HB3	6:AD:17:PHE:CZ	2.39	0.58
15:AH:102:CRT:H393	5:AI:36:HIS:HB3	1.86	0.58
9:AL:102:BCL:H3A	9:AL:102:BCL:CGA	2.33	0.58
6:G:43:ARG:HG3	5:I:55:TYR:CZ	2.38	0.58
15:A:103:CRT:H14	6:0:21:PHE:HA	1.86	0.58
15:A:103:CRT:H31A	6:0:17:PHE:HB2	1.84	0.58
6:E:40:TRP:HH2	6:E:46:LEU:HD12	1.67	0.58
5:S:48:ASP:OD1	5:S:48:ASP:N	2.36	0.58
6:X:45:TRP:HD1	6:X:46:LEU:HG	1.67	0.58
5:1:5:ASN:OD1	5:1:7:ASN:N	2.37	0.58
1:C:110:CYS:HA	1:C:123:THR:OG1	2.04	0.58
1:C:164:TYR:CD2	1:C:312:GLN:HG2	2.39	0.58
3:M:3:GLU:OE2	4:H:212:ASP:HB3	2.04	0.58
3:M:96:GLU:HG3	3:M:97:PRO:HD2	1.85	0.58
5:9:49:ASP:HB2	5:9:51:ILE:HG13	1.85	0.58
5:S:36:HIS:CE1	9:T:102:BCL:HMD1	2.39	0.58
5:7:44:LEU:HD12	5:9:47:LEU:HD22	1.85	0.58
5:A:17:PRO:HB3	6:B:17:PHE:CZ	2.39	0.58
3:M:7:ILE:HG13	12:M:407:PEF:H11	1.86	0.58
6:P:43:ARG:HG3	5:Q:55:TYR:OH	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:40:LEU:HD11	5:U:47:LEU:HD12	1.86	0.58
9:F:101:BCL:HBA1	6:G:28:TRP:HH2	1.69	0.57
9:I:101:BCL:HMD1	6:J:36:HIS:CE1	2.39	0.57
2:L:99:THR:HG1	2:L:157:TYR:HH	1.52	0.57
9:U:101:BCL:HMD1	6:V:36:HIS:CE1	3.24	0.57
4:H:44:ASP:HB3	4:H:48:ARG:HH21	1.68	0.57
5:U:40:LEU:HD13	5:U:46:TRP:CH2	2.38	0.57
15:4:101:CRT:H371	9:5:101:BCL:HMB2	1.85	0.57
1:C:232:THR:O	1:C:236:MET:HG2	2.04	0.57
1:C:128:ARG:HH21	7:C:501:HEM:HAD1	1.69	0.57
5:D:39:VAL:HG11	9:D:101:BCL:HBC1	2.29	0.57
5:W:8:LEU:HD11	15:AC:101:CRT:H133	70.36	0.57
5:F:23:SER:HB3	9:I:101:BCL:H143	1.86	0.57
4:H:45:ARG:HH12	12:H:301:PEF:H21	1.70	0.57
5:F:12:TRP:HB2	6:G:14:ALA:HB1	1.86	0.57
2:L:26:TRP:HZ3	4:H:99:PRO:HB3	1.69	0.57
5:S:17:PRO:HB3	6:T:17:PHE:CZ	2.38	0.57
5:W:40:LEU:O	5:W:45:ASN:ND2	3.11	0.57
5:AE:5:ASN:C	5:AE:7:ASN:H	2.06	0.57
5:D:18:ARG:HG3	5:AK:14:ILE:HG22	66.39	0.57
5:F:16:ASP:OD2	5:F:19:ARG:HG3	2.05	0.57
10:L:302:BPH:H111	9:L:305:BCL:H192	1.85	0.57
3:M:97:PRO:HD3	3:M:176:PRO:HB3	1.86	0.57
3:M:277:VAL:CG1	10:M:402:BPH:HAC2	2.34	0.57
9:Z:102:BCL:HMB2	9:Z:102:BCL:H93	1.86	0.57
6:2:40:TRP:HE3	6:2:45:TRP:CZ3	2.23	0.57
5:7:10:LYS:HA	5:7:13:LEU:HD13	1.86	0.57
6:AL:32:VAL:HG21	9:AL:102:BCL:HBA2	1.87	0.57
6:J:20:ILE:HD12	15:J:101:CRT:C6	2.35	0.57
3:M:178:GLY:O	3:M:182:HIS:HB3	2.05	0.57
9:W:101:BCL:H93	9:W:101:BCL:H152	1.87	0.57
9:W:101:BCL:HBD	9:W:101:BCL:HAA1	3.36	0.57
6:0:45:TRP:CD1	6:0:46:LEU:HG	2.40	0.57
5:AA:43:ASP:HB2	5:AC:48:ASP:HA	1.86	0.57
5:AC:43:ASP:HB2	5:AE:48:ASP:OD1	2.05	0.57
4:H:49:SER:O	12:H:303:PEF:N	2.38	0.57
5:AG:10:LYS:HA	5:AG:13:LEU:HD13	1.86	0.57
1:C:105:GLU:OE2	1:C:105:GLU:N	2.38	0.57
5:F:44:LEU:HD23	5:I:55:TYR:CE2	2.40	0.57
3:M:125:SER:OG	10:M:402:BPH:H2	2.04	0.57
3:M:267:ARG:HD3	12:H:304:PEF:C31	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:18:HIS:O	6:V:22:MET:HG2	2.03	0.57
5:3:40:LEU:HG	5:3:46:TRP:CZ3	2.39	0.57
4:H:157:VAL:HG12	4:H:163:VAL:HA	1.86	0.57
6:J:45:TRP:HZ2	9:J:102:BCL:H122	1.70	0.57
5:K:17:PRO:HB3	6:N:17:PHE:CZ	2.39	0.57
3:M:8:PHE:HB2	12:M:407:PEF:H42	1.86	0.57
6:B:45:TRP:HD1	6:B:46:LEU:HG	1.71	0.56
5:W:21:LEU:HD11	15:X:101:CRT:H133	1.87	0.56
6:X:40:TRP:HH2	6:X:46:LEU:OXT	1.87	0.56
5:Y:44:LEU:HD23	5:1:55:TYR:CE2	2.36	0.56
5:W:10:LYS:HD3	15:Z:101:CRT:H31A	1.86	0.56
5:W:17:PRO:HB3	6:Z:17:PHE:CZ	16.75	0.56
5:AK:49:ASP:OD2	6:AL:43:ARG:NH1	2.38	0.56
9:G:102:BCL:HBB2	9:G:102:BCL:H101	1.88	0.56
5:I:9:TYR:HB2	6:J:14:ALA:O	2.06	0.56
2:L:189:PHE:CE1	2:L:249:ALA:HB1	2.40	0.56
6:R:21:PHE:HA	15:R:101:CRT:H15	1.86	0.56
1:C:110:CYS:SG	7:C:501:HEM:CAC	2.93	0.56
9:AB:101:BCL:H42	9:AD:101:BCL:H172	1.88	0.56
5:AK:45:ASN:OD1	5:AK:47:LEU:N	2.34	0.56
6:P:21:PHE:CE1	15:P:102:CRT:H16	2.40	0.56
9:U:101:BCL:HBD	9:U:101:BCL:HAA2	1.87	0.56
9:Z:102:BCL:HAA2	9:Z:102:BCL:HED2	1.87	0.56
1:C:250:CYS:HA	1:C:263:THR:OG1	2.04	0.56
6:E:17:PHE:HB2	15:E:101:CRT:H23	4.59	0.56
9:U:101:BCL:H12	6:V:28:TRP:CZ2	3.11	0.56
6:8:21:PHE:HA	15:8:101:CRT:H11	1.88	0.56
1:C:72:ALA:N	1:C:85:LEU:O	2.30	0.56
5:W:12:TRP:O	6:Z:7:THR:OG1	16.51	0.56
9:D:102:BCL:HBA2	6:E:32:VAL:HG21	1.88	0.56
2:L:102:ALA:HB2	10:L:302:BPH:H121	1.87	0.56
5:U:3:THR:HB	5:U:8:LEU:HB3	11.23	0.56
9:W:101:BCL:HAA1	9:W:101:BCL:CBF	3.89	0.56
15:2:101:CRT:C32	9:3:101:BCL:H3A	2.36	0.56
5:AI:16:ASP:OD2	5:AI:19:ARG:HG3	2.06	0.56
9:1:102:BCL:HBA2	6:2:32:VAL:HG21	1.87	0.56
1:C:242:SER:HA	1:C:308:MET:CE	2.36	0.56
5:F:28:GLN:OE1	6:G:28:TRP:NE1	2.82	0.56
4:H:60:ASP:CG	4:H:61:LEU:H	2.09	0.56
5:F:5:ASN:N	6:J:23:GLN:OE1	2.39	0.56
5:3:5:ASN:ND2	6:6:23:GLN:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AE:104:BCL:HMA3	9:AH:101:BCL:HMB3	1.88	0.56
9:W:101:BCL:C1D	9:X:102:BCL:HMD2	2.36	0.56
5:U:8:LEU:HD21	9:W:101:BCL:H141	6.40	0.56
6:AB:45:TRP:HD1	6:AB:46:LEU:HG	1.69	0.55
1:C:200:LEU:HD22	1:C:204:LEU:HD12	1.87	0.55
6:E:16:GLU:O	6:E:20:ILE:HG13	2.07	0.55
4:H:140:LYS:H	4:H:140:LYS:HD2	1.71	0.55
5:I:26:ALA:O	5:I:29:ILE:HG22	2.05	0.55
3:M:152:ALA:O	3:M:155:PHE:HB3	2.05	0.55
3:M:34:PRO:CG	3:M:50:PRO:HD3	2.36	0.55
9:T:102:BCL:H3A	9:T:102:BCL:H43	1.88	0.55
5:W:41:SER:O	18:W:201:HOH:O	2.18	0.55
5:5:10:LYS:HD3	15:8:101:CRT:H22A	1.88	0.55
5:D:49:ASP:HB2	5:D:51:ILE:CG1	2.84	0.55
2:L:129:ALA:HB1	2:L:247:LEU:HD21	1.86	0.55
5:U:16:ASP:OD2	5:U:19:ARG:HG3	2.06	0.55
3:M:260:VAL:HG12	4:H:34:ASP:OD2	2.06	0.55
3:M:277:VAL:HG11	10:M:402:BPH:HAC2	1.88	0.55
6:Z:43:ARG:HD3	5:1:55:TYR:CE1	2.42	0.55
5:A:13:LEU:O	5:D:18:ARG:NH2	2.40	0.55
1:C:188:LYS:HB2	1:C:192:TYR:CZ	2.41	0.55
1:C:245:VAL:HG21	1:C:249:PHE:CD2	2.42	0.55
2:L:35:PHE:CD2	2:L:111:LEU:HB3	2.42	0.55
15:X:101:CRT:H181	15:X:101:CRT:C21	2.33	0.55
5:1:38:ILE:O	5:1:42:THR:HG23	2.06	0.55
15:AL:101:CRT:H27	9:AL:102:BCL:H11	1.89	0.55
5:D:5:ASN:OD1	5:D:7:ASN:N	7.24	0.55
9:D:101:BCL:HMD1	6:E:36:HIS:CE1	2.42	0.55
4:H:29:TYR:OH	12:H:304:PEF:C30	2.54	0.55
4:H:44:ASP:O	4:H:48:ARG:HB2	2.06	0.55
3:M:102:TYR:OH	3:M:111:GLU:OE1	2.16	0.55
5:5:43:ASP:HB2	5:7:48:ASP:HA	1.88	0.55
3:M:109:LEU:HD11	5:Q:42:THR:HG22	1.89	0.55
6:AL:45:TRP:CE2	9:AL:102:BCL:H2C	2.41	0.55
1:C:20:LEU:HA	1:C:21:LEU:CB	2.34	0.55
1:C:56:ASN:HB3	1:C:318:LEU:HA	1.88	0.55
5:D:12:TRP:HB3	5:D:17:PRO:HG3	1.87	0.55
6:R:40:TRP:CH2	6:R:46:LEU:HB2	2.42	0.55
5:S:25:VAL:HG21	9:S:102:BCL:H121	1.89	0.55
15:8:101:CRT:H293	9:9:103:BCL:H202	1.88	0.55
5:AA:14:ILE:HD11	15:AD:102:CRT:H31A	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:101:BCL:HAA2	9:F:101:BCL:HBD	1.89	0.55
6:G:46:LEU:HD22	6:J:42:TYR:CE2	2.41	0.55
6:J:21:PHE:HA	15:J:101:CRT:H14	1.87	0.55
2:L:184:LEU:HD23	2:L:252:TRP:CE2	2.42	0.55
2:L:222:ASN:HB3	2:L:226:ARG:NH1	2.22	0.55
5:7:4:MET:HG3	5:7:5:ASN:H	1.72	0.55
6:N:20:ILE:HB	15:N:101:CRT:H82	5.24	0.55
15:N:101:CRT:H393	5:O:36:HIS:HB3	1.89	0.55
5:U:25:VAL:HG22	9:U:101:BCL:H41	1.89	0.55
9:AI:101:BCL:CHD	9:AJ:102:BCL:HMD2	2.37	0.55
5:F:54:SER:HB3	5:F:57:ALA:HB3	1.89	0.55
5:F:17:PRO:HB3	6:G:17:PHE:CZ	2.42	0.55
4:H:193:VAL:HB	4:H:222:VAL:HG11	1.89	0.55
2:L:71:TRP:CD1	3:M:303:MET:HG2	2.42	0.55
15:N:101:CRT:H372	5:O:36:HIS:CD2	2.42	0.55
5:S:14:ILE:HD11	15:U:102:CRT:H31A	1.89	0.55
5:Y:51:ILE:CG2	5:Y:52:PRO:HA	2.35	0.55
1:C:124:LYS:HE3	7:C:501:HEM:C3D	2.42	0.54
6:P:43:ARG:HG3	5:Q:55:TYR:CZ	2.42	0.54
6:0:45:TRP:HD1	6:0:46:LEU:HG	1.71	0.54
6:4:20:ILE:HD12	15:4:101:CRT:C6	2.37	0.54
5:9:46:TRP:CD2	9:9:103:BCL:H2C	2.42	0.54
2:L:203:ILE:HG13	3:M:266:HIS:HD2	1.67	0.54
5:AA:10:LYS:HB3	15:AD:102:CRT:H33	1.89	0.54
5:AE:3:THR:OG1	5:AE:4:MET:N	2.40	0.54
9:F:101:BCL:CHD	9:G:102:BCL:HMD2	2.37	0.54
6:V:31:LEU:HD23	6:V:34:ILE:HD12	2.44	0.54
5:3:31:LEU:HD12	5:3:34:LEU:HD23	1.89	0.54
9:AL:102:BCL:HAA1	9:AL:102:BCL:CBD	2.37	0.54
15:A:103:CRT:H371	9:B:101:BCL:HMB2	1.88	0.54
9:I:101:BCL:CHD	9:J:102:BCL:HMD2	2.36	0.54
9:L:303:BCL:H111	9:M:401:BCL:H171	1.89	0.54
3:M:35:ILE:HG13	3:M:48:ILE:HB	1.89	0.54
5:S:17:PRO:HB3	6:T:17:PHE:CE1	2.43	0.54
5:AE:5:ASN:OD1	6:AH:23:GLN:NE2	2.40	0.54
3:M:197:TYR:CE1	9:M:401:BCL:HMC2	2.42	0.54
5:Q:9:TYR:HB2	6:R:14:ALA:O	2.07	0.54
5:1:44:LEU:HD23	5:3:55:TYR:HE2	1.70	0.54
5:AE:34:LEU:HD21	15:AE:103:CRT:H2M2	1.89	0.54
9:AI:101:BCL:HAA1	9:AI:101:BCL:HBD	1.89	0.54
4:H:154:MET:HE2	4:H:207:ARG:HA	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:18:ILE:HD12	2:L:35:PHE:CZ	2.43	0.54
2:L:228:ILE:O	3:M:132:ARG:NH2	2.39	0.54
6:Z:42:TYR:O	6:Z:43:ARG:HG3	2.08	0.54
6:0:32:VAL:HG21	9:0:101:BCL:HBA2	1.90	0.54
5:A:36:HIS:CD2	15:A:103:CRT:H372	2.43	0.54
6:B:28:TRP:CH2	9:B:101:BCL:H2	2.42	0.54
6:E:46:LEU:HD23	6:G:42:TYR:HE1	1.72	0.54
1:C:211:ARG:HD3	3:M:317:TYR:CE2	2.43	0.54
5:O:17:PRO:HB3	6:P:17:PHE:CZ	2.43	0.54
6:X:36:HIS:CD2	9:X:102:BCL:H8	2.42	0.54
1:C:237:MET:SD	2:L:174:LEU:HB3	2.46	0.54
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.89	0.54
9:O:101:BCL:HMD2	9:P:101:BCL:C1D	2.37	0.54
5:Q:51:ILE:CD1	6:R:43:ARG:HH22	2.21	0.54
5:U:26:ALA:O	5:U:29:ILE:HG22	4.38	0.54
9:1:101:BCL:H2	6:2:28:TRP:CH2	2.42	0.54
4:H:247:LYS:HA	4:H:254:ARG:HH11	1.72	0.54
5:W:9:TYR:CE1	5:W:10:LYS:HG3	2.43	0.54
9:X:102:BCL:CHB	9:X:102:BCL:H71	2.38	0.54
5:W:43:ASP:OD2	5:Y:55:TYR:HB2	2.08	0.54
5:7:40:LEU:HG	5:7:46:TRP:CH2	2.42	0.54
9:B:101:BCL:H61	5:9:2:PHE:CE1	2.43	0.54
5:F:17:PRO:HG2	6:G:9:LEU:HD21	2.81	0.54
5:I:45:ASN:O	5:I:49:ASP:OD2	2.25	0.54
9:Q:101:BCL:H191	6:R:31:LEU:HD22	1.90	0.54
5:U:34:LEU:O	5:U:38:ILE:HG13	2.14	0.54
6:T:43:ARG:HG3	5:U:55:TYR:CZ	2.43	0.54
5:Y:46:TRP:CD2	9:Y:101:BCL:H2C	2.43	0.54
6:AJ:43:ARG:HG3	5:AK:55:TYR:CE1	2.43	0.53
5:I:3:THR:HA	6:J:22:MET:HE2	1.88	0.53
4:H:96:PRO:HD3	6:0:7:THR:HA	1.90	0.53
5:7:35:ILE:HG12	15:8:101:CRT:H403	1.89	0.53
1:C:21:LEU:HD11	2:L:274:TRP:CD2	2.42	0.53
4:H:141:GLU:HG2	4:H:142:PHE:HD1	1.73	0.53
3:M:163:ILE:O	3:M:167:MET:HG3	2.07	0.53
5:U:51:ILE:HG23	5:U:52:PRO:HA	1.91	0.53
5:W:36:HIS:NE2	9:W:101:BCL:NB	2.56	0.53
5:A:33:LEU:HD23	15:A:103:CRT:H36	1.90	0.53
5:AI:3:THR:HG22	6:AJ:18:HIS:NE2	2.24	0.53
2:L:106:PHE:CD2	9:L:301:BCL:H91	2.43	0.53
3:M:175:VAL:CG1	3:M:176:PRO:HD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:265:ILE:CD1	14:M:403:MQ8:H121	2.38	0.53
9:S:102:BCL:HMB2	9:S:102:BCL:H93	15.42	0.53
9:V:101:BCL:HMA1	9:W:101:BCL:HMA1	1.90	0.53
5:AI:50:ASN:HB3	5:AI:54:SER:HA	1.89	0.53
5:AK:17:PRO:HG2	6:AL:9:LEU:HD11	1.91	0.53
9:W:101:BCL:CHD	9:X:102:BCL:HMD2	2.38	0.53
5:W:40:LEU:HG	5:W:46:TRP:CH2	2.43	0.53
5:Y:5:ASN:HA	6:2:23:GLN:HE22	1.72	0.53
4:H:57:GLY:H	12:H:301:PEF:C5	2.20	0.53
5:U:5:ASN:OD1	5:U:6:ALA:N	2.41	0.53
9:U:101:BCL:H2	6:V:28:TRP:CZ2	2.42	0.53
5:Y:23:SER:HB3	9:1:101:BCL:H151	1.90	0.53
5:5:43:ASP:OD2	5:7:50:ASN:HA	2.09	0.53
5:A:18:ARG:HH12	12:A:101:PEF:H51	1.74	0.53
9:B:101:BCL:H193	9:B:101:BCL:H8	1.91	0.53
1:C:311:HIS:HA	1:C:317:PRO:HG3	1.90	0.53
4:H:171:TRP:HB2	4:H:181:TYR:HB2	1.91	0.53
4:H:189:ASN:ND2	4:H:191:LYS:HB2	2.24	0.53
6:J:29:PHE:O	6:J:33:VAL:HG23	2.08	0.53
3:M:202:HIS:HE1	9:M:401:BCL:ND	2.07	0.53
5:O:35:ILE:HG12	5:O:38:ILE:HD12	1.91	0.53
5:S:16:ASP:OD1	5:S:18:ARG:N	2.41	0.53
5:Q:10:LYS:HB3	15:T:101:CRT:H22A	1.90	0.53
6:T:34:ILE:O	6:T:38:LEU:HG	2.08	0.53
5:7:28:GLN:OE1	6:8:28:TRP:NE1	2.39	0.53
5:5:18:ARG:O	5:5:21:LEU:HB2	2.09	0.53
9:AC:102:BCL:HMB2	9:AC:102:BCL:H8	1.89	0.53
6:AH:17:PHE:HA	15:AH:102:CRT:H6	1.90	0.53
6:AH:45:TRP:CD1	6:AH:46:LEU:HG	2.43	0.53
2:L:3:MET:HB3	2:L:7:GLU:HB3	1.91	0.53
9:M:401:BCL:H61	10:M:402:BPH:CHC	2.39	0.53
9:T:102:BCL:HMA1	9:U:101:BCL:HMA1	1.89	0.53
5:U:9:TYR:HB2	6:V:14:ALA:O	2.09	0.53
5:A:51:ILE:HG21	6:0:46:LEU:HA	1.90	0.53
5:5:46:TRP:CH2	9:5:101:BCL:H2C	2.43	0.53
9:AH:103:BCL:HED3	9:AH:103:BCL:HAA2	1.90	0.53
5:K:35:ILE:HD11	15:N:101:CRT:H403	1.89	0.53
6:B:17:PHE:HA	15:9:102:CRT:H83	1.91	0.53
4:H:124:ASP:HB2	4:H:233:LEU:HD21	1.91	0.53
2:L:179:ASN:HB3	2:L:182:HIS:HB2	1.91	0.53
6:4:21:PHE:CD1	15:4:101:CRT:H14	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:25:VAL:HG13	9:AH:101:BCL:H192	1.91	0.52
5:D:9:TYR:HB2	6:E:14:ALA:O	3.29	0.52
6:E:44:PRO:O	5:F:55:TYR:OH	2.24	0.52
4:H:64:PRO:HA	4:H:78:ALA:O	2.08	0.52
5:K:40:LEU:HD21	5:K:47:LEU:HD12	1.91	0.52
2:L:176:PHE:HE2	9:L:301:BCL:HMD3	1.73	0.52
3:M:208:PHE:CE2	3:M:275:LEU:HB3	2.44	0.52
3:M:18:TYR:CD2	3:M:20:GLY:HA2	2.44	0.52
3:M:63:PHE:CD1	5:Q:30:VAL:HG22	2.45	0.52
6:N:20:ILE:HD12	15:N:101:CRT:H82	4.09	0.52
5:Q:12:TRP:CH2	6:R:17:PHE:HE2	2.26	0.52
5:Q:42:THR:HG21	5:S:47:LEU:HD13	1.91	0.52
9:V:101:BCL:CHB	9:W:101:BCL:HMB3	2.39	0.52
5:1:57:ALA:N	5:1:58:LEU:C	2.62	0.52
5:5:40:LEU:HG	5:5:46:TRP:CH2	2.44	0.52
1:C:21:LEU:HD21	2:L:274:TRP:CZ2	2.44	0.52
3:M:64:GLY:HA3	10:M:402:BPH:H5C2	1.91	0.52
6:N:37:LEU:O	6:N:41:LEU:HG	2.09	0.52
5:O:29:ILE:O	5:O:33:LEU:HG	2.09	0.52
6:R:18:HIS:O	6:R:22:MET:HG2	2.08	0.52
9:AB:101:BCL:H93	9:AB:101:BCL:HMB2	1.91	0.52
15:AE:103:CRT:C14	6:AF:21:PHE:HA	2.40	0.52
5:D:24:ILE:HD11	9:F:101:BCL:H152	3.75	0.52
4:H:247:LYS:O	4:H:254:ARG:HD3	2.09	0.52
2:L:15:GLY:N	4:H:255:ALA:O	2.33	0.52
2:L:196:LEU:HD13	3:M:216:PHE:CD2	2.44	0.52
3:M:3:GLU:OE2	4:H:247:LYS:NZ	2.28	0.52
5:Y:46:TRP:CE3	9:Y:101:BCL:HAC1	2.45	0.52
5:9:14:ILE:HD11	15:9:102:CRT:C5	2.39	0.52
6:AD:28:TRP:O	6:AD:32:VAL:HG23	2.09	0.52
6:B:16:GLU:O	6:B:20:ILE:HG13	2.09	0.52
4:H:45:ARG:NH1	4:H:53:VAL:HG21	2.25	0.52
3:M:4:TYR:HE1	3:M:6:ASN:OD1	1.92	0.52
6:P:29:PHE:O	6:P:32:VAL:HB	2.10	0.52
5:Q:51:ILE:HD11	6:R:43:ARG:HH22	1.75	0.52
5:W:17:PRO:HB3	6:X:17:PHE:CZ	2.44	0.52
6:4:40:TRP:CG	9:4:102:BCL:H18	2.44	0.52
5:3:9:TYR:HB2	6:4:14:ALA:O	2.10	0.52
6:AH:29:PHE:CD1	9:AH:103:BCL:H2	2.45	0.52
6:B:31:LEU:HD23	6:B:34:ILE:HD12	1.91	0.52
1:C:167:VAL:HG12	1:C:301:ASP:OD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ASP:HB2	1:C:304:ARG:HH12	1.73	0.52
1:C:242:SER:HA	1:C:308:MET:HE2	1.90	0.52
9:G:102:BCL:HMB2	9:G:102:BCL:H71	1.92	0.52
2:L:199:HIS:HA	11:L:304:UQ8:O2	2.10	0.52
3:M:36:PHE:HA	3:M:46:ALA:O	2.09	0.52
6:R:40:TRP:CZ3	6:R:46:LEU:HB2	2.44	0.52
5:S:16:ASP:OD2	5:S:19:ARG:HG3	2.09	0.52
5:U:46:TRP:CD1	9:U:101:BCL:HMC2	3.83	0.52
6:2:7:THR:HG23	6:2:9:LEU:H	1.73	0.52
9:7:101:BCL:H111	9:7:101:BCL:H41	1.91	0.52
5:D:13:LEU:HA	6:E:7:THR:HG21	5.76	0.52
9:V:101:BCL:HAA1	9:V:101:BCL:HBD	1.90	0.52
5:AE:5:ASN:O	5:AE:7:ASN:N	2.42	0.52
9:L:301:BCL:NA	9:M:401:BCL:HBB2	2.25	0.52
15:T:101:CRT:H27	9:T:102:BCL:O1A	2.10	0.52
5:AC:34:LEU:O	5:AC:38:ILE:HG13	2.09	0.52
9:AK:101:BCL:HMD1	6:AL:36:HIS:ND1	2.24	0.52
2:L:59:THR:OG1	2:L:63:SER:OG	2.09	0.52
6:N:17:PHE:CD1	15:N:101:CRT:H9	2.44	0.52
5:U:54:SER:O	5:U:58:LEU:N	2.43	0.52
6:8:29:PHE:CD1	9:8:102:BCL:H12	2.45	0.52
6:8:32:VAL:HG21	9:8:102:BCL:H11	1.92	0.52
6:E:23:GLN:NE2	5:AK:3:THR:O	85.40	0.52
1:C:219:ALA:HB2	3:M:292:ASP:HB2	1.92	0.52
5:S:13:LEU:HD21	6:T:11:ASP:HA	1.91	0.52
5:1:49:ASP:O	5:1:51:ILE:HG13	2.10	0.52
5:Y:43:ASP:OD2	5:1:50:ASN:HA	2.10	0.52
6:AF:32:VAL:O	6:AF:36:HIS:ND1	2.41	0.52
6:N:31:LEU:HD23	6:N:34:ILE:HD12	3.70	0.52
6:0:12:ASP:O	6:0:15:LYS:HB2	2.10	0.51
6:0:40:TRP:CZ2	9:0:101:BCL:H191	2.44	0.51
5:1:24:ILE:HD13	9:3:101:BCL:H18	1.91	0.51
5:5:43:ASP:O	5:7:55:TYR:HB2	2.10	0.51
2:L:125:HIS:CE1	3:M:5:GLN:OE1	2.63	0.51
3:M:177:PHE:CD1	15:M:404:CRT:H16	2.41	0.51
2:L:275:TRP:NE1	3:M:88:LYS:O	2.42	0.51
5:O:36:HIS:CE1	9:O:101:BCL:HMD1	2.45	0.51
1:C:268:THR:HG21	7:C:504:HEM:C2A	2.45	0.51
3:M:240:HIS:NE2	4:H:69:LEU:HD11	2.26	0.51
3:M:187:ALA:HA	9:M:401:BCL:HBC2	1.91	0.51
5:7:38:ILE:O	5:7:41:SER:OG	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AH:32:VAL:HG21	9:AH:103:BCL:HBA2	1.93	0.51
6:E:17:PHE:HB2	15:E:101:CRT:H31A	1.91	0.51
6:E:44:PRO:O	5:F:52:PRO:HD2	2.10	0.51
4:H:135:PRO:HA	4:H:171:TRP:HA	1.92	0.51
6:J:40:TRP:CE2	9:J:102:BCL:H202	2.45	0.51
5:S:5:ASN:C	5:S:7:ASN:H	2.13	0.51
15:T:101:CRT:H372	5:U:36:HIS:CD2	2.45	0.51
5:Y:11:ILE:HD13	15:2:101:CRT:H10	1.92	0.51
9:AJ:102:BCL:CGA	9:AJ:102:BCL:H3A	2.41	0.51
6:B:44:PRO:O	5:D:55:TYR:OH	2.29	0.51
1:C:203:PHE:O	1:C:277:ARG:NH1	2.44	0.51
4:H:136:MET:HG3	4:H:170:VAL:O	2.09	0.51
9:S:102:BCL:H92	9:S:102:BCL:H41	1.93	0.51
6:R:43:ARG:HG3	5:S:55:TYR:CE1	2.44	0.51
5:AE:9:TYR:HB2	6:AF:14:ALA:O	2.10	0.51
5:F:34:LEU:O	5:F:38:ILE:HG13	2.41	0.51
6:O:40:TRP:HZ3	6:O:45:TRP:H	1.57	0.51
4:H:130:LEU:HB3	4:H:174:ARG:NH2	2.26	0.51
3:M:274:VAL:O	3:M:278:ILE:HG12	2.11	0.51
6:P:18:HIS:O	6:P:22:MET:HG2	2.11	0.51
5:S:19:ARG:NH1	17:S:101:PGW:H01	2.26	0.51
6:N:44:PRO:O	5:O:52:PRO:HD3	2.11	0.51
9:U:101:BCL:C1D	9:V:101:BCL:HMD2	2.40	0.51
5:U:11:ILE:HD13	15:Z:101:CRT:H10	19.35	0.51
5:1:17:PRO:HA	5:1:20:VAL:HG22	1.92	0.51
5:Y:10:LYS:HB3	15:2:101:CRT:H5	1.92	0.51
5:5:43:ASP:OD1	5:7:56:GLN:HG2	2.10	0.51
5:AE:25:VAL:HG21	9:AE:102:BCL:C15	2.41	0.51
10:L:302:BPH:H141	9:L:305:BCL:CBB	2.40	0.51
6:P:45:TRP:HD1	6:P:46:LEU:HG	1.76	0.51
6:B:20:ILE:CG2	5:9:5:ASN:HB3	2.41	0.51
9:J:102:BCL:HBA1	9:J:102:BCL:H2	1.93	0.51
3:M:243:THR:O	3:M:247:ARG:HD2	2.10	0.51
5:Q:36:HIS:CE1	9:R:102:BCL:HMD1	2.46	0.51
6:B:44:PRO:HG2	5:D:52:PRO:CD	2.39	0.51
2:L:155:PHE:HA	2:L:165:TRP:CD1	2.46	0.51
2:L:170:GLY:HA2	2:L:176:PHE:CD2	2.46	0.51
3:M:6:ASN:HD22	3:M:227:SER:CB	2.24	0.51
9:AA:101:BCL:HBD	9:AA:101:BCL:HBA2	1.91	0.50
6:AH:33:VAL:HG22	9:AH:103:BCL:H92	1.93	0.50
5:AI:20:VAL:O	5:AI:24:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:11:ILE:HD12	5:I:14:ILE:HD12	1.92	0.50
12:M:407:PEF:H51	12:M:408:PEF:O2P	2.11	0.50
6:R:29:PHE:O	6:R:33:VAL:HG23	2.12	0.50
5:D:56:GLN:O	5:D:58:LEU:N	2.44	0.50
5:F:51:ILE:HD13	6:G:43:ARG:HH22	3.67	0.50
2:L:179:ASN:HB3	2:L:182:HIS:CB	2.41	0.50
15:P:102:CRT:H372	5:Q:36:HIS:CD2	2.45	0.50
9:1:102:BCL:H2	6:2:29:PHE:CE1	2.46	0.50
5:1:42:THR:HG21	5:3:47:LEU:HD13	1.91	0.50
5:I:25:VAL:HG13	9:I:101:BCL:H62	1.92	0.50
2:L:133:ALA:HB1	9:L:301:BCL:H62	1.94	0.50
9:O:101:BCL:HMB2	9:O:101:BCL:H93	1.93	0.50
15:X:101:CRT:H372	5:Y:36:HIS:CD2	2.46	0.50
6:E:46:LEU:HD21	5:F:46:TRP:HB2	9.45	0.50
5:F:9:TYR:O	6:G:14:ALA:HB1	3.43	0.50
3:M:121:PHE:HZ	5:Q:34:LEU:HA	1.77	0.50
3:M:219:HIS:CE1	3:M:223:ILE:HD11	2.46	0.50
5:Y:40:LEU:HG	5:Y:46:TRP:CH2	2.47	0.50
5:AE:51:ILE:O	5:AE:55:TYR:HE2	1.95	0.50
9:D:101:BCL:HMB1	9:D:101:BCL:HBB3	1.93	0.50
4:H:141:GLU:HG2	4:H:142:PHE:N	2.26	0.50
6:E:46:LEU:HA	5:F:51:ILE:HG22	5.13	0.50
6:G:32:VAL:HG21	9:G:102:BCL:HBA2	1.93	0.50
2:L:120:LEU:HD11	3:M:250:LEU:HB2	1.94	0.50
9:L:303:BCL:HED1	3:M:179:ILE:HG23	1.94	0.50
6:P:21:PHE:HA	15:P:102:CRT:H14	1.92	0.50
6:X:20:ILE:HD12	15:X:101:CRT:C5	2.42	0.50
9:9:103:BCL:HED1	6:0:28:TRP:CZ3	2.47	0.50
6:6:21:PHE:HA	15:6:101:CRT:H14	1.94	0.50
1:C:19:MET:HB2	1:C:21:LEU:HD13	1.93	0.50
5:A:7:ASN:ND2	6:E:23:GLN:OE1	2.45	0.50
9:D:102:BCL:HED1	6:E:28:TRP:HZ2	1.76	0.50
6:E:45:TRP:CD1	6:E:46:LEU:HG	6.48	0.50
3:M:63:PHE:CE1	5:Q:30:VAL:HG22	2.46	0.50
1:C:183:GLN:O	1:C:184:ASN:HB2	2.12	0.50
1:C:236:MET:HB3	7:C:503:HEM:C4B	2.45	0.50
2:L:244:PHE:HB2	11:L:304:UQ8:H45	1.94	0.50
5:Q:10:LYS:HD3	15:T:101:CRT:H21A	1.93	0.50
9:T:102:BCL:H3A	9:T:102:BCL:CGA	2.42	0.50
5:U:44:LEU:HD13	9:V:101:BCL:HAC1	1.94	0.50
5:S:43:ASP:HB3	5:U:47:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:39:VAL:HG11	9:3:101:BCL:HBC1	1.93	0.50
6:4:40:TRP:CD2	9:4:102:BCL:H18	2.47	0.50
9:AA:101:BCL:CHD	9:AB:101:BCL:HMD2	2.42	0.50
5:AE:14:ILE:HD11	15:AH:102:CRT:C5	2.42	0.50
9:AK:101:BCL:HMD1	6:AL:36:HIS:CE1	2.47	0.50
5:D:40:LEU:HG	5:D:46:TRP:CH2	2.47	0.50
4:H:251:THR:OG1	4:H:254:ARG:HG3	2.12	0.50
2:L:271:TRP:HZ3	2:L:272:TRP:CH2	2.30	0.50
2:L:65:LEU:HD13	3:M:308:PRO:HG3	1.94	0.50
5:AG:11:ILE:HD13	15:AJ:101:CRT:C10	2.42	0.49
1:C:24:GLU:O	2:L:263:PHE:HA	2.11	0.49
1:C:124:LYS:HG3	7:C:501:HEM:HMD3	1.94	0.49
2:L:228:ILE:HD13	3:M:133:THR:HG22	1.94	0.49
2:L:61:PRO:HA	2:L:66:GLN:HG3	1.92	0.49
3:M:219:HIS:ND1	14:M:403:MQ8:O1	2.41	0.49
6:V:29:PHE:O	6:V:32:VAL:HB	2.12	0.49
5:Y:46:TRP:NE1	9:Y:101:BCL:OBB	2.43	0.49
15:2:101:CRT:H291	9:3:101:BCL:H11	1.94	0.49
9:5:102:BCL:H12	6:6:32:VAL:HG11	1.94	0.49
4:H:257:PRO:HG3	5:7:19:ARG:CZ	2.42	0.49
6:AJ:14:ALA:CB	6:AJ:17:PHE:HB3	2.42	0.49
1:C:316:LYS:HE3	7:C:504:HEM:CGA	2.42	0.49
5:D:27:PHE:CD2	9:F:101:BCL:H191	14.27	0.49
5:F:44:LEU:HD12	5:I:47:LEU:HD22	1.93	0.49
2:L:162:HIS:CE1	2:L:163:LEU:HD23	2.47	0.49
2:L:78:PRO:HB2	2:L:82:TYR:CD2	2.47	0.49
3:M:39:TRP:O	3:M:40:LEU:C	2.51	0.49
6:X:24:SER:CB	15:X:101:CRT:H14	2.41	0.49
5:9:17:PRO:HB3	6:0:17:PHE:CE1	2.47	0.49
6:AH:39:ALA:HB2	9:AH:101:BCL:HMD3	1.93	0.49
6:AH:32:VAL:HG11	9:AH:103:BCL:HBA1	1.95	0.49
1:C:181:THR:C	1:C:183:GLN:H	2.16	0.49
2:L:217:THR:HG23	2:L:220:HIS:CE1	2.47	0.49
6:R:36:HIS:CE1	9:S:102:BCL:HMD1	15.40	0.49
5:W:5:ASN:OD1	5:W:6:ALA:N	2.45	0.49
5:AC:11:ILE:HD13	15:AE:103:CRT:H10	1.94	0.49
5:AA:8:LEU:HD11	15:AD:102:CRT:H133	1.93	0.49
6:AH:29:PHE:CE1	9:AH:103:BCL:H2	2.47	0.49
6:AJ:20:ILE:HD12	15:AJ:101:CRT:C5	2.43	0.49
6:AJ:45:TRP:HD1	6:AJ:46:LEU:HG	1.78	0.49
4:H:46:THR:HG23	4:H:51:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:80:HIS:O	3:M:81:TRP:HB2	2.13	0.49
5:O:40:LEU:HG	5:O:46:TRP:CH2	2.47	0.49
5:S:49:ASP:HB3	5:S:51:ILE:HG13	1.93	0.49
5:W:44:LEU:HD12	5:Y:47:LEU:HD22	1.94	0.49
6:B:17:PHE:CD1	15:9:102:CRT:H5	2.41	0.49
1:C:99:THR:HA	1:C:103:PRO:HB3	1.94	0.49
4:H:77:VAL:O	4:H:80:ARG:NE	2.43	0.49
9:K:101:BCL:CHD	9:N:102:BCL:HMD2	2.42	0.49
3:M:114:TRP:CE3	3:M:114:TRP:HA	2.47	0.49
9:1:101:BCL:HMD1	6:2:36:HIS:ND1	2.27	0.49
6:AH:21:PHE:CD2	15:AH:102:CRT:H14	2.47	0.49
1:C:155:CYS:SG	1:C:310:CYS:SG	3.10	0.49
1:C:98:THR:HA	7:C:501:HEM:HMC3	1.93	0.49
9:D:101:BCL:O2D	9:D:101:BCL:H2A	3.05	0.49
11:L:304:UQ8:H3MA	11:L:304:UQ8:H4MB	1.95	0.49
2:L:137:TYR:CE1	9:L:305:BCL:HBB1	2.48	0.49
3:M:260:VAL:HG22	14:M:403:MQ8:C4	2.43	0.49
6:V:29:PHE:CD1	9:V:101:BCL:H2	2.48	0.49
6:Z:43:ARG:HD3	5:1:55:TYR:CZ	2.48	0.49
9:8:102:BCL:HED2	9:8:102:BCL:O1A	2.12	0.49
6:B:16:GLU:OE2	5:9:10:LYS:HE3	2.13	0.49
5:AK:49:ASP:HB3	5:AK:51:ILE:HG22	1.94	0.49
1:C:280:ASN:OD1	1:C:304:ARG:HB2	2.12	0.49
4:H:36:ARG:C	4:H:37:GLU:HG2	2.33	0.49
2:L:237:ALA:O	2:L:240:ARG:N	2.46	0.49
2:L:86:MET:HA	2:L:96:GLN:HE22	1.77	0.49
6:T:16:GLU:HB3	15:T:101:CRT:H33	1.94	0.49
15:U:102:CRT:H36	5:W:33:LEU:HD23	1.94	0.49
6:V:10:THR:OG1	6:V:13:GLU:N	3.50	0.49
6:V:40:TRP:CH2	6:V:46:LEU:HB2	2.48	0.49
5:A:18:ARG:HG3	5:9:15:LEU:HD23	1.95	0.49
6:AJ:25:MET:HG2	6:AJ:29:PHE:CZ	2.48	0.49
9:B:101:BCL:H91	9:B:101:BCL:H121	1.93	0.49
1:C:137:ALA:HA	1:C:141:TRP:CD1	2.46	0.49
1:C:19:MET:C	1:C:21:LEU:HD13	2.33	0.49
5:F:3:THR:HG22	5:I:2:PHE:CE2	2.48	0.49
5:I:12:TRP:HB3	5:I:17:PRO:HG3	1.95	0.49
2:L:239:HIS:NE2	3:M:223:ILE:HG13	2.27	0.49
3:M:60:SER:HB2	3:M:128:LEU:HB3	1.95	0.49
9:Z:102:BCL:HMB3	9:1:101:BCL:HMA3	1.94	0.49
6:O:40:TRP:HH2	6:O:46:LEU:OXT	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1:102:BCL:H12	9:1:102:BCL:H3A	1.94	0.49
1:C:126:VAL:HG13	1:C:287:LEU:HD13	1.94	0.49
5:F:35:ILE:HA	5:F:38:ILE:HD12	2.42	0.49
6:AD:28:TRP:CZ2	9:AD:101:BCL:H43	2.47	0.49
5:AI:5:ASN:HB3	6:AL:23:GLN:OE1	2.13	0.49
2:L:172:GLN:HG3	2:L:172:GLN:O	2.11	0.49
9:L:303:BCL:HMB1	9:L:303:BCL:HBB2	1.93	0.49
5:AE:34:LEU:O	5:AE:38:ILE:HG13	2.12	0.48
3:M:71:ILE:O	3:M:75:MET:HG3	2.13	0.48
15:AD:102:CRT:H26	15:AD:102:CRT:H241	1.66	0.48
5:AE:12:TRP:CZ3	5:AE:20:VAL:HG11	2.48	0.48
9:AK:101:BCL:HBB3	9:AK:101:BCL:HMB1	1.94	0.48
1:C:263:THR:HG22	3:M:311:VAL:CG1	2.41	0.48
9:D:101:BCL:C4C	9:D:102:BCL:HMD2	2.43	0.48
2:L:206:VAL:HB	2:L:216:LYS:HB2	1.95	0.48
3:M:253:ARG:HH12	12:M:406:PEF:HN2	1.58	0.48
5:S:40:LEU:HD13	5:S:46:TRP:CH2	2.48	0.48
5:9:40:LEU:HD21	5:9:47:LEU:HD12	1.95	0.48
5:A:49:ASP:HB2	5:A:51:ILE:HG13	1.95	0.48
15:AH:102:CRT:H342	9:AI:101:BCL:O1A	2.14	0.48
9:AL:102:BCL:HAA1	9:AL:102:BCL:HBD	1.94	0.48
9:D:101:BCL:HMD1	6:E:36:HIS:ND1	2.42	0.48
4:H:113:PRO:HG2	4:H:249:TYR:CE2	2.48	0.48
5:I:44:LEU:HD13	9:J:102:BCL:CAC	2.42	0.48
2:L:30:PHE:CE1	3:M:257:GLY:HA3	2.49	0.48
6:N:17:PHE:CE1	15:N:101:CRT:H9	2.48	0.48
9:O:101:BCL:C1B	9:Q:101:BCL:HMB3	2.44	0.48
6:6:17:PHE:HA	15:6:101:CRT:H6	1.94	0.48
15:AD:102:CRT:H372	5:AE:36:HIS:CD2	2.49	0.48
5:AG:44:LEU:HD23	5:AI:55:TYR:CD2	2.48	0.48
1:C:67:SER:HA	1:C:68:THR:OG1	2.14	0.48
5:Q:8:LEU:HD11	15:T:101:CRT:H133	1.95	0.48
9:S:102:BCL:C1B	9:U:101:BCL:HMB3	14.52	0.48
9:1:102:BCL:H3A	9:1:102:BCL:HBA1	1.51	0.48
5:5:32:GLY:HA2	9:5:102:BCL:O1D	2.13	0.48
9:AC:102:BCL:HMA1	9:AE:102:BCL:HMA1	1.94	0.48
9:AH:103:BCL:CHB	9:AI:101:BCL:HMB3	2.43	0.48
5:D:44:LEU:HD11	6:E:45:TRP:HB2	3.90	0.48
9:AE:104:BCL:H61	9:AE:104:BCL:HMB2	1.95	0.48
2:L:34:PHE:O	2:L:38:VAL:HG23	2.13	0.48
2:L:48:LEU:HB3	5:9:34:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:25:VAL:CG1	9:U:101:BCL:H71	7.61	0.48
5:5:46:TRP:CZ3	9:5:101:BCL:HAC2	2.49	0.48
5:3:10:LYS:HE3	6:6:16:GLU:OE2	2.13	0.48
5:AC:38:ILE:O	5:AC:42:THR:HG23	2.14	0.48
5:AI:6:ALA:HB2	6:AL:23:GLN:OE1	2.13	0.48
1:C:21:LEU:HD21	2:L:274:TRP:CE2	2.49	0.48
1:C:67:SER:CB	1:C:86:SER:HG	2.24	0.48
9:D:101:BCL:H142	9:D:101:BCL:H91	1.96	0.48
15:T:101:CRT:H22A	15:T:101:CRT:H5	1.69	0.48
6:T:12:ASP:O	6:T:15:LYS:HB2	2.13	0.48
9:U:101:BCL:HBB3	9:U:101:BCL:HMB1	2.01	0.48
5:U:42:THR:HG21	5:W:47:LEU:HD13	2.92	0.48
5:5:9:TYR:HD1	5:5:9:TYR:H	1.62	0.48
5:AI:34:LEU:HA	5:AI:37:MET:HE3	1.94	0.48
1:C:97:VAL:HG21	1:C:131:PHE:HZ	1.74	0.48
6:G:45:TRP:HD1	6:G:46:LEU:HG	1.75	0.48
4:H:214:ILE:HB	4:H:218:HIS:HB2	1.96	0.48
2:L:241:LEU:HD21	11:L:304:UQ8:H13	1.94	0.48
3:M:215:LEU:HD23	3:M:215:LEU:HA	1.64	0.48
3:M:225:SER:O	3:M:228:ARG:HD2	2.13	0.48
3:M:233:ARG:NH2	4:H:124:ASP:OD2	2.47	0.48
3:M:65:LEU:HD21	10:M:402:BPH:H7C2	1.95	0.48
9:N:102:BCL:H71	9:N:102:BCL:HMB2	1.96	0.48
9:W:101:BCL:HBA1	6:X:28:TRP:HH2	1.79	0.48
9:8:102:BCL:HMB1	9:8:102:BCL:HBB2	1.96	0.48
5:A:56:GLN:HG2	5:9:43:ASP:CG	2.34	0.48
5:D:28:GLN:NE2	6:E:28:TRP:HE1	4.24	0.48
3:M:290:VAL:HG12	3:M:291:VAL:HG23	1.96	0.48
3:M:65:LEU:HD11	10:M:402:BPH:H122	1.95	0.48
5:9:5:ASN:C	5:9:7:ASN:H	2.12	0.48
6:AH:40:TRP:HH2	6:AH:46:LEU:OXT	1.97	0.48
2:L:194:LEU:HD11	10:M:402:BPH:ND	2.29	0.48
9:R:102:BCL:H142	9:R:102:BCL:H112	1.71	0.48
9:Z:102:BCL:H3A	9:Z:102:BCL:HBA1	1.71	0.48
6:8:18:HIS:O	6:8:22:MET:HG2	2.13	0.47
6:AJ:14:ALA:HB1	6:AJ:17:PHE:HB3	1.95	0.47
6:B:20:ILE:HB	15:9:102:CRT:H82	1.95	0.47
5:D:12:TRP:HZ3	5:D:20:VAL:HG21	2.21	0.47
9:F:101:BCL:C1D	9:G:102:BCL:HMD2	2.43	0.47
9:F:101:BCL:H2	6:G:28:TRP:CH2	2.49	0.47
5:F:45:ASN:OD1	5:F:46:TRP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:43:THR:HA	10:L:302:BPH:H7C1	1.96	0.47
2:L:99:THR:OG1	2:L:157:TYR:OH	2.28	0.47
9:W:101:BCL:H102	9:W:101:BCL:H171	5.70	0.47
5:U:15:LEU:HD23	5:W:18:ARG:HG3	1.95	0.47
5:W:51:ILE:HD11	5:Y:58:LEU:CB	2.44	0.47
5:1:33:LEU:O	5:1:37:MET:HG3	2.13	0.47
15:8:101:CRT:H241	15:8:101:CRT:H26	1.75	0.47
9:G:102:BCL:H62	9:G:102:BCL:H41	1.61	0.47
9:I:101:BCL:HAA2	9:I:101:BCL:HBD	1.96	0.47
9:U:101:BCL:HBA1	6:V:28:TRP:HH2	1.80	0.47
6:B:21:PHE:HA	15:9:102:CRT:H14	1.95	0.47
5:9:11:ILE:HG23	5:9:12:TRP:CD2	2.48	0.47
5:D:22:VAL:HG13	9:D:101:BCL:H191	1.94	0.47
4:H:64:PRO:HA	4:H:79:PRO:HD2	1.96	0.47
1:C:263:THR:C	3:M:313:ALA:HB2	2.34	0.47
5:Y:44:LEU:HA	5:1:55:TYR:CE2	2.49	0.47
5:AA:11:ILE:HD13	15:AD:102:CRT:H132	1.96	0.47
5:D:28:GLN:HE21	6:E:28:TRP:HE1	4.98	0.47
6:G:20:ILE:HD12	15:G:101:CRT:C6	2.44	0.47
4:H:35:LYS:HG2	4:H:39:TYR:CE1	2.49	0.47
2:L:193:CYS:SG	10:M:402:BPH:HMC3	2.54	0.47
3:M:177:PHE:CD1	15:M:404:CRT:H19	2.47	0.47
6:P:40:TRP:HH2	6:P:46:LEU:OXT	1.97	0.47
9:S:102:BCL:HBA1	9:S:102:BCL:H12	5.06	0.47
9:4:102:BCL:HBB2	9:4:102:BCL:H121	1.96	0.47
6:B:17:PHE:HE1	5:9:14:ILE:HD13	1.80	0.47
15:E:101:CRT:C31	9:F:101:BCL:HBA2	4.26	0.47
12:H:301:PEF:O4	5:D:18:ARG:HD3	2.14	0.47
2:L:112:ARG:NH2	3:M:255:THR:O	2.28	0.47
3:M:268:TRP:CD2	4:H:30:LEU:HD13	2.48	0.47
5:W:10:LYS:HE3	6:AB:16:GLU:OE2	55.94	0.47
6:X:45:TRP:CD1	6:X:46:LEU:HG	2.49	0.47
9:L:301:BCL:HBB3	9:L:303:BCL:HMD2	1.96	0.47
5:Y:51:ILE:HG12	5:1:59:GLY:HA3	1.95	0.47
5:AI:39:VAL:HG11	9:AI:101:BCL:HBC1	1.97	0.47
5:F:40:LEU:HG	5:F:46:TRP:CH2	2.54	0.47
4:H:36:ARG:O	4:H:37:GLU:HG2	2.14	0.47
2:L:235:ALA:N	11:L:304:UQ8:O4	2.48	0.47
2:L:52:TRP:O	2:L:56:ILE:HG23	2.14	0.47
5:U:24:ILE:HD11	9:W:101:BCL:H202	1.96	0.47
6:X:14:ALA:HB1	6:X:17:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:8:101:CRT:H342	9:9:103:BCL:HBA2	1.97	0.47
5:AC:35:ILE:HA	5:AC:38:ILE:HD12	1.97	0.47
15:AE:103:CRT:H14	6:AF:21:PHE:CD2	2.49	0.47
6:AH:45:TRP:HD1	6:AH:46:LEU:HG	1.79	0.47
5:AI:11:ILE:HD13	15:AL:101:CRT:H10	1.95	0.47
7:C:503:HEM:HBC2	7:C:503:HEM:CMC	2.45	0.47
5:A:2:PHE:HE2	6:E:23:GLN:HE21	1.58	0.47
2:L:176:PHE:CE2	9:L:301:BCL:HMD3	2.50	0.47
3:M:222:THR:O	3:M:225:SER:N	2.48	0.47
9:O:101:BCL:HMD2	9:P:101:BCL:CHD	2.45	0.47
5:S:43:ASP:OD2	5:U:50:ASN:HA	2.15	0.47
5:Y:16:ASP:OD2	5:Y:19:ARG:HB2	2.14	0.47
5:1:40:LEU:HG	5:1:46:TRP:CH2	2.50	0.47
6:2:13:GLU:HB3	15:2:101:CRT:H23	1.96	0.47
6:AD:21:PHE:HA	15:AD:102:CRT:H15	1.96	0.47
5:AE:14:ILE:HD13	6:AH:17:PHE:CE1	2.49	0.47
1:C:174:TYR:CZ	1:C:180:PRO:HA	2.49	0.47
12:H:303:PEF:C11	6:E:8:GLY:HA3	2.45	0.47
2:L:17:LEU:O	4:H:258:LEU:HB2	2.15	0.47
5:K:38:ILE:O	5:K:42:THR:HG23	2.15	0.47
2:L:239:HIS:CD2	3:M:223:ILE:HG21	2.49	0.47
5:AG:21:LEU:HA	5:AG:21:LEU:HD23	1.67	0.47
15:AE:103:CRT:C32	9:AH:101:BCL:H3A	2.45	0.47
5:A:9:TYR:HB3	6:B:18:HIS:CG	2.50	0.47
4:H:63:ASP:OD2	5:F:19:ARG:NH2	2.47	0.47
15:J:101:CRT:H27	9:J:102:BCL:O1A	2.15	0.47
5:K:39:VAL:HG11	9:K:101:BCL:HBC1	1.97	0.47
6:N:17:PHE:CD1	15:N:101:CRT:H5	4.95	0.47
9:O:101:BCL:H3A	9:O:101:BCL:H12	1.97	0.47
6:X:20:ILE:HB	15:X:101:CRT:C9	2.44	0.47
15:A:103:CRT:C14	6:O:21:PHE:HA	2.44	0.47
5:5:38:ILE:O	5:5:42:THR:HG23	2.15	0.47
6:4:46:LEU:HD22	6:6:42:TYR:CE2	2.50	0.47
5:9:10:LYS:HB3	15:9:102:CRT:H41	1.96	0.47
5:AC:49:ASP:O	5:AE:57:ALA:HB3	2.14	0.47
9:AK:101:BCL:HED3	6:AL:28:TRP:CH2	2.50	0.47
1:C:200:LEU:HD21	1:C:238:ASN:OD1	2.15	0.47
6:G:30:GLY:O	6:G:34:ILE:HG12	2.15	0.47
9:I:101:BCL:H91	9:I:101:BCL:H112	1.60	0.47
5:I:3:THR:OG1	5:I:5:ASN:N	2.48	0.47
2:L:170:GLY:HA2	2:L:176:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:ARG:HH11	3:M:305:PRO:HA	1.80	0.47
5:U:9:TYR:OH	6:V:11:ASP:OD1	3.88	0.47
5:Y:10:LYS:HB3	15:2:101:CRT:H31A	1.96	0.47
9:1:101:BCL:O2D	9:1:101:BCL:H2A	2.15	0.46
5:3:27:PHE:CE1	5:5:29:ILE:HD13	2.49	0.46
9:AE:102:BCL:H72	9:AE:102:BCL:H112	1.50	0.46
5:AE:14:ILE:HD13	6:AH:17:PHE:HE1	1.81	0.46
15:G:101:CRT:C32	9:I:101:BCL:H3A	2.45	0.46
2:L:57:GLY:HA3	2:L:66:GLN:HA	1.97	0.46
9:V:101:BCL:HAA1	9:V:101:BCL:CBD	2.44	0.46
9:1:102:BCL:H12	9:1:102:BCL:HBA1	1.56	0.46
9:B:101:BCL:HMA1	9:0:101:BCL:HMA1	1.98	0.46
7:C:503:HEM:HMC2	7:C:503:HEM:HBC2	1.97	0.46
5:D:56:GLN:C	5:D:58:LEU:H	2.18	0.46
5:F:36:HIS:CE1	9:G:102:BCL:HMD1	2.50	0.46
6:E:46:LEU:HD23	6:G:42:TYR:CE1	2.50	0.46
4:H:106:PRO:HB3	4:H:249:TYR:CD1	2.50	0.46
4:H:141:GLU:HG2	4:H:142:PHE:CD1	2.50	0.46
3:M:13:VAL:HG22	4:H:178:GLN:HA	1.98	0.46
2:L:210:GLN:HB2	3:M:141:GLY:O	2.15	0.46
5:Q:45:ASN:O	5:Q:49:ASP:OD2	2.33	0.46
9:X:102:BCL:HBD	9:X:102:BCL:HED2	1.60	0.46
5:AE:10:LYS:HB3	15:AH:102:CRT:H33	1.97	0.46
5:AK:44:LEU:HD11	6:AL:45:TRP:HB2	1.97	0.46
1:C:183:GLN:HA	1:C:196:PRO:HA	1.96	0.46
5:D:9:TYR:C	5:D:11:ILE:H	2.19	0.46
9:F:101:BCL:HED3	6:G:35:ALA:HB2	1.97	0.46
4:H:136:MET:HE2	4:H:152:ARG:HH22	1.80	0.46
4:H:149:PRO:HG3	4:H:204:LYS:HD3	1.97	0.46
3:M:155:PHE:O	3:M:159:VAL:HG23	2.15	0.46
3:M:4:TYR:CE1	3:M:6:ASN:HA	2.50	0.46
5:S:22:VAL:HG22	9:S:102:BCL:H18	1.96	0.46
6:V:32:VAL:HG21	9:V:101:BCL:HBA2	1.96	0.46
9:8:102:BCL:HBA1	9:8:102:BCL:H3A	1.45	0.46
15:A:103:CRT:H403	5:9:35:ILE:HG12	1.97	0.46
5:A:44:LEU:HD23	5:D:55:TYR:CE2	2.50	0.46
5:AG:28:GLN:HB3	9:AH:101:BCL:H12	1.97	0.46
5:D:12:TRP:CZ3	5:D:20:VAL:HG11	2.51	0.46
5:D:39:VAL:HG12	5:D:46:TRP:HZ3	1.81	0.46
5:I:3:THR:HB	6:J:18:HIS:NE2	2.30	0.46
6:J:24:SER:O	6:J:27:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:132:PHE:CD2	2:L:247:LEU:HB3	2.49	0.46
9:Z:102:BCL:H111	9:Z:102:BCL:H143	4.05	0.46
5:AK:40:LEU:HG	5:AK:46:TRP:CH2	2.50	0.46
3:M:204:LEU:HD13	4:H:19:PHE:CE2	2.50	0.46
5:I:10:LYS:HD3	15:N:101:CRT:H22A	1.97	0.46
6:J:17:PHE:CD1	15:J:101:CRT:H9	2.50	0.46
6:J:21:PHE:CD2	15:J:101:CRT:H14	2.51	0.46
3:M:126:ILE:HD11	9:M:401:BCL:H142	1.97	0.46
3:M:65:LEU:CD2	10:M:402:BPH:H7C2	2.45	0.46
5:O:43:ASP:HB2	5:Q:48:ASP:OD1	2.15	0.46
5:W:25:VAL:HG11	9:W:101:BCL:H192	1.97	0.46
6:Z:20:ILE:HD12	15:Z:101:CRT:C6	2.75	0.46
5:3:45:ASN:OD1	5:3:46:TRP:N	2.49	0.46
5:7:27:PHE:CZ	5:7:31:LEU:HD22	2.51	0.46
9:A:102:BCL:HBD	9:B:101:BCL:HBD	1.98	0.46
1:C:305:VAL:HG22	7:C:502:HEM:HAC	1.97	0.46
5:D:46:TRP:CD2	9:D:101:BCL:H2C	2.51	0.46
1:C:178:LEU:HA	3:M:110:SER:HB2	1.96	0.46
3:M:242:GLY:O	3:M:246:GLU:HG3	2.15	0.46
5:S:19:ARG:NH2	17:S:101:PGW:H04A	2.31	0.46
5:Y:21:LEU:HD23	5:Y:21:LEU:HA	1.83	0.46
1:C:216:ALA:C	3:M:296:LEU:HD12	2.36	0.46
5:D:46:TRP:CE2	9:D:101:BCL:H2C	2.51	0.46
2:L:240:ARG:NE	3:M:6:ASN:O	2.49	0.46
3:M:228:ARG:HG3	3:M:228:ARG:H	1.40	0.46
15:N:101:CRT:H372	6:P:36:HIS:CD2	14.03	0.46
4:H:16:ILE:HD12	4:H:16:ILE:HA	1.78	0.46
1:C:36:ARG:HD2	2:L:77:PRO:O	2.15	0.46
2:L:126:VAL:HG11	3:M:251:PHE:CE2	2.50	0.46
6:X:24:SER:HB2	15:X:101:CRT:C14	2.45	0.46
5:Y:46:TRP:CE3	9:Y:101:BCL:H2C	2.50	0.46
9:Z:102:BCL:HMB2	9:Z:102:BCL:H101	1.97	0.46
9:Y:101:BCL:C1D	9:Z:102:BCL:HMD2	2.46	0.46
5:1:5:ASN:HB3	5:1:8:LEU:HB2	1.97	0.46
5:AC:17:PRO:HB3	6:AD:17:PHE:CE1	2.51	0.46
9:AI:101:BCL:C4C	9:AJ:102:BCL:HMD2	2.46	0.46
5:D:10:LYS:HG2	5:D:13:LEU:HD12	1.98	0.46
5:F:31:LEU:O	5:F:34:LEU:HB3	2.16	0.46
3:M:126:ILE:HD13	9:M:401:BCL:C9	2.44	0.46
3:M:233:ARG:NH1	4:H:133:ILE:HD11	2.31	0.46
3:M:59:LEU:HB3	3:M:128:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:101:CRT:H181	15:N:101:CRT:H20	1.87	0.46
6:X:36:HIS:CD2	9:X:102:BCL:H112	2.51	0.46
5:A:21:LEU:HD23	5:A:21:LEU:HA	1.62	0.46
9:AB:101:BCL:H61	9:AB:101:BCL:H93	1.79	0.46
1:C:119:ASP:OD1	1:C:124:LYS:HE2	2.16	0.46
5:D:29:ILE:HD11	9:D:101:BCL:H101	1.98	0.46
5:D:2:PHE:O	5:D:3:THR:OG1	2.26	0.46
15:G:101:CRT:H20	15:G:101:CRT:H181	1.78	0.46
5:K:17:PRO:HB3	6:N:17:PHE:CE2	2.49	0.46
3:M:5:GLN:HG2	12:M:407:PEF:O1P	2.15	0.46
5:O:7:ASN:HB3	5:O:10:LYS:HD2	1.98	0.46
9:T:102:BCL:HBB3	9:U:101:BCL:CHC	2.46	0.46
5:W:10:LYS:HB3	15:Z:101:CRT:C3	2.45	0.46
5:Y:23:SER:CB	9:1:101:BCL:H151	2.46	0.45
1:C:148:THR:HG23	1:C:321:ALA:O	2.17	0.45
2:L:140:LEU:HD11	9:L:301:BCL:HED2	1.97	0.45
3:M:150:PHE:CA	10:M:402:BPH:HMD3	2.46	0.45
6:N:20:ILE:HB	15:N:101:CRT:C8	4.34	0.45
5:O:5:ASN:HB2	5:O:8:LEU:HB2	1.97	0.45
9:U:101:BCL:HBA1	9:U:101:BCL:HED2	4.49	0.45
9:W:101:BCL:HBB3	9:W:101:BCL:HMB1	1.98	0.45
2:L:52:TRP:CZ3	5:A:40:LEU:HD13	2.50	0.45
6:AD:18:HIS:O	6:AD:22:MET:HG2	2.16	0.45
9:F:101:BCL:H61	6:G:28:TRP:CZ3	2.51	0.45
4:H:120:PRO:HB3	4:H:122:HIS:CD2	2.51	0.45
5:O:59:GLY:C	5:O:61:LYS:HA	2.36	0.45
6:T:45:TRP:CD1	6:T:46:LEU:HG	2.50	0.45
9:U:101:BCL:H112	9:U:101:BCL:H142	3.39	0.45
5:W:39:VAL:HG12	5:W:46:TRP:HZ3	1.80	0.45
9:A:102:BCL:H102	9:A:102:BCL:H62	1.51	0.45
9:AC:102:BCL:HBA2	6:AD:32:VAL:CG2	2.46	0.45
5:D:24:ILE:HD13	5:D:24:ILE:HA	4.36	0.45
4:H:171:TRP:CE2	4:H:194:LEU:HD21	2.51	0.45
5:1:57:ALA:H	5:1:59:GLY:CA	2.30	0.45
9:7:101:BCL:H162	9:7:101:BCL:H122	1.57	0.45
6:AD:31:LEU:HB3	9:AD:101:BCL:HED3	1.97	0.45
15:AE:103:CRT:H342	9:AH:101:BCL:O1A	2.15	0.45
6:B:11:ASP:O	6:B:15:LYS:HG3	2.17	0.45
1:C:155:CYS:SG	7:C:502:HEM:CAC	3.05	0.45
6:E:17:PHE:HA	15:E:101:CRT:H42	1.99	0.45
15:N:101:CRT:H27	9:N:102:BCL:H12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:101:CRT:H342	9:P:101:BCL:O1A	2.17	0.45
6:P:40:TRP:CE3	6:P:44:PRO:HA	2.52	0.45
6:P:45:TRP:CD1	6:P:46:LEU:HG	2.51	0.45
9:S:102:BCL:H92	9:S:102:BCL:H61	1.71	0.45
9:X:102:BCL:C1C	9:Y:101:BCL:HBB3	2.46	0.45
6:Z:40:TRP:CE2	9:Z:102:BCL:H202	2.52	0.45
5:3:35:ILE:HG21	9:4:102:BCL:C1D	2.47	0.45
9:5:101:BCL:H72	9:5:101:BCL:H112	1.33	0.45
6:6:10:THR:HG23	6:6:13:GLU:CD	2.36	0.45
5:7:4:MET:HB2	6:0:23:GLN:OE1	2.16	0.45
6:AD:28:TRP:CE3	9:AD:101:BCL:H101	2.51	0.45
9:AK:101:BCL:H2C	9:AK:101:BCL:HBC2	1.79	0.45
5:D:55:TYR:CZ	6:AL:43:ARG:HG2	153.10	0.45
6:G:10:THR:HG23	6:G:13:GLU:CD	3.42	0.45
2:L:199:HIS:CE1	2:L:239:HIS:CE1	3.05	0.45
11:L:304:UQ8:H37A	11:L:304:UQ8:H40	1.61	0.45
2:L:109:TRP:CZ2	14:M:403:MQ8:H291	2.51	0.45
5:O:4:MET:N	6:R:23:GLN:OE1	2.50	0.45
5:U:11:ILE:HG12	9:W:101:BCL:H142	1.98	0.45
9:A:102:BCL:H3A	9:A:102:BCL:HBA1	1.78	0.45
9:AI:101:BCL:HMD1	6:AJ:36:HIS:ND1	2.32	0.45
5:D:17:PRO:HG2	6:E:9:LEU:HD21	3.82	0.45
6:E:21:PHE:HA	15:E:101:CRT:H14	2.51	0.45
6:E:20:ILE:HB	15:E:101:CRT:H9	3.04	0.45
6:G:33:VAL:O	6:G:37:LEU:HG	2.17	0.45
4:H:89:ALA:HB1	4:H:101:VAL:O	2.17	0.45
4:H:149:PRO:HG3	4:H:204:LYS:HB3	1.98	0.45
3:M:128:LEU:HA	3:M:128:LEU:HD23	1.61	0.45
6:N:20:ILE:HD12	15:N:101:CRT:C6	2.46	0.45
5:O:44:LEU:HD12	5:Q:47:LEU:HD22	1.99	0.45
9:Q:101:BCL:H51	9:Q:101:BCL:C12	2.46	0.45
6:V:28:TRP:O	6:V:32:VAL:HG23	2.17	0.45
5:Y:46:TRP:O	5:Y:47:LEU:HD23	2.17	0.45
15:2:101:CRT:C29	9:3:101:BCL:H11	2.47	0.45
9:AH:101:BCL:H203	9:AH:101:BCL:H102	1.99	0.45
1:C:212:ILE:HD11	7:C:503:HEM:HMA3	1.98	0.45
1:C:46:LYS:O	1:C:49:ARG:HB3	2.17	0.45
5:D:55:TYR:HD1	5:D:61:LYS:O	11.57	0.45
3:M:268:TRP:NE1	4:H:30:LEU:HB3	2.32	0.45
2:L:35:PHE:CE2	2:L:111:LEU:HB3	2.51	0.45
2:L:177:HIS:NE2	9:L:301:BCL:HMC2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:184:LEU:O	2:L:187:SER:N	2.49	0.45
2:L:252:TRP:HE1	11:L:304:UQ8:H35A	1.81	0.45
9:O:101:BCL:H141	9:O:101:BCL:H193	1.99	0.45
5:K:14:ILE:HG22	5:O:18:ARG:HG2	1.97	0.45
5:Q:2:PHE:HD1	6:R:26:TYR:HE2	1.64	0.45
5:A:8:LEU:HB2	6:E:20:ILE:HD13	1.98	0.45
1:C:127:SER:OG	7:C:501:HEM:HAC	2.17	0.45
1:C:191:ALA:O	1:C:192:TYR:HB2	2.17	0.45
5:D:8:LEU:HD23	5:D:8:LEU:HA	1.75	0.45
6:E:17:PHE:HD1	15:E:101:CRT:H33	1.82	0.45
4:H:154:MET:HB3	4:H:207:ARG:O	2.16	0.45
4:H:45:ARG:NH1	4:H:53:VAL:HG11	2.31	0.45
3:M:6:ASN:ND2	3:M:227:SER:HB2	2.31	0.45
5:Q:9:TYR:HD1	5:Q:9:TYR:H	1.64	0.45
9:W:101:BCL:H41	9:W:101:BCL:H61	2.62	0.45
9:Y:101:BCL:HHC	9:Y:101:BCL:HMC2	1.62	0.45
9:7:101:BCL:HBB3	9:7:101:BCL:HMB1	1.98	0.45
9:AC:102:BCL:HMB1	9:AC:102:BCL:HBB2	1.98	0.45
9:AI:101:BCL:H3A	9:AI:101:BCL:HBA1	1.78	0.45
6:B:43:ARG:HG3	5:D:55:TYR:CE1	2.52	0.45
2:L:65:LEU:CD1	3:M:308:PRO:HG3	2.46	0.45
3:M:33:ARG:HA	3:M:34:PRO:HD3	1.66	0.45
5:7:18:ARG:HG2	5:7:18:ARG:H	1.54	0.45
15:6:101:CRT:H393	5:7:36:HIS:CD2	2.52	0.45
5:9:46:TRP:CZ3	9:9:103:BCL:HBC3	2.53	0.45
5:AC:44:LEU:HD12	5:AE:47:LEU:HD22	1.99	0.45
15:AH:102:CRT:H5	15:AH:102:CRT:H33	1.66	0.45
1:C:207:ALA:HB1	1:C:277:ARG:HH21	1.82	0.45
1:C:27:PRO:HD3	5:3:41:SER:HB2	1.99	0.45
1:C:54:GLN:HA	1:C:54:GLN:OE1	2.16	0.45
5:D:12:TRP:HZ3	5:D:20:VAL:HG11	1.82	0.45
5:F:11:ILE:CD1	15:J:101:CRT:H10	2.47	0.45
2:L:236:LEU:O	2:L:239:HIS:HB2	2.17	0.45
2:L:192:ASN:OD1	2:L:246:ALA:HB2	2.16	0.45
5:O:12:TRP:HB2	6:P:14:ALA:HB1	1.99	0.45
6:R:17:PHE:HB2	15:R:101:CRT:H22A	1.98	0.45
5:U:3:THR:OG1	5:U:5:ASN:N	7.35	0.45
9:W:101:BCL:HBC3	9:W:101:BCL:H2C	1.77	0.45
9:X:102:BCL:HMB2	9:X:102:BCL:H102	1.99	0.45
6:6:20:ILE:O	6:6:24:SER:OG	2.19	0.44
9:A:102:BCL:HAA2	9:A:102:BCL:HED3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AE:102:BCL:H43	6:AF:28:TRP:CH2	2.52	0.44
1:C:199:PRO:O	1:C:203:PHE:HD2	1.99	0.44
5:D:20:VAL:O	5:D:23:SER:HB2	2.17	0.44
15:G:101:CRT:H36	5:I:33:LEU:HD23	1.98	0.44
5:I:7:ASN:OD1	5:I:9:TYR:HE2	2.00	0.44
3:M:42:LYS:NZ	12:M:408:PEF:H52	2.32	0.44
6:T:45:TRP:CZ2	9:T:102:BCL:H143	2.52	0.44
6:Z:43:ARG:HG3	5:AA:55:TYR:OH	128.92	0.44
5:7:35:ILE:CG1	15:8:101:CRT:H403	2.47	0.44
5:7:9:TYR:OH	6:8:11:ASP:OD2	2.26	0.44
6:AH:18:HIS:O	6:AH:22:MET:HG2	2.17	0.44
6:AL:20:ILE:HD12	15:AL:101:CRT:C6	2.46	0.44
1:C:128:ARG:HH21	7:C:501:HEM:CAD	2.29	0.44
6:J:26:TYR:HD1	6:J:29:PHE:CD2	2.36	0.44
2:L:130:PHE:CE2	2:L:134:ILE:HD11	2.52	0.44
3:M:162:PHE:C	3:M:165:PRO:HD2	2.36	0.44
5:Y:13:LEU:O	6:Z:7:THR:HG23	2.16	0.44
9:AH:103:BCL:H151	9:AH:103:BCL:H18	1.60	0.44
9:D:101:BCL:H93	9:D:101:BCL:H111	1.85	0.44
2:L:196:LEU:HB2	3:M:216:PHE:CD2	2.52	0.44
6:T:11:ASP:O	6:T:15:LYS:HG3	2.18	0.44
5:A:11:ILE:HG23	5:A:12:TRP:CD2	2.53	0.44
9:F:101:BCL:HBA1	6:G:28:TRP:CH2	2.51	0.44
2:L:132:PHE:CE2	11:L:304:UQ8:H40B	2.53	0.44
3:M:23:LEU:HD22	3:M:139:ALA:HB1	1.99	0.44
3:M:37:SER:OG	3:M:37:SER:O	2.30	0.44
9:L:303:BCL:H151	15:M:404:CRT:H133	1.99	0.44
3:M:42:LYS:HE3	12:M:408:PEF:O2P	2.17	0.44
3:M:81:TRP:CD1	5:U:40:LEU:HG	2.52	0.44
5:1:44:LEU:HA	5:3:55:TYR:CD2	2.52	0.44
6:8:21:PHE:HA	15:8:101:CRT:H14	1.99	0.44
5:AE:12:TRP:HZ3	5:AE:20:VAL:HG11	1.82	0.44
5:AC:42:THR:HG21	5:AE:47:LEU:HD13	1.99	0.44
5:AE:43:ASP:OD2	5:AG:55:TYR:HD2	2.00	0.44
9:D:101:BCL:HBD	9:D:101:BCL:HAA2	1.99	0.44
9:F:101:BCL:H192	9:F:101:BCL:H161	1.71	0.44
9:G:102:BCL:CGA	9:G:102:BCL:H3A	2.47	0.44
6:G:31:LEU:O	6:G:34:ILE:HB	2.17	0.44
5:U:5:ASN:HA	5:U:6:ALA:HA	4.38	0.44
6:X:10:THR:OG1	6:X:13:GLU:HG3	2.18	0.44
5:3:50:ASN:HB3	5:3:54:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4:102:BCL:H111	9:4:102:BCL:H93	1.65	0.44
9:A:102:BCL:H11	9:A:102:BCL:HBA1	1.67	0.44
9:AD:101:BCL:H62	9:AD:101:BCL:H41	1.30	0.44
9:D:101:BCL:H62	9:D:101:BCL:H41	3.07	0.44
2:L:7:GLU:OE1	2:L:11:ARG:NE	2.42	0.44
3:M:215:LEU:HD21	14:M:403:MQ8:C19	2.48	0.44
5:Q:45:ASN:OD1	5:Q:46:TRP:N	2.51	0.44
5:5:46:TRP:CZ3	9:5:101:BCL:H2C	2.53	0.44
5:5:9:TYR:HB2	6:6:14:ALA:O	2.18	0.44
1:C:172:PRO:HG3	1:C:185:TYR:CE1	2.53	0.44
15:E:101:CRT:H181	15:E:101:CRT:H20	1.94	0.44
4:H:29:TYR:HH	12:H:304:PEF:C10	2.29	0.44
2:L:167:SER:HA	9:L:301:BCL:CBC	2.47	0.44
3:M:260:VAL:HG12	4:H:34:ASP:CG	2.38	0.44
3:M:8:PHE:HB2	12:M:407:PEF:C4	2.48	0.44
5:S:19:ARG:HH22	17:S:101:PGW:H04A	1.82	0.44
5:S:40:LEU:HD11	5:S:47:LEU:HD12	1.99	0.44
6:V:32:VAL:CG2	9:V:101:BCL:HBA2	2.48	0.44
9:4:102:BCL:H192	9:4:102:BCL:H162	1.75	0.44
9:3:101:BCL:H2	6:4:28:TRP:CH2	2.53	0.44
9:AH:103:BCL:C4A	9:AI:101:BCL:HMB3	2.48	0.44
1:C:33:ILE:HG21	1:C:248:THR:O	2.17	0.44
4:H:68:VAL:O	4:H:68:VAL:HG12	2.18	0.44
6:J:26:TYR:HD1	6:J:29:PHE:HD2	1.66	0.44
2:L:75:ILE:N	2:L:75:ILE:HD12	2.33	0.44
3:M:156:PHE:CD2	9:M:401:BCL:H43	2.53	0.44
5:S:25:VAL:HG21	9:S:102:BCL:H152	1.99	0.44
9:Y:101:BCL:H111	9:Y:101:BCL:H151	1.42	0.44
6:Z:40:TRP:CH2	6:Z:46:LEU:HB2	2.53	0.44
5:1:20:VAL:O	5:1:23:SER:HB2	2.18	0.44
15:6:101:CRT:H36	5:7:33:LEU:HD23	1.99	0.44
5:AA:7:ASN:HB3	5:AA:10:LYS:HD2	1.99	0.44
9:AE:102:BCL:H43	6:AF:28:TRP:CZ2	2.53	0.44
6:B:42:TYR:OH	6:B:43:ARG:NH2	2.51	0.44
1:C:53:ILE:HA	1:C:319:TYR:CE1	2.52	0.44
4:H:162:GLU:HB2	4:H:216:ALA:CB	2.48	0.44
9:J:102:BCL:H161	9:J:102:BCL:H192	1.83	0.44
9:L:301:BCL:HBC3	3:M:197:TYR:OH	2.18	0.44
3:M:182:HIS:CD2	15:M:404:CRT:H20	2.53	0.44
9:T:102:BCL:CHB	9:T:102:BCL:H62	2.47	0.44
6:V:45:TRP:HA	5:W:55:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:43:ASP:C	5:Y:45:ASN:H	2.20	0.44
5:5:14:ILE:HG21	15:8:101:CRT:H1M1	2.00	0.43
9:7:101:BCL:HED2	6:8:32:VAL:HG22	1.99	0.43
15:8:101:CRT:H30	9:8:102:BCL:H41	1.99	0.43
5:AE:45:ASN:O	5:AE:49:ASP:OD2	2.36	0.43
5:AG:16:ASP:OD2	5:AG:19:ARG:HG3	2.18	0.43
4:H:76:VAL:HG12	4:H:77:VAL:N	2.33	0.43
2:L:12:VAL:HG22	2:L:13:ARG:N	2.33	0.43
15:M:404:CRT:H26	15:M:404:CRT:H241	1.85	0.43
3:M:63:PHE:CE2	3:M:124:LEU:HB3	2.53	0.43
6:N:43:ARG:HG3	5:O:55:TYR:CZ	2.53	0.43
15:P:102:CRT:H10	15:P:102:CRT:H81	1.90	0.43
5:W:31:LEU:HD12	5:W:34:LEU:HD23	2.00	0.43
5:W:4:MET:O	5:W:5:ASN:HB2	2.17	0.43
5:Y:35:ILE:HG12	15:Z:101:CRT:H392	2.00	0.43
9:4:102:BCL:H122	9:4:102:BCL:H162	1.87	0.43
9:7:101:BCL:HHC	9:7:101:BCL:HMC2	1.78	0.43
9:AH:101:BCL:H2C	9:AH:101:BCL:HBC3	1.72	0.43
15:AJ:101:CRT:H15	15:AJ:101:CRT:H131	1.88	0.43
1:C:152:CYS:HA	7:C:502:HEM:HAB	2.00	0.43
1:C:71:LYS:HB2	1:C:74:GLU:OE2	2.17	0.43
5:D:39:VAL:HG21	9:D:102:BCL:H3C	1.99	0.43
3:M:242:GLY:CA	4:H:119:ARG:HD2	2.48	0.43
2:L:225:PHE:HD1	2:L:225:PHE:HA	1.56	0.43
2:L:48:LEU:HD13	5:9:34:LEU:HD22	1.99	0.43
9:Q:101:BCL:HMB1	9:Q:101:BCL:HBB3	2.00	0.43
9:T:102:BCL:HBC3	9:T:102:BCL:H2C	1.62	0.43
5:U:3:THR:HG23	5:U:5:ASN:H	9.04	0.43
5:U:4:MET:O	5:U:5:ASN:HB2	4.44	0.43
9:X:102:BCL:H161	9:X:102:BCL:H122	1.60	0.43
5:1:12:TRP:HZ3	5:1:20:VAL:HG21	1.83	0.43
5:1:24:ILE:CD1	9:3:101:BCL:H18	2.48	0.43
1:C:274:ARG:N	1:C:274:ARG:HD2	2.33	0.43
1:C:167:VAL:HG11	1:C:297:GLY:HA3	2.00	0.43
4:H:184:VAL:HB	4:H:193:VAL:HG22	2.00	0.43
15:P:102:CRT:H36	5:Q:33:LEU:HD23	2.00	0.43
6:P:46:LEU:O	6:R:42:TYR:OH	2.22	0.43
5:O:14:ILE:HD11	15:R:101:CRT:H21A	1.98	0.43
6:T:40:TRP:HH2	6:T:46:LEU:OXT	2.02	0.43
6:X:14:ALA:CB	6:X:17:PHE:HB3	2.48	0.43
5:9:8:LEU:HG	6:0:18:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AA:101:BCL:C4C	9:AB:101:BCL:HMD2	2.48	0.43
5:AG:5:ASN:C	5:AG:7:ASN:N	2.68	0.43
6:AH:44:PRO:O	5:AI:52:PRO:HD2	2.18	0.43
9:AI:101:BCL:HBA2	9:AJ:102:BCL:O2D	2.17	0.43
9:D:101:BCL:H152	5:AK:23:SER:OG	88.26	0.43
6:AL:21:PHE:CD1	15:AL:101:CRT:H14	2.43	0.43
9:AL:102:BCL:H93	9:AL:102:BCL:H111	1.55	0.43
6:E:8:GLY:C	6:E:9:LEU:HD12	2.39	0.43
2:L:26:TRP:CZ3	4:H:99:PRO:HB3	2.51	0.43
9:K:101:BCL:H162	9:K:101:BCL:H122	1.79	0.43
2:L:184:LEU:HD12	2:L:184:LEU:HA	1.74	0.43
3:M:21:VAL:HA	3:M:22:PRO:HD3	1.73	0.43
15:6:101:CRT:H10	15:6:101:CRT:H81	1.85	0.43
5:7:46:TRP:CE3	9:7:101:BCL:HBC3	2.53	0.43
6:AB:20:ILE:HD12	15:AC:101:CRT:C5	2.49	0.43
9:AE:104:BCL:H111	9:AE:104:BCL:H91	1.71	0.43
9:AH:101:BCL:H122	9:AH:101:BCL:H162	1.64	0.43
2:L:188:PHE:HB3	2:L:249:ALA:HB2	2.00	0.43
3:M:63:PHE:CD2	3:M:124:LEU:HB3	2.54	0.43
9:L:305:BCL:HMD1	3:M:206:ILE:HD13	2.00	0.43
3:M:39:TRP:O	3:M:42:LYS:N	2.50	0.43
5:Q:12:TRP:O	6:R:9:LEU:HD12	2.18	0.43
5:W:15:LEU:O	5:W:17:PRO:HD3	2.18	0.43
6:X:31:LEU:HA	6:X:31:LEU:HD23	1.74	0.43
15:4:101:CRT:H293	9:5:101:BCL:H11	2.01	0.43
5:9:10:LYS:HB3	15:9:102:CRT:C4	2.49	0.43
9:AB:101:BCL:H61	9:AB:101:BCL:H41	1.72	0.43
6:AB:40:TRP:HH2	6:AB:46:LEU:OXT	2.01	0.43
9:AH:103:BCL:H2C	9:AH:103:BCL:HBC3	1.79	0.43
5:A:36:HIS:NE2	9:B:101:BCL:NB	2.66	0.43
6:R:17:PHE:HD1	15:R:101:CRT:H22A	1.83	0.43
9:V:101:BCL:H72	9:V:101:BCL:HMB2	1.99	0.43
9:W:101:BCL:H143	9:W:101:BCL:H112	1.67	0.43
5:Y:17:PRO:HB3	6:Z:17:PHE:CZ	2.53	0.43
9:AD:101:BCL:H3A	9:AD:101:BCL:HBA1	1.68	0.43
5:AG:36:HIS:CE1	9:AH:103:BCL:HMD1	2.54	0.43
9:AI:101:BCL:H121	9:AI:101:BCL:H161	1.38	0.43
1:C:189:THR:HG23	1:C:238:ASN:HD21	1.83	0.43
6:G:10:THR:OG1	6:G:13:GLU:HG3	2.71	0.43
9:L:303:BCL:H2C	9:L:303:BCL:HBC2	1.73	0.43
3:M:98:PRO:HG3	3:M:107:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:235:ILE:CG2	3:M:236:ASP:N	2.82	0.43
2:L:276:LEU:O	3:M:88:LYS:HE3	2.19	0.43
6:N:25:MET:HG3	15:N:101:CRT:C20	2.48	0.43
6:P:28:TRP:CH2	9:P:101:BCL:HBA1	2.52	0.43
6:V:16:GLU:O	6:V:20:ILE:HG13	2.18	0.43
9:4:102:BCL:HMB1	9:4:102:BCL:HBB3	2.00	0.43
5:7:49:ASP:O	5:7:50:ASN:HB2	2.18	0.43
5:A:20:VAL:HG22	9:D:101:BCL:H162	1.99	0.43
9:AB:101:BCL:HMA1	9:AD:101:BCL:HMA1	2.00	0.43
6:AB:31:LEU:O	6:AB:34:ILE:HB	2.18	0.43
6:AD:33:VAL:O	6:AD:37:LEU:HG	2.19	0.43
6:AJ:40:TRP:CE3	6:AJ:44:PRO:HA	2.53	0.43
9:AL:102:BCL:H141	9:AL:102:BCL:H162	1.76	0.43
9:AL:102:BCL:HBB2	9:AL:102:BCL:HMB1	1.99	0.43
6:B:17:PHE:CD1	15:9:102:CRT:H83	2.53	0.43
4:H:100:LEU:HB2	4:H:111:PHE:CZ	2.53	0.43
9:K:101:BCL:H171	9:K:101:BCL:H13	1.83	0.43
3:M:18:TYR:HA	3:M:19:PRO:HD2	1.87	0.43
9:L:305:BCL:O1D	3:M:203:MET:HB3	2.19	0.43
3:M:263:GLU:OE1	3:M:267:ARG:NH2	2.49	0.43
3:M:37:SER:HG	3:M:40:LEU:N	2.11	0.43
2:L:230:GLY:HA3	3:M:51:ILE:HD12	2.01	0.43
3:M:91:PHE:N	3:M:91:PHE:CD1	2.86	0.43
9:R:102:BCL:CED	9:R:102:BCL:HAA2	2.49	0.43
5:U:36:HIS:CE1	9:V:101:BCL:HMD1	2.53	0.43
5:W:9:TYR:H	5:W:9:TYR:HD1	1.67	0.43
15:AD:102:CRT:H36	5:AE:33:LEU:HD23	2.01	0.43
15:J:101:CRT:H15	15:J:101:CRT:H131	1.82	0.43
2:L:130:PHE:CD1	10:L:302:BPH:C4D	3.01	0.43
3:M:149:ALA:O	3:M:152:ALA:N	2.46	0.43
5:Q:21:LEU:HA	5:Q:21:LEU:HD23	1.87	0.43
5:Q:39:VAL:HG12	5:Q:46:TRP:HZ3	1.83	0.43
9:W:101:BCL:HMD2	9:Z:102:BCL:CHD	18.94	0.43
6:0:32:VAL:HG11	9:0:101:BCL:HBA1	2.00	0.43
9:AC:102:BCL:HBA1	9:AC:102:BCL:H3A	1.40	0.43
5:AI:12:TRP:HE1	6:AJ:18:HIS:HB2	1.83	0.43
1:C:169:ASP:OD1	1:C:169:ASP:C	2.56	0.43
5:D:46:TRP:NE1	9:D:101:BCL:HHC	2.33	0.43
15:E:101:CRT:H372	5:F:36:HIS:CD2	2.54	0.43
2:L:116:ILE:HD13	3:M:254:TRP:CB	2.49	0.43
14:M:403:MQ8:H262	14:M:403:MQ8:H221	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:101:CRT:H372	5:O:36:HIS:CG	2.53	0.43
6:N:31:LEU:HD23	6:N:31:LEU:HA	2.30	0.43
6:R:43:ARG:HG3	5:S:55:TYR:OH	2.19	0.43
6:X:13:GLU:HA	6:X:14:ALA:HA	1.77	0.43
9:Y:101:BCL:H162	9:Y:101:BCL:H143	1.91	0.43
6:4:32:VAL:HG21	9:4:102:BCL:HBA2	2.00	0.42
9:7:101:BCL:H62	9:7:101:BCL:H41	1.78	0.42
6:B:36:HIS:ND1	9:B:101:BCL:HMD1	2.34	0.42
1:C:81:VAL:HG11	1:C:131:PHE:HB3	2.00	0.42
6:E:34:ILE:HA	6:E:34:ILE:HD13	1.88	0.42
6:G:24:SER:O	6:G:27:ALA:HB3	2.35	0.42
9:L:305:BCL:CHD	9:L:305:BCL:HBC2	2.49	0.42
3:M:18:TYR:CE2	3:M:20:GLY:CA	2.95	0.42
3:M:63:PHE:HB2	3:M:125:SER:HB2	2.01	0.42
6:N:24:SER:O	6:N:27:ALA:HB3	2.25	0.42
6:P:25:MET:HG2	6:P:29:PHE:CE2	2.54	0.42
9:R:102:BCL:C2	9:R:102:BCL:H3A	2.39	0.42
15:U:102:CRT:H393	5:W:36:HIS:CD2	2.54	0.42
5:W:43:ASP:O	5:Y:56:GLN:NE2	2.52	0.42
6:4:21:PHE:HA	15:4:101:CRT:H14	2.00	0.42
6:AH:32:VAL:HA	9:AH:101:BCL:HED2	2.00	0.42
5:AI:9:TYR:CE1	5:AI:10:LYS:HG3	2.54	0.42
6:AJ:25:MET:HG3	15:AJ:101:CRT:C21	2.49	0.42
6:AJ:40:TRP:HH2	6:AJ:46:LEU:OXT	2.02	0.42
9:AK:101:BCL:H41	9:AK:101:BCL:H61	1.65	0.42
9:D:102:BCL:C9	6:E:33:VAL:HG22	2.45	0.42
1:C:253:THR:HG21	2:L:171:TYR:CB	2.49	0.42
2:L:17:LEU:HA	2:L:17:LEU:HD23	1.78	0.42
2:L:248:SER:O	2:L:251:PHE:HB3	2.19	0.42
2:L:196:LEU:HB2	3:M:216:PHE:HD2	1.83	0.42
9:N:102:BCL:HBA1	9:N:102:BCL:H3A	1.78	0.42
9:O:101:BCL:C2	9:O:101:BCL:HBA1	2.48	0.42
5:S:36:HIS:O	5:S:40:LEU:HB2	2.19	0.42
6:T:45:TRP:CZ2	9:T:102:BCL:H151	2.54	0.42
5:U:43:ASP:CB	5:W:50:ASN:HD21	7.33	0.42
5:Y:50:ASN:C	5:Y:51:ILE:HD12	2.40	0.42
9:0:101:BCL:H91	9:0:101:BCL:H111	1.78	0.42
5:1:57:ALA:HB3	5:1:58:LEU:CB	2.49	0.42
5:1:5:ASN:OD1	5:1:6:ALA:N	2.52	0.42
15:2:101:CRT:C31	9:3:101:BCL:H3A	2.49	0.42
9:AE:104:BCL:H192	6:AF:40:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AI:10:LYS:O	5:AI:13:LEU:HB2	2.19	0.42
1:C:141:TRP:C	1:C:145:VAL:HG22	2.39	0.42
1:C:195:LEU:HA	1:C:195:LEU:HD23	1.76	0.42
6:E:40:TRP:HZ3	6:E:45:TRP:H	1.67	0.42
5:D:43:ASP:OD1	5:F:56:GLN:HG2	2.48	0.42
5:I:4:MET:O	5:I:5:ASN:HB2	2.19	0.42
2:L:179:ASN:O	2:L:182:HIS:HB3	2.18	0.42
9:L:301:BCL:H111	10:L:302:BPH:HHB	2.01	0.42
3:M:122:LEU:HD12	3:M:122:LEU:HA	1.67	0.42
6:N:32:VAL:HG12	9:N:102:BCL:H92	2.00	0.42
9:K:101:BCL:HMD1	6:N:36:HIS:CE1	2.54	0.42
9:T:102:BCL:H61	9:T:102:BCL:H93	1.76	0.42
6:T:18:HIS:O	6:T:22:MET:HG2	2.18	0.42
5:W:2:PHE:O	5:W:3:THR:HG23	2.18	0.42
9:X:102:BCL:H41	9:X:102:BCL:H61	1.71	0.42
5:1:39:VAL:HG12	5:1:46:TRP:HZ3	1.84	0.42
6:6:9:LEU:HD23	6:6:13:GLU:O	2.19	0.42
6:AD:31:LEU:HA	6:AD:31:LEU:HD23	1.91	0.42
5:AG:40:LEU:HA	5:AG:40:LEU:HD12	1.73	0.42
9:AI:101:BCL:HBC3	9:AI:101:BCL:H2C	1.82	0.42
9:D:101:BCL:HBC3	9:D:101:BCL:H2C	3.49	0.42
15:J:101:CRT:H5	15:J:101:CRT:H21A	1.68	0.42
2:L:237:ALA:HA	2:L:240:ARG:CG	2.50	0.42
9:M:401:BCL:HMA1	9:M:401:BCL:HHB	1.76	0.42
15:T:101:CRT:H10	15:T:101:CRT:H81	1.85	0.42
9:V:101:BCL:C1B	9:W:101:BCL:HMB3	2.49	0.42
9:1:101:BCL:H61	9:1:101:BCL:H41	1.91	0.42
5:1:9:TYR:HB2	6:2:14:ALA:O	2.20	0.42
6:4:21:PHE:HA	15:4:101:CRT:H11	2.00	0.42
5:AA:44:LEU:HD13	6:AB:43:ARG:HD3	2.01	0.42
5:AC:28:GLN:OE1	6:AD:28:TRP:NE1	2.49	0.42
9:AI:101:BCL:HMD1	6:AJ:36:HIS:CE1	2.54	0.42
15:AJ:101:CRT:H2M1	5:AK:37:MET:HG3	2.02	0.42
6:AL:40:TRP:CH2	9:AL:102:BCL:H193	2.54	0.42
9:L:303:BCL:HAC2	9:L:303:BCL:HHD	1.19	0.42
3:M:200:PRO:HD2	3:M:294:TRP:CZ3	2.55	0.42
3:M:63:PHE:CB	3:M:125:SER:HB2	2.50	0.42
5:W:45:ASN:HB3	5:Y:56:GLN:HE22	1.84	0.42
6:Z:10:THR:OG1	6:Z:13:GLU:HG3	2.20	0.42
5:AI:12:TRP:HE1	6:AJ:18:HIS:HD1	1.67	0.42
9:AL:102:BCL:CBB	9:AL:102:BCL:HMB1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:31:LEU:HD23	6:B:31:LEU:HA	1.86	0.42
1:C:169:ASP:HA	1:C:170:PRO:HD3	1.89	0.42
9:D:101:BCL:H141	9:D:101:BCL:H162	1.52	0.42
2:L:157:TYR:CG	10:L:302:BPH:H151	2.55	0.42
3:M:230:GLY:O	3:M:233:ARG:HB2	2.20	0.42
2:L:281:TRP:CB	3:M:88:LYS:HD2	2.49	0.42
5:Q:11:ILE:O	5:Q:15:LEU:N	2.43	0.42
5:AG:11:ILE:HG23	5:AG:12:TRP:CD2	2.55	0.42
1:C:258:ASP:O	1:C:262:SER:OG	2.33	0.42
5:D:39:VAL:HG12	5:D:46:TRP:CZ3	2.55	0.42
4:H:66:THR:HG22	4:H:77:VAL:CG2	2.50	0.42
2:L:125:HIS:HE1	3:M:5:GLN:OE1	2.03	0.42
9:O:101:BCL:H13	9:O:101:BCL:H172	1.57	0.42
15:P:102:CRT:H342	9:Q:101:BCL:H11	2.01	0.42
15:X:101:CRT:H10	15:X:101:CRT:H81	1.62	0.42
9:X:102:BCL:HBB2	9:X:102:BCL:HMB1	2.01	0.42
6:Z:40:TRP:HZ3	6:Z:46:LEU:H	1.67	0.42
5:3:31:LEU:O	5:3:34:LEU:HB3	2.20	0.42
9:5:102:BCL:H111	9:5:102:BCL:H93	1.72	0.42
9:AE:104:BCL:H71	6:AF:36:HIS:CG	2.55	0.42
9:D:101:BCL:HHB	15:AL:101:CRT:H32	113.92	0.42
1:C:179:LYS:HA	1:C:180:PRO:HD3	1.92	0.42
9:D:102:BCL:H93	9:D:102:BCL:H111	1.72	0.42
6:E:40:TRP:CH2	6:E:46:LEU:HD12	2.50	0.42
5:F:28:GLN:HB3	9:F:101:BCL:H12	2.02	0.42
4:H:136:MET:SD	4:H:152:ARG:NH2	2.93	0.42
4:H:224:THR:OG1	4:H:225:LEU:N	2.52	0.42
4:H:4:GLY:O	4:H:6:THR:N	2.53	0.42
5:I:3:THR:H	5:I:4:MET:HA	1.85	0.42
2:L:153:HIS:O	2:L:165:TRP:HZ2	2.03	0.42
2:L:183:MET:HB3	9:L:303:BCL:O1D	2.20	0.42
6:P:21:PHE:CD1	15:P:102:CRT:H16	2.55	0.42
6:P:32:VAL:HG22	9:P:101:BCL:HED2	2.02	0.42
9:U:101:BCL:H102	9:U:101:BCL:H62	4.59	0.42
5:U:21:LEU:HA	5:U:21:LEU:HD23	1.99	0.42
5:A:49:ASP:O	5:A:50:ASN:HB2	2.19	0.42
5:AE:18:ARG:NH1	17:AE:101:PGW:OAE	2.53	0.42
15:AD:102:CRT:H372	5:AE:36:HIS:CG	2.54	0.42
4:H:197:ILE:O	4:H:200:SER:OG	2.34	0.42
4:H:181:TYR:OH	4:H:236:GLU:OE1	2.23	0.42
5:I:13:LEU:HB2	15:N:101:CRT:H1M1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:PHE:CE1	2:L:32:VAL:HG21	2.54	0.42
15:N:101:CRT:H26	15:N:101:CRT:H241	1.91	0.42
15:R:101:CRT:H10	15:R:101:CRT:H81	1.78	0.42
6:T:21:PHE:HA	15:T:101:CRT:H14	2.02	0.42
6:V:30:GLY:O	6:V:34:ILE:HG13	2.46	0.42
15:Z:101:CRT:C27	9:Z:102:BCL:H11	2.50	0.42
6:Z:29:PHE:O	6:Z:32:VAL:HB	2.20	0.42
15:4:101:CRT:H81	15:4:101:CRT:H10	1.86	0.42
5:7:21:LEU:HD23	5:7:21:LEU:HA	1.83	0.42
5:7:31:LEU:HD23	9:8:102:BCL:HED1	2.01	0.42
5:AA:40:LEU:HD23	5:AA:40:LEU:HA	1.95	0.42
9:AB:101:BCL:HBD	9:AB:101:BCL:HED2	1.69	0.42
9:AI:101:BCL:H62	9:AI:101:BCL:H201	2.01	0.42
1:C:189:THR:CG2	1:C:238:ASN:HD21	2.33	0.42
1:C:275:HIS:O	1:C:275:HIS:HD2	2.03	0.42
9:F:101:BCL:H2	6:G:28:TRP:CZ2	2.55	0.42
4:H:66:THR:HG22	4:H:77:VAL:HG23	2.02	0.42
5:I:33:LEU:O	5:I:37:MET:HG2	2.19	0.42
2:L:196:LEU:HD13	3:M:216:PHE:CB	2.50	0.42
3:M:303:MET:HB3	3:M:303:MET:HE2	1.86	0.42
1:C:263:THR:O	3:M:313:ALA:HB2	2.20	0.42
15:N:101:CRT:H291	15:N:101:CRT:H31	2.20	0.42
5:O:30:VAL:HA	5:O:33:LEU:HD12	2.02	0.42
5:O:35:ILE:HA	5:O:38:ILE:HD12	2.02	0.42
5:Q:17:PRO:HB3	6:R:17:PHE:CE2	2.54	0.42
5:U:38:ILE:O	5:U:42:THR:HG23	2.19	0.42
5:3:18:ARG:O	5:3:22:VAL:HG22	2.20	0.41
5:7:12:TRP:HZ3	5:7:20:VAL:HG11	1.85	0.41
6:B:20:ILE:CG2	5:9:3:THR:HG22	2.50	0.41
9:AA:101:BCL:HBB3	9:AA:101:BCL:HMB1	2.02	0.41
5:AA:35:ILE:HG12	15:AC:101:CRT:H403	2.02	0.41
4:H:154:MET:O	4:H:167:VAL:HG23	2.20	0.41
4:H:223:PRO:HG2	4:H:238:LYS:O	2.19	0.41
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.02	0.41
9:T:102:BCL:HAA1	9:T:102:BCL:HBD	2.02	0.41
9:W:101:BCL:H13	9:W:101:BCL:H171	4.02	0.41
9:7:101:BCL:C4C	9:8:102:BCL:HMD2	2.50	0.41
5:AA:7:ASN:OD1	5:AA:9:TYR:HE1	2.03	0.41
15:AE:103:CRT:H14	6:AF:21:PHE:HA	2.01	0.41
5:AK:40:LEU:HD21	5:AK:47:LEU:HD12	2.01	0.41
1:C:205:ASP:CG	1:C:285:TRP:HE1	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:101:CRT:H393	5:F:36:HIS:HB3	2.01	0.41
4:H:107:MET:HB3	4:H:107:MET:HE3	1.91	0.41
4:H:31:ARG:HD2	4:H:31:ARG:HA	1.86	0.41
9:J:102:BCL:HBD	9:J:102:BCL:HED2	1.90	0.41
2:L:235:ALA:O	2:L:238:ILE:HG22	2.19	0.41
2:L:271:TRP:O	2:L:273:ASN:N	2.53	0.41
2:L:68:TYR:CA	2:L:73:ILE:HD11	2.49	0.41
15:M:404:CRT:H31	15:M:404:CRT:H291	1.89	0.41
3:M:31:ILE:HD11	3:M:53:LEU:HB2	2.02	0.41
5:O:3:THR:O	5:O:4:MET:HG2	2.19	0.41
6:P:21:PHE:C	6:P:21:PHE:HD1	2.23	0.41
9:Q:101:BCL:H51	9:Q:101:BCL:H122	2.02	0.41
9:S:102:BCL:O2D	9:S:102:BCL:H2A	2.20	0.41
15:T:101:CRT:H241	15:T:101:CRT:H26	1.88	0.41
15:X:101:CRT:H393	5:Y:36:HIS:HB3	2.02	0.41
6:X:36:HIS:CG	9:X:102:BCL:H8	2.56	0.41
6:Z:46:LEU:HA	6:Z:46:LEU:HD23	1.96	0.41
6:4:17:PHE:HA	15:4:101:CRT:H6	2.02	0.41
6:8:32:VAL:HG12	9:8:102:BCL:H121	2.01	0.41
15:9:102:CRT:H181	15:9:102:CRT:H20	1.89	0.41
9:AE:104:BCL:HBD	9:AE:104:BCL:HED2	1.80	0.41
5:AK:35:ILE:HG12	15:AL:101:CRT:H403	2.02	0.41
1:C:21:LEU:HD11	2:L:274:TRP:CE3	2.55	0.41
1:C:21:LEU:HA	1:C:21:LEU:HD12	1.69	0.41
9:D:102:BCL:H3A	9:D:102:BCL:HBA1	1.77	0.41
3:M:242:GLY:HA2	4:H:119:ARG:HD2	2.02	0.41
4:H:45:ARG:HD3	4:H:45:ARG:HA	1.83	0.41
2:L:161:SER:O	2:L:164:ASP:HB2	2.20	0.41
3:M:143:SER:HB2	3:M:145:HIS:CE1	2.55	0.41
2:L:177:HIS:HB3	3:M:183:LEU:HD22	2.02	0.41
14:M:403:MQ8:H361	14:M:403:MQ8:H401	1.79	0.41
9:N:102:BCL:H161	9:N:102:BCL:H192	1.64	0.41
6:P:21:PHE:C	6:P:21:PHE:CD1	2.93	0.41
5:W:21:LEU:HD23	5:W:21:LEU:HA	1.81	0.41
5:W:24:ILE:HD13	5:W:24:ILE:HA	1.83	0.41
9:Z:102:BCL:H62	9:Z:102:BCL:H41	1.54	0.41
9:9:103:BCL:H152	9:9:103:BCL:H112	1.48	0.41
9:AD:101:BCL:HBD	9:AD:101:BCL:HAA1	2.01	0.41
6:AJ:25:MET:HB2	15:AJ:101:CRT:H182	2.01	0.41
9:D:101:BCL:HMB2	15:AL:101:CRT:H371	118.30	0.41
6:B:46:LEU:C	5:D:51:ILE:HG21	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:101:CRT:H82	5:AK:14:ILE:CD1	71.63	0.41
6:E:17:PHE:N	15:E:101:CRT:H23	4.67	0.41
15:J:101:CRT:H26	15:J:101:CRT:H241	1.83	0.41
6:J:40:TRP:CZ2	9:J:102:BCL:H202	2.55	0.41
2:L:189:PHE:HB3	3:M:209:LEU:HD21	2.01	0.41
9:L:301:BCL:CBB	9:L:303:BCL:HMD2	2.51	0.41
3:M:159:VAL:HG13	3:M:285:LEU:HG	2.01	0.41
15:R:101:CRT:H31A	15:R:101:CRT:H5	1.82	0.41
9:T:102:BCL:HBD	9:T:102:BCL:HED2	1.77	0.41
5:U:9:TYR:HA	6:V:18:HIS:CG	2.97	0.41
5:W:49:ASP:HB3	5:W:51:ILE:HG13	2.01	0.41
6:X:32:VAL:HG21	9:X:102:BCL:HBA2	2.03	0.41
6:Z:29:PHE:CZ	9:Z:102:BCL:H2	2.55	0.41
9:8:102:BCL:CAB	9:8:102:BCL:H172	2.51	0.41
15:E:101:CRT:H132	5:AK:11:ILE:HD13	81.08	0.41
5:D:40:LEU:HD23	5:D:40:LEU:HA	2.30	0.41
4:H:102:PRO:HB3	4:H:111:PHE:HD2	1.86	0.41
5:I:17:PRO:HB3	6:J:17:PHE:CE1	2.55	0.41
5:I:17:PRO:HB3	6:J:17:PHE:CE2	2.55	0.41
2:L:155:PHE:HA	2:L:165:TRP:NE1	2.35	0.41
15:4:101:CRT:H342	9:5:101:BCL:HBA1	2.03	0.41
6:AD:28:TRP:HH2	9:AD:101:BCL:HAA2	1.85	0.41
9:AD:101:BCL:HBB3	9:AD:101:BCL:HMB1	2.02	0.41
6:AJ:12:ASP:C	6:AJ:15:LYS:H	2.23	0.41
4:H:14:ILE:HA	4:H:17:TRP:CD1	2.56	0.41
4:H:21:LEU:HD23	4:H:21:LEU:HA	1.75	0.41
4:H:31:ARG:O	4:H:34:ASP:HB2	2.21	0.41
2:L:26:TRP:HZ2	3:M:254:TRP:CZ3	2.37	0.41
10:L:302:BPH:HBA2	10:L:302:BPH:H3A	1.86	0.41
9:L:303:BCL:H13	9:L:303:BCL:H172	1.91	0.41
3:M:96:GLU:HA	3:M:97:PRO:HD3	1.89	0.41
5:O:10:LYS:HE3	6:R:16:GLU:OE2	2.20	0.41
9:V:101:BCL:HBB3	9:W:101:BCL:CHC	2.51	0.41
5:U:17:PRO:HB3	6:V:17:PHE:CZ	2.87	0.41
6:V:33:VAL:O	6:V:37:LEU:HG	2.58	0.41
6:Z:28:TRP:O	6:Z:32:VAL:HG23	2.21	0.41
5:1:56:GLN:O	5:1:59:GLY:HA2	2.21	0.41
6:2:31:LEU:HD23	6:2:31:LEU:HA	1.83	0.41
5:9:40:LEU:HD12	5:9:40:LEU:HA	1.75	0.41
5:9:8:LEU:HG	6:0:18:HIS:CE1	2.55	0.41
5:AA:60:LYS:HA	5:AA:61:LYS:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AD:41:LEU:HA	6:AD:41:LEU:HD23	1.84	0.41
9:AE:104:BCL:HMB1	9:AE:104:BCL:HBB2	2.02	0.41
5:AG:39:VAL:HG11	9:AH:101:BCL:HBC1	2.03	0.41
9:AI:101:BCL:C1D	9:AJ:102:BCL:HMD2	2.51	0.41
1:C:21:LEU:HD23	2:L:271:TRP:CH2	2.56	0.41
6:E:8:GLY:O	6:E:9:LEU:HD12	2.20	0.41
4:H:247:LYS:HA	4:H:254:ARG:NH1	2.34	0.41
4:H:60:ASP:CG	4:H:61:LEU:N	2.70	0.41
9:I:101:BCL:H2	9:I:101:BCL:H61	1.84	0.41
2:L:15:GLY:O	2:L:118:ARG:NE	2.47	0.41
3:M:159:VAL:CG1	3:M:285:LEU:HG	2.51	0.41
3:M:256:MET:HE2	3:M:256:MET:HB2	1.70	0.41
2:L:204:LEU:HD11	3:M:266:HIS:O	2.21	0.41
15:N:101:CRT:H10	15:N:101:CRT:H132	2.54	0.41
15:N:101:CRT:H393	6:P:36:HIS:CD2	15.08	0.41
5:W:11:ILE:HG23	5:W:12:TRP:CD2	2.76	0.41
5:W:9:TYR:CD2	6:X:15:LYS:HG2	2.55	0.41
9:Y:101:BCL:HED1	6:Z:31:LEU:HB3	2.02	0.41
5:Y:10:LYS:CB	15:2:101:CRT:H5	2.50	0.41
6:B:46:LEU:HA	5:D:51:ILE:HD13	2.03	0.41
1:C:101:VAL:HG22	1:C:152:CYS:HB3	2.03	0.41
1:C:213:THR:HG1	7:C:503:HEM:CGA	2.33	0.41
3:M:232:ASP:C	3:M:234:GLU:H	2.24	0.41
1:C:38:VAL:HG22	3:M:307:TYR:CD2	2.55	0.41
3:M:157:TYR:CZ	15:M:404:CRT:H293	2.56	0.41
5:S:20:VAL:O	5:S:24:ILE:HG13	2.21	0.41
5:S:28:GLN:OE1	6:T:28:TRP:NE1	2.38	0.41
6:T:16:GLU:HB3	15:T:101:CRT:C3	2.50	0.41
6:T:28:TRP:O	6:T:32:VAL:HG23	2.20	0.41
5:1:29:ILE:O	5:1:33:LEU:HG	2.20	0.41
6:2:41:LEU:HA	6:2:41:LEU:HD23	1.80	0.41
9:AI:101:BCL:HMC2	9:AI:101:BCL:HHC	1.82	0.41
1:C:272:ALA:HB1	7:C:504:HEM:C4B	2.55	0.41
5:D:35:ILE:HG12	15:E:101:CRT:H403	2.02	0.41
6:E:21:PHE:CD1	6:E:21:PHE:C	2.94	0.41
5:I:18:ARG:HB2	5:I:18:ARG:HE	1.73	0.41
2:L:239:HIS:CD2	3:M:223:ILE:CG1	2.95	0.41
2:L:239:HIS:CE1	3:M:234:GLU:CD	2.94	0.41
9:L:303:BCL:CMA	9:L:303:BCL:H142	2.50	0.41
5:K:36:HIS:CE1	9:N:102:BCL:HMD1	2.56	0.41
9:T:102:BCL:HBB2	9:T:102:BCL:HMB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:53:VAL:HG13	5:U:55:TYR:CZ	2.55	0.41
9:W:101:BCL:H203	15:Z:101:CRT:H131	24.42	0.41
9:AB:101:BCL:H3A	9:AB:101:BCL:HBA1	1.73	0.41
6:AD:25:MET:HG3	15:AD:102:CRT:C21	2.51	0.41
6:AL:32:VAL:CG2	9:AL:102:BCL:HBA2	2.49	0.41
1:C:167:VAL:HG22	1:C:303:LEU:HD23	2.03	0.41
1:C:196:PRO:HB2	1:C:231:TRP:CZ3	2.55	0.41
1:C:269:ALA:HB2	7:C:504:HEM:HMA1	2.02	0.41
5:A:44:LEU:HD23	5:D:55:TYR:HE2	1.86	0.41
6:E:20:ILE:HD12	15:E:101:CRT:C6	2.59	0.41
5:D:27:PHE:CE1	5:F:29:ILE:HG21	2.56	0.41
5:I:12:TRP:CZ3	5:I:20:VAL:HG11	2.56	0.41
9:J:102:BCL:O2D	9:J:102:BCL:HAA2	2.21	0.41
5:K:42:THR:HG21	5:O:47:LEU:HB3	2.03	0.41
3:M:84:PHE:CD1	5:W:37:MET:HG3	2.56	0.41
9:V:101:BCL:H2C	9:V:101:BCL:HBC3	1.60	0.41
5:1:20:VAL:O	5:1:24:ILE:HG12	2.20	0.41
5:5:44:LEU:HD23	5:7:55:TYR:CD2	2.55	0.41
9:8:102:BCL:HBA2	9:8:102:BCL:H11	1.62	0.41
6:8:46:LEU:HA	6:8:46:LEU:HD23	1.90	0.41
5:AK:46:TRP:CD1	9:AK:101:BCL:HMC2	2.56	0.41
4:H:179:ILE:HG22	4:H:197:ILE:HD13	2.03	0.41
4:H:249:TYR:C	4:H:251:THR:H	2.23	0.41
9:J:102:BCL:H3A	9:J:102:BCL:H12	2.03	0.41
2:L:207:THR:HG21	3:M:238:ILE:HD13	2.03	0.41
3:M:121:PHE:CD1	3:M:121:PHE:N	2.89	0.41
3:M:42:LYS:HZ3	12:M:408:PEF:H52	1.84	0.41
6:N:16:GLU:O	6:N:20:ILE:HG13	2.20	0.41
9:P:101:BCL:H62	9:P:101:BCL:H41	1.70	0.41
6:V:40:TRP:CZ3	6:V:46:LEU:HB2	2.72	0.41
9:W:101:BCL:HMD1	6:X:36:HIS:ND1	2.36	0.41
5:W:21:LEU:O	5:W:25:VAL:HG23	2.59	0.41
5:W:34:LEU:O	5:W:38:ILE:HG13	2.21	0.41
5:W:4:MET:HG2	5:W:8:LEU:HD22	2.03	0.41
9:Z:102:BCL:HMC2	9:Z:102:BCL:HHC	2.32	0.41
5:W:9:TYR:HB2	6:Z:14:ALA:O	17.40	0.41
6:2:17:PHE:CD1	15:2:101:CRT:H6	2.56	0.40
9:4:102:BCL:CHB	9:5:101:BCL:HMB3	2.51	0.40
6:8:25:MET:HG3	15:8:101:CRT:C20	2.51	0.40
5:W:45:ASN:HB3	5:AA:56:GLN:OE1	130.09	0.40
9:AC:102:BCL:H61	9:AC:102:BCL:HHB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:51:ILE:HA	5:AE:52:PRO:HA	1.84	0.40
5:AG:9:TYR:HA	6:AH:18:HIS:CG	2.56	0.40
4:H:246:GLY:O	4:H:250:ALA:HB3	2.21	0.40
9:K:101:BCL:HBB3	9:K:101:BCL:HMB1	2.03	0.40
2:L:225:PHE:CD2	11:L:304:UQ8:C7	3.00	0.40
11:L:304:UQ8:H27A	11:L:304:UQ8:H30	1.90	0.40
5:S:16:ASP:C	5:S:16:ASP:OD1	2.59	0.40
6:T:20:ILE:HD12	15:T:101:CRT:C6	2.50	0.40
6:Z:32:VAL:HG13	6:Z:36:HIS:CE1	3.55	0.40
6:2:12:ASP:O	6:2:15:LYS:HB2	2.21	0.40
6:2:45:TRP:CD1	6:2:46:LEU:HG	2.56	0.40
9:AC:102:BCL:H91	6:AD:36:HIS:CD2	2.57	0.40
15:AE:103:CRT:H26	15:AE:103:CRT:H241	1.89	0.40
5:AE:39:VAL:HG12	5:AE:46:TRP:HZ3	1.86	0.40
5:D:27:PHE:HE1	5:F:29:ILE:HG21	1.87	0.40
5:F:44:LEU:HD23	5:I:55:TYR:CD2	2.56	0.40
3:M:275:LEU:HD23	3:M:275:LEU:HA	1.53	0.40
15:P:102:CRT:H372	5:Q:36:HIS:CG	2.56	0.40
5:W:46:TRP:CH2	9:W:101:BCL:H2C	3.09	0.40
5:W:10:LYS:HB3	15:Z:101:CRT:H31A	2.02	0.40
5:5:53:VAL:HG22	5:5:54:SER:O	2.22	0.40
5:AA:36:HIS:CE1	9:AB:101:BCL:HMD1	2.56	0.40
5:AE:25:VAL:HG21	9:AE:102:BCL:H152	2.01	0.40
9:AK:101:BCL:C1D	9:AL:102:BCL:HMD2	2.51	0.40
9:AL:102:BCL:HMB2	9:AL:102:BCL:H92	2.03	0.40
1:C:311:HIS:HB3	1:C:314:VAL:O	2.21	0.40
5:F:29:ILE:HD13	9:F:101:BCL:H193	12.85	0.40
15:G:101:CRT:H36	5:I:33:LEU:CD2	2.52	0.40
4:H:29:TYR:CZ	12:H:304:PEF:C30	3.04	0.40
15:G:101:CRT:H2M1	5:I:33:LEU:HD22	2.03	0.40
6:J:16:GLU:O	6:J:20:ILE:HG13	2.20	0.40
9:L:303:BCL:CHA	9:L:303:BCL:HED3	2.51	0.40
3:M:164:ARG:HD3	3:M:284:ILE:HG22	2.01	0.40
3:M:68:ILE:HG21	3:M:68:ILE:HD13	1.91	0.40
5:O:39:VAL:HG11	9:P:101:BCL:CBC	2.51	0.40
6:T:24:SER:O	6:T:27:ALA:HB3	2.21	0.40
5:U:17:PRO:HB3	6:V:17:PHE:CE1	3.07	0.40
5:U:28:GLN:HB3	9:U:101:BCL:C1	2.51	0.40
5:U:3:THR:HB	5:U:8:LEU:CB	11.08	0.40
5:1:40:LEU:HA	5:1:40:LEU:HD23	1.93	0.40
5:7:36:HIS:NE2	9:7:101:BCL:NB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:24:SER:HB2	15:8:101:CRT:C14	2.51	0.40
6:8:43:ARG:HG3	5:9:55:TYR:CE1	2.56	0.40
5:9:25:VAL:O	5:9:29:ILE:HG13	2.22	0.40
9:AA:101:BCL:H51	6:AB:28:TRP:CZ3	2.57	0.40
15:AE:103:CRT:H5	15:AE:103:CRT:H22A	1.65	0.40
5:AE:52:PRO:HD2	5:AE:55:TYR:OH	2.22	0.40
5:AE:5:ASN:C	5:AE:7:ASN:N	2.74	0.40
7:C:504:HEM:HHA	7:C:504:HEM:HBD1	2.04	0.40
9:F:101:BCL:HAA2	9:F:101:BCL:CBD	2.51	0.40
5:K:10:LYS:O	5:K:13:LEU:HB2	2.22	0.40
5:S:5:ASN:C	5:S:7:ASN:N	2.75	0.40
6:V:40:TRP:HZ3	6:V:46:LEU:HB2	2.40	0.40
9:W:101:BCL:CBD	9:W:101:BCL:HAA2	2.47	0.40
5:W:40:LEU:HG	5:W:46:TRP:CZ3	2.56	0.40
9:0:101:BCL:H3A	9:0:101:BCL:HBA1	1.69	0.40
5:1:12:TRP:HB2	6:2:14:ALA:HB1	2.04	0.40
9:9:103:BCL:H91	9:9:103:BCL:H112	1.84	0.40
9:AC:102:BCL:H112	9:AC:102:BCL:H91	1.84	0.40
9:AE:104:BCL:H121	6:AF:45:TRP:HZ2	1.86	0.40
1:C:212:ILE:HD11	7:C:503:HEM:CMA	2.52	0.40
6:G:46:LEU:HD12	9:G:102:BCL:H141	2.03	0.40
4:H:27:ILE:HD12	4:H:27:ILE:HG23	1.83	0.40
4:H:46:THR:OG1	4:H:53:VAL:O	2.29	0.40
6:J:21:PHE:CD2	15:J:101:CRT:H16	2.56	0.40
2:L:190:PHE:HA	2:L:190:PHE:HD1	1.70	0.40
2:L:271:TRP:HZ3	2:L:272:TRP:CZ3	2.40	0.40
11:L:304:UQ8:H15	11:L:304:UQ8:H12A	1.79	0.40
2:L:51:VAL:CG1	5:A:37:MET:HG3	2.51	0.40
3:M:140:LEU:HD23	3:M:140:LEU:HA	1.94	0.40
6:Z:41:LEU:HA	6:Z:41:LEU:HD23	1.75	0.40

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
4	H	250	ALA
5	A	60	LYS
5	F	3	THR
5	O	59	GLY
5	Y	60	LYS
5	3	6	ALA
6	0	8	GLY
1	o	21	LEU
1	o	66	ASP
1	o	195	LEU
2	x	262	PRO
4	t	5	ILE
4	t	38	GLY
4	t	142	PHE
4	t	250	ALA
5	m	60	LYS
5	p	57	ALA

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Mol	Chain	Res	Type
5	r	3	THR
5	AC	4	MET
5	AE	6	ALA
5	AG	6	ALA
5	AK	60	LYS
5	d	58	LEU
5	f	5	ASN
1	C	21	LEU
2	L	21	ASP
2	L	262	PRO
4	H	5	ILE
4	H	140	LYS
4	H	188	ALA
5	F	10	LYS
5	I	59	GLY
5	Q	6	ALA
5	S	6	ALA
5	S	58	LEU
5	U	54	SER
5	W	5	ASN
6	X	8	GLY
5	Y	59	GLY
5	1	3	THR
5	3	56	GLN
1	o	83	LYS
1	o	84	ASP
2	x	21	ASP
4	t	140	LYS
4	t	188	ALA
5	m	10	LYS
5	p	6	ALA
5	p	56	GLN
5	p	60	LYS
5	r	59	GLY
5	AE	59	GLY
5	l	4	MET
1	C	83	LYS
1	C	184	ASN
3	M	3	GLU
3	M	29	PRO
3	M	34	PRO
4	H	177	PRO

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Mol	Chain	Res	Type
5	A	10	LYS
5	D	5	ASN
5	Q	10	LYS
5	S	60	LYS
5	3	57	ALA
5	5	10	LYS
5	7	6	ALA
5	7	10	LYS
5	9	6	ALA
5	9	59	GLY
1	o	67	SER
3	y	3	GLU
3	y	29	PRO
3	y	34	PRO
4	t	177	PRO
5	AC	6	ALA
5	AE	58	LEU
5	AI	10	LYS
5	f	59	GLY
5	h	6	ALA
5	j	6	ALA
5	l	10	LYS
1	C	253	THR
5	I	10	LYS
5	I	60	LYS
6	N	8	GLY
6	P	8	GLY
5	W	6	ALA
5	3	10	LYS
5	5	50	ASN
1	o	253	THR
5	p	5	ASN
5	w	10	LYS
5	d	10	LYS
5	h	8	LEU
3	M	38	TYR
5	D	57	ALA
5	I	6	ALA
5	Q	8	LEU
1	o	184	ASN
3	y	38	TYR
5	r	60	LYS

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Mol	Chain	Res	Type
5	u	5	ASN
5	AK	10	LYS
5	h	10	LYS
4	H	213	ALA
5	Q	4	MET
5	Q	59	GLY
5	9	10	LYS
5	9	50	ASN
5	r	10	LYS
2	L	32	VAL
6	B	8	GLY
2	x	32	VAL
6	T	8	GLY
5	l	59	GLY
4	t	227	ASN
5	AA	59	GLY
2	L	141	VAL
4	H	227	ASN
4	t	59	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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	l	52/56 (93%)	50 (96%)	2 (4%)	38	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	z	33/39 (85%)	33 (100%)	0	100	100
All	All	4640/4990 (93%)	4462 (96%)	178 (4%)	38	70

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	LEU
1	C	23	CYS
1	C	48	GLN
1	C	74	GLU
1	C	86	SER
1	C	128	ARG
1	C	130	MET
1	C	167	VAL
1	C	169	ASP
1	C	181	THR
1	C	183	GLN
1	C	190	VAL
1	C	212	ILE
1	C	221	SER
1	C	238	ASN
1	C	277	ARG
1	C	282	ASN
1	C	289	ASP
1	C	304	ARG
1	C	307	CYS
2	L	120	LEU
2	L	125	HIS
2	L	148	MET
2	L	163	LEU
2	L	172	GLN
2	L	175	HIS
2	L	176	PHE
2	L	208	ASN
2	L	210	GLN
2	L	225	PHE
2	L	248	SER
2	L	256	CYS
2	L	281	TRP
3	M	3	GLU
3	M	25	LYS
3	M	31	ILE

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Mol	Chain	Res	Type
3	M	33	ARG
3	M	37	SER
3	M	42	LYS
3	M	45	ASP
3	M	79	VAL
3	M	182	HIS
3	M	216	PHE
3	M	228	ARG
3	M	232	ASP
3	M	256	MET
3	M	264	SER
3	M	279	THR
3	M	310	VAL
3	M	311	VAL
3	M	312	THR
4	H	45	ARG
4	H	81	VAL
4	H	106	PRO
4	H	116	SER
4	H	128	GLU
4	H	131	PRO
4	H	140	LYS
4	H	143	SER
4	H	157	VAL
4	H	159	LEU
4	H	160	ASP
4	H	177	PRO
4	H	200	SER
4	H	230	GLN
4	H	258	LEU
4	H	259	LEU
6	B	20	ILE
6	B	24	SER
5	D	9	TYR
5	F	14	ILE
5	I	3	THR
5	K	43	ASP
5	O	5	ASN
5	O	37	MET
6	P	21	PHE
5	Q	2	PHE
5	Q	3	THR

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Mol	Chain	Res	Type
5	Q	9	TYR
5	S	48	ASP
5	S	51	ILE
5	U	53	VAL
5	W	9	TYR
5	W	50	ASN
6	X	13	GLU
5	1	51	ILE
5	1	55	TYR
5	3	44	LEU
5	3	50	ASN
5	5	9	TYR
5	7	48	ASP
5	9	8	LEU
1	o	21	LEU
1	o	47	ARG
1	o	48	GLN
1	o	66	ASP
1	o	68	THR
1	o	74	GLU
1	o	86	SER
1	o	128	ARG
1	o	130	MET
1	o	169	ASP
1	o	181	THR
1	o	190	VAL
1	o	212	ILE
1	o	238	ASN
1	o	277	ARG
1	o	281	GLN
1	o	282	ASN
1	o	304	ARG
1	o	307	CYS
2	x	59	THR
2	x	128	PHE
2	x	147	LEU
2	x	148	MET
2	x	163	LEU
2	x	172	GLN
2	x	176	PHE
2	x	208	ASN
2	x	210	GLN

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Mol	Chain	Res	Type
2	x	225	PHE
2	x	248	SER
2	x	256	CYS
2	x	281	TRP
3	y	3	GLU
3	y	25	LYS
3	y	31	ILE
3	y	33	ARG
3	y	37	SER
3	y	42	LYS
3	y	45	ASP
3	y	182	HIS
3	y	216	PHE
3	y	228	ARG
3	y	232	ASP
3	y	256	MET
3	y	277	VAL
3	y	279	THR
3	y	285	LEU
3	y	310	VAL
3	y	311	VAL
3	y	312	THR
4	t	45	ARG
4	t	60	ASP
4	t	81	VAL
4	t	116	SER
4	t	128	GLU
4	t	131	PRO
4	t	140	LYS
4	t	143	SER
4	t	157	VAL
4	t	159	LEU
4	t	160	ASP
4	t	166	THR
4	t	177	PRO
4	t	200	SER
4	t	218	HIS
4	t	221	ASN
4	t	224	THR
4	t	230	GLN
4	t	259	LEU
5	r	37	MET

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Mol	Chain	Res	Type
5	u	3	THR
5	w	5	ASN
5	AA	5	ASN
5	AA	43	ASP
5	AA	44	LEU
5	AC	2	PHE
5	AC	3	THR
5	AE	8	LEU
5	AG	2	PHE
6	AJ	13	GLU
5	f	3	THR
5	h	14	ILE
5	j	9	TYR
5	j	48	ASP
5	l	8	LEU
5	l	40	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	238	ASN
2	L	125	HIS
3	M	6	ASN
3	M	27	ASN
4	H	122	HIS
4	H	189	ASN
6	X	36	HIS
5	Y	5	ASN
5	Y	36	HIS
5	Y	56	GLN
6	Z	23	GLN
6	2	23	GLN
2	x	182	HIS
2	x	192	ASN
2	x	273	ASN
3	y	240	HIS
3	y	301	HIS
5	m	7	ASN
5	w	50	ASN
5	w	56	GLN
6	e	23	GLN
5	l	56	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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%)

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

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



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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
9	4	102	BCL	O1D-CGD	-4.26	1.10	1.21
9	s	102	BCL	O1D-CGD	-4.23	1.10	1.21
9	p	104	BCL	O1D-CGD	-4.20	1.10	1.21
9	g	101	BCL	O1D-CGD	-4.17	1.10	1.21
9	h	101	BCL	O1D-CGD	-4.16	1.10	1.21
7	C	501	HEM	C1B-NB	-4.16	1.31	1.36
9	D	101	BCL	O1D-CGD	-4.15	1.10	1.21
9	G	102	BCL	O1D-CGD	-4.14	1.10	1.21
9	AK	101	BCL	O1D-CGD	-4.13	1.10	1.21
9	m	102	BCL	O1D-CGD	-4.13	1.10	1.21
9	V	101	BCL	O1D-CGD	-4.12	1.10	1.21
9	Y	101	BCL	O1D-CGD	-4.06	1.10	1.21
9	AI	101	BCL	O1D-CGD	-4.06	1.10	1.21
9	AL	102	BCL	O1D-CGD	-4.06	1.11	1.21
9	x	301	BCL	O1D-CGD	-4.04	1.11	1.21
9	5	101	BCL	O1D-CGD	-4.03	1.11	1.21
9	f	101	BCL	O1D-CGD	-4.02	1.11	1.21
9	M	401	BCL	O2A-CGA	-4.01	1.21	1.33
9	U	101	BCL	O1D-CGD	-4.00	1.11	1.21
9	P	101	BCL	O1D-CGD	-3.99	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	u	101	BCL	O1D-CGD	-3.99	1.11	1.21
9	9	103	BCL	O1D-CGD	-3.96	1.11	1.21
9	c	102	BCL	O1D-CGD	-3.96	1.11	1.21
9	T	102	BCL	O1D-CGD	-3.95	1.11	1.21
9	D	102	BCL	O1D-CGD	-3.95	1.11	1.21
9	k	102	BCL	O1D-CGD	-3.95	1.11	1.21
9	l	102	BCL	O1D-CGD	-3.94	1.11	1.21
9	v	102	BCL	O1D-CGD	-3.94	1.11	1.21
9	M	401	BCL	O1D-CGD	-3.94	1.11	1.21
7	C	502	HEM	C3B-C2B	-3.93	1.35	1.40
9	AB	101	BCL	O1D-CGD	-3.92	1.11	1.21
9	m	103	BCL	O1D-CGD	-3.91	1.11	1.21
9	AH	103	BCL	O1D-CGD	-3.91	1.11	1.21
9	x	303	BCL	C3D-C2D	-3.91	1.31	1.39
9	AH	101	BCL	O1D-CGD	-3.89	1.11	1.21
9	y	401	BCL	O1D-CGD	-3.87	1.11	1.21
9	AA	101	BCL	O1D-CGD	-3.87	1.11	1.21
9	W	101	BCL	O1D-CGD	-3.87	1.11	1.21
9	j	101	BCL	O1D-CGD	-3.86	1.11	1.21
9	L	303	BCL	C3D-C2D	-3.85	1.31	1.39
7	C	501	HEM	C3B-C2B	-3.85	1.35	1.40
9	5	102	BCL	O1D-CGD	-3.85	1.11	1.21
9	I	101	BCL	O1D-CGD	-3.84	1.11	1.21
9	AE	102	BCL	O1D-CGD	-3.84	1.11	1.21
9	Z	102	BCL	O1D-CGD	-3.84	1.11	1.21
9	8	102	BCL	O1D-CGD	-3.82	1.11	1.21
9	A	102	BCL	O1D-CGD	-3.82	1.11	1.21
9	p	102	BCL	O1D-CGD	-3.82	1.11	1.21
9	l	101	BCL	O1D-CGD	-3.82	1.11	1.21
9	Q	101	BCL	O1D-CGD	-3.80	1.11	1.21
9	K	101	BCL	O1D-CGD	-3.79	1.11	1.21
9	e	102	BCL	O1D-CGD	-3.79	1.11	1.21
9	i	102	BCL	O1D-CGD	-3.79	1.11	1.21
9	x	303	BCL	O1D-CGD	-3.78	1.11	1.21
7	C	502	HEM	C1B-NB	-3.78	1.32	1.36
9	z	102	BCL	O1D-CGD	-3.77	1.11	1.21
9	w	101	BCL	O1D-CGD	-3.77	1.11	1.21
9	S	102	BCL	O1D-CGD	-3.76	1.11	1.21
9	AC	102	BCL	O1D-CGD	-3.76	1.11	1.21
9	B	101	BCL	O1D-CGD	-3.75	1.11	1.21
9	3	101	BCL	O1D-CGD	-3.75	1.11	1.21
9	AD	101	BCL	O1D-CGD	-3.73	1.11	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	102	BCL	C3D-C2D	-3.72	1.31	1.39
9	F	101	BCL	O1D-CGD	-3.72	1.11	1.21
9	0	101	BCL	O1D-CGD	-3.71	1.11	1.21
9	1	101	BCL	O1D-CGD	-3.67	1.11	1.21
9	AJ	102	BCL	O1D-CGD	-3.67	1.11	1.21
7	C	504	HEM	C3B-C2B	-3.65	1.35	1.40
9	U	101	BCL	O2D-CGD	-3.65	1.23	1.33
9	AE	104	BCL	O1D-CGD	-3.65	1.12	1.21
9	X	102	BCL	O1D-CGD	-3.64	1.12	1.21
9	N	102	BCL	O1D-CGD	-3.63	1.12	1.21
9	7	101	BCL	O1D-CGD	-3.63	1.12	1.21
9	L	305	BCL	O1D-CGD	-3.58	1.12	1.21
9	U	101	BCL	O2A-CGA	-3.57	1.22	1.33
9	AL	102	BCL	C3D-C2D	-3.53	1.32	1.39
9	J	102	BCL	O1D-CGD	-3.50	1.12	1.21
9	O	101	BCL	O1D-CGD	-3.50	1.12	1.21
9	d	101	BCL	O1D-CGD	-3.50	1.12	1.21
9	r	101	BCL	O1D-CGD	-3.48	1.12	1.21
9	R	102	BCL	O1D-CGD	-3.47	1.12	1.21
9	x	303	BCL	O2D-CGD	-3.44	1.24	1.33
9	L	301	BCL	O1D-CGD	-3.43	1.12	1.21
9	x	305	BCL	O1A-CGA	-3.39	1.12	1.22
9	N	102	BCL	C3D-C2D	-3.29	1.32	1.39
7	o	504	HEM	C3B-C2B	-3.29	1.36	1.40
7	o	501	HEM	C1B-NB	-3.29	1.32	1.36
7	C	503	HEM	C3B-C2B	-3.28	1.36	1.40
9	AH	101	BCL	O2D-CGD	-3.27	1.24	1.33
10	y	402	BPH	C1B-C2B	-3.24	1.38	1.45
9	x	301	BCL	C3D-C2D	-3.24	1.32	1.39
9	AL	102	BCL	O2A-CGA	-3.24	1.23	1.33
9	h	101	BCL	O2D-CGD	-3.24	1.25	1.33
9	D	101	BCL	O2D-CGD	-3.23	1.25	1.33
9	w	101	BCL	O2D-CGD	-3.22	1.25	1.33
9	V	101	BCL	O2A-CGA	-3.22	1.23	1.33
10	L	302	BPH	C1C-NC	-3.21	1.30	1.37
7	o	503	HEM	C3B-C2B	-3.20	1.36	1.40
9	AK	101	BCL	O2D-CGD	-3.19	1.25	1.33
9	M	401	BCL	O1A-CGA	-3.18	1.13	1.22
9	Q	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	v	102	BCL	O2D-CGD	-3.16	1.25	1.33
9	p	104	BCL	O1A-CGA	-3.16	1.13	1.22
9	D	101	BCL	O2A-CGA	-3.14	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	y	401	BCL	O1A-CGA	-3.14	1.13	1.22
7	o	504	HEM	C1B-NB	-3.14	1.33	1.36
9	9	103	BCL	C3D-C2D	-3.13	1.33	1.39
9	m	102	BCL	O2D-CGD	-3.13	1.25	1.33
7	C	504	HEM	C1B-NB	-3.12	1.33	1.36
9	z	102	BCL	C3D-C2D	-3.11	1.33	1.39
9	AH	103	BCL	O2D-CGD	-3.09	1.25	1.33
9	p	104	BCL	O2D-CGD	-3.09	1.25	1.33
9	Z	102	BCL	O1A-CGA	-3.08	1.13	1.22
9	D	102	BCL	O2A-CGA	-3.07	1.24	1.33
9	U	101	BCL	O1A-CGA	-3.07	1.13	1.22
9	I	101	BCL	O2D-CGD	-3.06	1.25	1.33
9	T	102	BCL	O2D-CGD	-3.05	1.25	1.33
9	L	303	BCL	O2D-CGD	-3.05	1.25	1.33
9	L	301	BCL	O1A-CGA	-3.04	1.13	1.22
9	AA	101	BCL	O2D-CGD	-3.03	1.25	1.33
9	G	102	BCL	O2A-CGA	-3.02	1.24	1.33
9	V	101	BCL	O2D-CGD	-3.02	1.25	1.33
9	k	102	BCL	O2D-CGD	-3.02	1.25	1.33
9	AJ	102	BCL	O2A-CGA	-3.02	1.24	1.33
9	3	101	BCL	O1A-CGA	-3.01	1.13	1.22
9	G	102	BCL	O2D-CGD	-3.01	1.25	1.33
9	AD	101	BCL	O2D-CGD	-3.00	1.25	1.33
9	8	102	BCL	O2A-CGA	-2.99	1.24	1.33
9	L	301	BCL	C3D-C2D	-2.99	1.33	1.39
9	w	101	BCL	C3D-C2D	-2.99	1.33	1.39
9	x	303	BCL	O2A-CGA	-2.98	1.24	1.33
9	S	102	BCL	O1A-CGA	-2.97	1.13	1.22
9	X	102	BCL	O1A-CGA	-2.97	1.13	1.22
9	N	102	BCL	O2A-CGA	-2.96	1.24	1.33
9	p	104	BCL	O2A-CGA	-2.95	1.24	1.33
9	w	101	BCL	O1A-CGA	-2.95	1.13	1.22
9	P	101	BCL	O2D-CGD	-2.95	1.25	1.33
9	4	102	BCL	O1A-CGA	-2.94	1.13	1.22
9	Z	102	BCL	O2A-CGA	-2.94	1.24	1.33
9	X	102	BCL	O2A-CGA	-2.94	1.24	1.33
9	AB	101	BCL	O2D-CGD	-2.94	1.25	1.33
9	O	101	BCL	O2A-CGA	-2.93	1.24	1.33
9	l	101	BCL	C3D-C2D	-2.93	1.33	1.39
9	u	101	BCL	O2D-CGD	-2.93	1.25	1.33
9	g	101	BCL	O1A-CGA	-2.92	1.13	1.22
9	y	401	BCL	O2D-CGD	-2.91	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	s	102	BCL	O2D-CGD	-2.91	1.25	1.33
9	AH	103	BCL	O2A-CGA	-2.91	1.24	1.33
9	j	101	BCL	O2D-CGD	-2.91	1.25	1.33
9	AI	101	BCL	O2D-CGD	-2.91	1.25	1.33
9	T	102	BCL	O1A-CGA	-2.91	1.13	1.22
9	m	103	BCL	O2A-CGA	-2.91	1.24	1.33
9	m	103	BCL	O1A-CGA	-2.90	1.13	1.22
9	x	303	BCL	O1A-CGA	-2.90	1.13	1.22
9	r	101	BCL	O1A-CGA	-2.90	1.13	1.22
9	B	101	BCL	C3D-C2D	-2.89	1.33	1.39
9	AC	102	BCL	O2A-CGA	-2.89	1.24	1.33
9	p	102	BCL	O2A-CGA	-2.89	1.24	1.33
9	K	101	BCL	C3D-C2D	-2.89	1.33	1.39
9	p	102	BCL	C3D-C2D	-2.88	1.33	1.39
9	T	102	BCL	O2A-CGA	-2.88	1.24	1.33
10	x	302	BPH	C1B-C2B	-2.87	1.39	1.45
9	8	102	BCL	O1A-CGA	-2.87	1.14	1.22
9	s	102	BCL	O2A-CGA	-2.87	1.24	1.33
9	l	101	BCL	O2A-CGA	-2.87	1.24	1.33
9	y	401	BCL	O2A-CGA	-2.86	1.24	1.33
9	f	101	BCL	O2D-CGD	-2.85	1.25	1.33
9	AA	101	BCL	O2A-CGA	-2.85	1.24	1.33
9	AH	103	BCL	O1A-CGA	-2.85	1.14	1.22
9	AJ	102	BCL	O1A-CGA	-2.85	1.14	1.22
9	g	101	BCL	O2A-CGA	-2.84	1.24	1.33
9	I	101	BCL	O1A-CGA	-2.83	1.14	1.22
10	y	402	BPH	C4C-NC	-2.83	1.31	1.37
9	K	101	BCL	O2D-CGD	-2.83	1.26	1.33
9	5	101	BCL	O1A-CGA	-2.82	1.14	1.22
9	s	102	BCL	O1A-CGA	-2.82	1.14	1.22
9	A	102	BCL	O2D-CGD	-2.82	1.26	1.33
9	AI	101	BCL	O1A-CGA	-2.82	1.14	1.22
9	O	101	BCL	O1A-CGA	-2.82	1.14	1.22
10	y	402	BPH	C1C-NC	-2.82	1.31	1.37
9	J	102	BCL	O2A-CGA	-2.82	1.25	1.33
9	AH	101	BCL	O2A-CGA	-2.81	1.25	1.33
9	A	102	BCL	O2A-CGA	-2.81	1.25	1.33
9	g	101	BCL	O2D-CGD	-2.81	1.26	1.33
9	3	101	BCL	O2A-CGA	-2.80	1.25	1.33
9	K	101	BCL	O1A-CGA	-2.80	1.14	1.22
9	AD	101	BCL	O1A-CGA	-2.80	1.14	1.22
9	G	102	BCL	O1A-CGA	-2.80	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	102	BCL	O2D-CGD	-2.80	1.26	1.33
9	L	305	BCL	O2D-CGD	-2.80	1.26	1.33
9	D	101	BCL	O1A-CGA	-2.79	1.14	1.22
9	p	102	BCL	O2D-CGD	-2.79	1.26	1.33
9	AE	102	BCL	O1A-CGA	-2.79	1.14	1.22
9	0	101	BCL	O1A-CGA	-2.79	1.14	1.22
9	AB	101	BCL	O2A-CGA	-2.78	1.25	1.33
9	AA	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	x	305	BCL	C3D-C2D	-2.78	1.33	1.39
9	e	102	BCL	O2A-CGA	-2.78	1.25	1.33
9	4	102	BCL	C3D-C2D	-2.78	1.33	1.39
9	k	102	BCL	C3D-C2D	-2.78	1.33	1.39
9	m	102	BCL	O2A-CGA	-2.77	1.25	1.33
9	L	305	BCL	O2A-CGA	-2.77	1.25	1.33
9	AD	101	BCL	O2A-CGA	-2.77	1.25	1.33
9	AC	102	BCL	O2D-CGD	-2.77	1.26	1.33
9	S	102	BCL	O2A-CGA	-2.77	1.25	1.33
9	c	102	BCL	O2A-CGA	-2.77	1.25	1.33
9	r	101	BCL	O2A-CGA	-2.77	1.25	1.33
9	AK	101	BCL	C3D-C2D	-2.76	1.33	1.39
9	AB	101	BCL	O1A-CGA	-2.76	1.14	1.22
9	AC	102	BCL	O1A-CGA	-2.76	1.14	1.22
9	z	102	BCL	O2A-CGA	-2.75	1.25	1.33
7	o	501	HEM	C3B-C2B	-2.75	1.36	1.40
9	Y	101	BCL	O1A-CGA	-2.75	1.14	1.22
9	N	102	BCL	O1A-CGA	-2.74	1.14	1.22
9	X	102	BCL	O2D-CGD	-2.74	1.26	1.33
9	L	305	BCL	O1A-CGA	-2.74	1.14	1.22
9	I	101	BCL	C3D-C2D	-2.74	1.33	1.39
9	0	101	BCL	O2A-CGA	-2.74	1.25	1.33
9	P	101	BCL	O1A-CGA	-2.74	1.14	1.22
9	5	101	BCL	O2D-CGD	-2.74	1.26	1.33
9	v	102	BCL	O2A-CGA	-2.73	1.25	1.33
9	5	101	BCL	O2A-CGA	-2.72	1.25	1.33
9	W	101	BCL	O2D-CGD	-2.72	1.26	1.33
9	AE	104	BCL	O1A-CGA	-2.72	1.14	1.22
9	D	102	BCL	O1A-CGA	-2.72	1.14	1.22
9	4	102	BCL	O2A-CGA	-2.72	1.25	1.33
9	J	102	BCL	O1A-CGA	-2.71	1.14	1.22
9	AC	102	BCL	C3D-C2D	-2.71	1.33	1.39
9	5	102	BCL	O2A-CGA	-2.71	1.25	1.33
9	c	102	BCL	O2D-CGD	-2.71	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	101	BCL	O1A-CGA	-2.70	1.14	1.22
9	L	301	BCL	O2D-CGD	-2.70	1.26	1.33
9	d	101	BCL	O2D-CGD	-2.70	1.26	1.33
9	AE	102	BCL	O2A-CGA	-2.70	1.25	1.33
9	e	102	BCL	O1A-CGA	-2.69	1.14	1.22
9	m	103	BCL	O2D-CGD	-2.69	1.26	1.33
9	Y	101	BCL	O2A-CGA	-2.69	1.25	1.33
9	P	101	BCL	O2A-CGA	-2.69	1.25	1.33
9	1	101	BCL	O1A-CGA	-2.69	1.14	1.22
9	O	101	BCL	C3D-C2D	-2.69	1.33	1.39
9	1	101	BCL	O2A-CGA	-2.68	1.25	1.33
9	A	102	BCL	C3D-C2D	-2.68	1.33	1.39
9	I	101	BCL	O2A-CGA	-2.67	1.25	1.33
9	l	101	BCL	O1A-CGA	-2.67	1.14	1.22
9	1	101	BCL	O2D-CGD	-2.67	1.26	1.33
9	R	102	BCL	O2A-CGA	-2.67	1.25	1.33
9	p	102	BCL	O1A-CGA	-2.66	1.14	1.22
9	S	102	BCL	O2D-CGD	-2.66	1.26	1.33
9	AD	101	BCL	C3D-C2D	-2.66	1.34	1.39
9	i	102	BCL	O2A-CGA	-2.65	1.25	1.33
9	AK	101	BCL	O2A-CGA	-2.65	1.25	1.33
9	R	102	BCL	O1A-CGA	-2.65	1.14	1.22
9	AL	102	BCL	O2D-CGD	-2.65	1.26	1.33
9	F	101	BCL	O1A-CGA	-2.65	1.14	1.22
9	j	101	BCL	O2A-CGA	-2.65	1.25	1.33
9	k	102	BCL	O1A-CGA	-2.64	1.14	1.22
7	o	501	HEM	C4D-ND	-2.64	1.33	1.36
9	g	101	BCL	C3D-C2D	-2.64	1.34	1.39
9	Y	101	BCL	O2D-CGD	-2.64	1.26	1.33
9	A	102	BCL	O1A-CGA	-2.64	1.14	1.22
9	x	303	BCL	CHD-C4C	-2.64	1.33	1.41
9	u	101	BCL	C3D-C2D	-2.64	1.34	1.39
9	AE	102	BCL	O2D-CGD	-2.63	1.26	1.33
9	B	101	BCL	O1A-CGA	-2.63	1.14	1.22
10	x	302	BPH	C4C-NC	-2.63	1.31	1.37
9	c	102	BCL	O1A-CGA	-2.63	1.14	1.22
9	4	102	BCL	O2D-CGD	-2.63	1.26	1.33
9	5	102	BCL	O1A-CGA	-2.62	1.14	1.22
9	j	101	BCL	O1A-CGA	-2.62	1.14	1.22
9	9	103	BCL	O1A-CGA	-2.62	1.14	1.22
9	j	101	BCL	C3D-C2D	-2.62	1.34	1.39
9	D	102	BCL	O2D-CGD	-2.61	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	1	102	BCL	O1A-CGA	-2.61	1.14	1.22
9	W	101	BCL	O1A-CGA	-2.61	1.14	1.22
9	R	102	BCL	C3D-C2D	-2.61	1.34	1.39
9	f	101	BCL	O1A-CGA	-2.61	1.14	1.22
9	AE	104	BCL	O2A-CGA	-2.61	1.25	1.33
9	e	102	BCL	O2D-CGD	-2.60	1.26	1.33
9	0	101	BCL	O2D-CGD	-2.60	1.26	1.33
9	z	102	BCL	O1A-CGA	-2.60	1.14	1.22
9	m	102	BCL	O1A-CGA	-2.59	1.14	1.22
9	AH	101	BCL	O1A-CGA	-2.59	1.14	1.22
9	L	303	BCL	C3B-C2B	-2.59	1.34	1.39
9	k	102	BCL	O2A-CGA	-2.59	1.25	1.33
9	h	101	BCL	O2A-CGA	-2.58	1.25	1.33
9	i	102	BCL	O1A-CGA	-2.57	1.14	1.22
10	x	302	BPH	C1A-NA	-2.57	1.32	1.37
9	AK	101	BCL	O1A-CGA	-2.56	1.14	1.22
9	K	101	BCL	O2A-CGA	-2.56	1.25	1.33
10	M	402	BPH	C1B-C2B	-2.56	1.40	1.45
9	7	101	BCL	C3D-C2D	-2.56	1.34	1.39
9	r	101	BCL	C3D-C2D	-2.56	1.34	1.39
9	7	101	BCL	O2A-CGA	-2.56	1.25	1.33
9	v	102	BCL	C3D-C2D	-2.56	1.34	1.39
9	i	102	BCL	O2D-CGD	-2.55	1.26	1.33
10	y	402	BPH	C1A-NA	-2.55	1.32	1.37
9	i	102	BCL	C3D-C2D	-2.55	1.34	1.39
9	h	101	BCL	O1A-CGA	-2.55	1.15	1.22
9	l	101	BCL	O2D-CGD	-2.55	1.26	1.33
9	AE	104	BCL	C3D-C2D	-2.53	1.34	1.39
9	7	101	BCL	O1A-CGA	-2.53	1.15	1.22
9	1	102	BCL	O2A-CGA	-2.53	1.25	1.33
9	9	103	BCL	O2A-CGA	-2.53	1.25	1.33
9	Z	102	BCL	C3B-C2B	-2.53	1.34	1.39
9	F	101	BCL	O2D-CGD	-2.52	1.26	1.33
9	L	301	BCL	O2A-CGA	-2.51	1.25	1.33
9	Q	101	BCL	O1A-CGA	-2.51	1.15	1.22
10	y	402	BPH	OBD-CAD	-2.51	1.18	1.22
9	9	103	BCL	O2D-CGD	-2.50	1.26	1.33
9	N	102	BCL	O2D-CGD	-2.50	1.26	1.33
9	AL	102	BCL	O1A-CGA	-2.50	1.15	1.22
9	v	102	BCL	O1A-CGA	-2.50	1.15	1.22
9	d	101	BCL	C3D-C2D	-2.49	1.34	1.39
9	R	102	BCL	O2D-CGD	-2.49	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	101	BCL	O2D-CGD	-2.48	1.26	1.33
9	B	101	BCL	O2A-CGA	-2.48	1.25	1.33
9	z	102	BCL	O2D-CGD	-2.48	1.26	1.33
9	X	102	BCL	C3D-C2D	-2.48	1.34	1.39
9	5	101	BCL	C3D-C2D	-2.47	1.34	1.39
9	P	101	BCL	C3D-C2D	-2.47	1.34	1.39
9	W	101	BCL	O2A-CGA	-2.47	1.26	1.33
9	3	101	BCL	C3D-C2D	-2.46	1.34	1.39
9	T	102	BCL	C3D-C2D	-2.46	1.34	1.39
9	w	101	BCL	O2A-CGA	-2.46	1.26	1.33
7	o	502	HEM	C1B-NB	-2.46	1.33	1.36
9	8	102	BCL	O2D-CGD	-2.46	1.26	1.33
9	M	401	BCL	O2D-CGD	-2.45	1.26	1.33
9	B	101	BCL	O2D-CGD	-2.43	1.27	1.33
9	d	101	BCL	O1A-CGA	-2.42	1.15	1.22
9	L	305	BCL	C3D-C2D	-2.41	1.34	1.39
9	u	101	BCL	O2A-CGA	-2.41	1.26	1.33
9	V	101	BCL	C3D-C2D	-2.41	1.34	1.39
7	o	501	HEM	C4B-NB	-2.41	1.30	1.36
10	L	302	BPH	C4C-NC	-2.40	1.32	1.37
9	AI	101	BCL	O2A-CGA	-2.40	1.26	1.33
9	AJ	102	BCL	C3D-C2D	-2.39	1.34	1.39
9	0	101	BCL	C3D-C2D	-2.39	1.34	1.39
9	c	102	BCL	C3D-C2D	-2.39	1.34	1.39
9	x	305	BCL	O2A-CGA	-2.38	1.26	1.33
9	s	102	BCL	C3D-C2D	-2.38	1.34	1.39
9	u	101	BCL	O1A-CGA	-2.38	1.15	1.22
9	l	102	BCL	O2D-CGD	-2.37	1.27	1.33
9	S	102	BCL	C3D-C2D	-2.37	1.34	1.39
9	G	102	BCL	C3D-C2D	-2.37	1.34	1.39
9	Q	101	BCL	C3D-C2D	-2.36	1.34	1.39
9	f	101	BCL	O2A-CGA	-2.36	1.26	1.33
9	F	101	BCL	C3D-C2D	-2.35	1.34	1.39
9	Q	101	BCL	O2A-CGA	-2.35	1.26	1.33
7	C	504	HEM	C4D-ND	-2.35	1.34	1.36
9	AE	104	BCL	O2D-CGD	-2.34	1.27	1.33
9	x	305	BCL	O2D-CGD	-2.33	1.27	1.33
9	x	303	BCL	C2C-C3C	-2.32	1.47	1.54
9	F	101	BCL	O2A-CGA	-2.31	1.26	1.33
9	x	305	BCL	C3B-C2B	-2.30	1.34	1.39
9	h	101	BCL	C3D-C2D	-2.30	1.34	1.39
9	x	301	BCL	O1A-CGA	-2.29	1.15	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	x	301	BCL	O2A-CGA	-2.28	1.26	1.33
9	AE	102	BCL	C3D-C2D	-2.28	1.34	1.39
9	B	101	BCL	CHD-C4C	-2.27	1.34	1.41
7	C	502	HEM	C4B-NB	-2.27	1.31	1.36
9	D	101	BCL	C3B-C2B	-2.27	1.34	1.39
9	x	301	BCL	C3B-C2B	-2.26	1.34	1.39
10	L	302	BPH	C1A-NA	-2.26	1.32	1.37
9	O	101	BCL	O2D-CGD	-2.26	1.27	1.33
9	1	102	BCL	C3D-C2D	-2.25	1.34	1.39
9	e	102	BCL	C3D-C2D	-2.25	1.34	1.39
9	AB	101	BCL	C3D-C2D	-2.25	1.34	1.39
9	3	101	BCL	C2C-C3C	-2.24	1.48	1.54
9	Z	102	BCL	C3D-C2D	-2.24	1.34	1.39
9	AL	102	BCL	C3B-C2B	-2.24	1.34	1.39
9	u	101	BCL	C3B-C2B	-2.24	1.34	1.39
9	3	101	BCL	O2D-CGD	-2.24	1.27	1.33
10	L	302	BPH	C1B-C2B	-2.23	1.41	1.45
9	7	101	BCL	C3B-C2B	-2.23	1.34	1.39
9	7	101	BCL	O2D-CGD	-2.22	1.27	1.33
7	C	501	HEM	C4B-NB	-2.21	1.31	1.36
9	5	102	BCL	C3D-C2D	-2.21	1.35	1.39
9	1	102	BCL	C3B-C2B	-2.21	1.35	1.39
7	o	502	HEM	C4D-ND	-2.20	1.34	1.36
9	AJ	102	BCL	O2D-CGD	-2.20	1.27	1.33
9	h	101	BCL	C3B-C2B	-2.18	1.35	1.39
9	i	102	BCL	CHD-C4C	-2.18	1.34	1.41
9	8	102	BCL	C3B-C2B	-2.16	1.35	1.39
9	x	305	BCL	C2C-C3C	-2.16	1.48	1.54
9	x	305	BCL	CHD-C4C	-2.16	1.35	1.41
9	5	101	BCL	C2C-C3C	-2.15	1.48	1.54
9	D	101	BCL	C3D-C2D	-2.14	1.35	1.39
9	p	104	BCL	C3D-C2D	-2.14	1.35	1.39
10	x	302	BPH	CHC-C4B	-2.13	1.35	1.40
9	1	101	BCL	C3D-C2D	-2.13	1.35	1.39
9	p	104	BCL	C3B-C2B	-2.12	1.35	1.39
7	C	501	HEM	CAA-C2A	-2.11	1.48	1.52
9	L	303	BCL	O1A-CGA	-2.11	1.16	1.22
9	L	305	BCL	CHD-C4C	-2.10	1.35	1.41
9	M	401	BCL	OBB-CAB	-2.10	1.15	1.22
9	AH	101	BCL	C3D-C2D	-2.08	1.35	1.39
9	e	102	BCL	CHD-C4C	-2.08	1.35	1.41
9	AE	104	BCL	C2C-C3C	-2.08	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	y	401	BCL	C3B-C2B	-2.07	1.35	1.39
7	o	502	HEM	C3B-CAB	-2.06	1.43	1.47
9	5	102	BCL	C3B-C2B	-2.06	1.35	1.39
9	4	102	BCL	C3B-C2B	-2.06	1.35	1.39
9	4	102	BCL	C4B-CHC	-2.06	1.34	1.40
9	W	101	BCL	C3B-C2B	-2.05	1.35	1.39
9	1	101	BCL	C3B-C2B	-2.04	1.35	1.39
9	y	401	BCL	C2C-C3C	-2.03	1.48	1.54
9	f	101	BCL	C1A-CHA	-2.02	1.34	1.43
9	D	102	BCL	CHD-C4C	-2.02	1.35	1.41
9	m	102	BCL	C3D-C2D	-2.02	1.35	1.39
9	AK	101	BCL	CHD-C4C	-2.02	1.35	1.41
7	o	501	HEM	C3B-CAB	-2.01	1.43	1.47
9	AA	101	BCL	C3D-C2D	-2.01	1.35	1.39
9	r	101	BCL	C3B-C2B	-2.01	1.35	1.39
9	k	102	BCL	CHD-C4C	-2.01	1.35	1.41
11	L	304	UQ8	C42-C43	2.00	1.57	1.50
9	m	102	BCL	C3D-CAD	2.01	1.51	1.46
11	L	304	UQ8	C6-C5	2.01	1.52	1.46
9	T	102	BCL	C5-C3	2.01	1.55	1.51
9	AH	103	BCL	C3D-CAD	2.01	1.51	1.46
12	t	303	PEF	C3-C2	2.01	1.56	1.50
9	x	301	BCL	C3A-C2A	2.02	1.60	1.54
9	g	101	BCL	C5-C3	2.03	1.55	1.51
9	L	303	BCL	C6-C5	2.03	1.59	1.52
14	y	403	MQ8	C47-C48	2.03	1.38	1.32
9	v	102	BCL	C3C-C4C	2.03	1.54	1.51
14	M	403	MQ8	C17-C18	2.04	1.38	1.33
9	v	102	BCL	C3B-CAB	2.04	1.54	1.49
7	C	501	HEM	C1C-NC	2.04	1.39	1.36
9	W	101	BCL	C3D-CAD	2.04	1.52	1.46
9	P	101	BCL	C5-C3	2.05	1.55	1.51
9	p	104	BCL	C3D-CAD	2.05	1.52	1.46
15	k	101	CRT	C4-C5	2.05	1.53	1.50
9	AI	101	BCL	C5-C3	2.05	1.55	1.51
14	y	403	MQ8	C17-C18	2.05	1.38	1.33
9	R	102	BCL	C3B-CAB	2.06	1.54	1.49
15	y	404	CRT	C25-C23	2.06	1.50	1.45
9	Y	101	BCL	C3D-CAD	2.07	1.52	1.46
9	AH	101	BCL	C3D-CAD	2.07	1.52	1.46
9	M	401	BCL	C3D-CAD	2.08	1.52	1.46
10	y	402	BPH	CHC-C1C	2.08	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	102	BCL	C3B-CAB	2.08	1.54	1.49
12	H	301	PEF	O3-C30	2.09	1.43	1.33
14	y	403	MQ8	C42-C43	2.09	1.38	1.33
9	AJ	102	BCL	C5-C3	2.10	1.55	1.51
9	S	102	BCL	C3B-CAB	2.10	1.54	1.49
9	e	102	BCL	C5-C3	2.10	1.55	1.51
9	r	101	BCL	C5-C3	2.11	1.55	1.51
9	l	102	BCL	C5-C3	2.11	1.55	1.51
9	W	101	BCL	C3B-CAB	2.11	1.54	1.49
11	x	304	UQ8	C43-C44	2.11	1.38	1.32
9	AA	101	BCL	C5-C3	2.12	1.55	1.51
9	i	102	BCL	C3B-CAB	2.12	1.54	1.49
9	Q	101	BCL	C3B-CAB	2.13	1.54	1.49
11	L	304	UQ8	O5-C5	2.13	1.28	1.23
11	L	304	UQ8	C43-C44	2.13	1.38	1.32
9	K	101	BCL	C5-C3	2.13	1.56	1.51
9	V	101	BCL	C3B-CAB	2.13	1.54	1.49
9	K	101	BCL	C3B-CAB	2.13	1.54	1.49
9	5	102	BCL	C2A-C1A	2.14	1.57	1.52
9	M	401	BCL	C5-C3	2.15	1.56	1.51
12	H	304	PEF	C3-C2	2.15	1.56	1.50
9	L	301	BCL	C3A-C2A	2.15	1.60	1.54
9	AH	101	BCL	C3B-CAB	2.15	1.54	1.49
9	AC	102	BCL	C5-C3	2.16	1.56	1.51
9	V	101	BCL	C3C-C4C	2.16	1.54	1.51
9	m	103	BCL	C5-C3	2.16	1.56	1.51
9	3	101	BCL	C3C-C4C	2.17	1.54	1.51
9	s	102	BCL	C3B-CAB	2.17	1.54	1.49
9	V	101	BCL	C5-C3	2.18	1.56	1.51
9	I	101	BCL	C5-C3	2.19	1.56	1.51
9	AE	102	BCL	C3B-CAB	2.19	1.55	1.49
9	Z	102	BCL	C5-C3	2.20	1.56	1.51
9	M	401	BCL	C2A-C1A	2.20	1.57	1.52
9	z	102	BCL	C3B-CAB	2.23	1.55	1.49
9	0	101	BCL	C5-C3	2.23	1.56	1.51
9	Y	101	BCL	C3B-CAB	2.23	1.55	1.49
11	L	304	UQ8	C23-C24	2.23	1.38	1.33
9	w	101	BCL	C3C-C4C	2.23	1.54	1.51
9	i	102	BCL	C5-C3	2.24	1.56	1.51
9	J	102	BCL	C3C-C4C	2.24	1.54	1.51
9	0	101	BCL	C3C-C4C	2.25	1.54	1.51
9	AL	102	BCL	C5-C3	2.25	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	502	HEM	C3C-C2C	2.27	1.43	1.40
9	p	104	BCL	C3C-C4C	2.27	1.54	1.51
7	C	501	HEM	C4C-NC	2.28	1.39	1.36
10	M	402	BPH	O2D-CGD	2.28	1.39	1.33
12	y	408	PEF	C1-C2	2.29	1.57	1.50
9	L	301	BCL	C3B-CAB	2.30	1.55	1.49
7	C	502	HEM	C3C-C2C	2.33	1.43	1.40
9	AH	103	BCL	C3B-CAB	2.34	1.55	1.49
9	x	303	BCL	CHB-C4A	2.34	1.36	1.33
9	AH	103	BCL	C3C-C4C	2.35	1.54	1.51
14	M	403	MQ8	C42-C43	2.37	1.38	1.33
9	f	101	BCL	C3C-C4C	2.37	1.54	1.51
9	7	101	BCL	C3C-C4C	2.37	1.54	1.51
9	5	102	BCL	C3B-CAB	2.37	1.55	1.49
9	S	102	BCL	C3C-C4C	2.38	1.54	1.51
9	J	102	BCL	C3B-CAB	2.40	1.55	1.49
9	s	102	BCL	C3C-C4C	2.40	1.54	1.51
9	3	101	BCL	C5-C3	2.40	1.56	1.51
12	H	303	PEF	O3-C30	2.43	1.45	1.33
9	1	102	BCL	C3C-C4C	2.43	1.54	1.51
9	h	101	BCL	C5-C3	2.43	1.56	1.51
9	Q	101	BCL	C3C-C4C	2.45	1.54	1.51
9	U	101	BCL	C5-C3	2.46	1.56	1.51
9	m	102	BCL	C3C-C4C	2.46	1.54	1.51
14	y	403	MQ8	C32-C33	2.48	1.39	1.33
9	L	305	BCL	C3B-CAB	2.49	1.55	1.49
9	l	101	BCL	C3B-CAB	2.51	1.55	1.49
12	p	101	PEF	O3-C30	2.51	1.45	1.33
9	L	301	BCL	C5-C3	2.51	1.56	1.51
9	u	101	BCL	C3C-C4C	2.52	1.54	1.51
9	d	101	BCL	C3C-C4C	2.53	1.54	1.51
9	9	103	BCL	C3C-C4C	2.53	1.54	1.51
9	w	101	BCL	C5-C3	2.54	1.56	1.51
9	m	102	BCL	C5-C3	2.58	1.57	1.51
9	p	104	BCL	CHB-C4A	2.58	1.36	1.33
9	F	101	BCL	C3C-C4C	2.60	1.54	1.51
11	L	304	UQ8	C4-C3	2.60	1.46	1.35
12	x	306	PEF	O3-C30	2.62	1.46	1.33
9	m	103	BCL	C3C-C4C	2.62	1.55	1.51
9	s	102	BCL	O2D-CED	2.65	1.51	1.45
10	M	402	BPH	CHB-C1B	2.65	1.43	1.38
12	y	406	PEF	O3-C30	2.67	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	402	BPH	CHC-C1C	2.68	1.41	1.36
9	m	102	BCL	C3B-CAB	2.68	1.56	1.49
9	m	103	BCL	C3D-CAD	2.69	1.53	1.46
17	S	101	PGW	O01-C1	2.70	1.41	1.35
14	y	403	MQ8	C9-C10	2.71	1.44	1.39
9	l	101	BCL	C5-C3	2.72	1.57	1.51
12	m	101	PEF	O3-C30	2.72	1.46	1.33
9	U	101	BCL	O2D-CED	2.74	1.51	1.45
9	f	101	BCL	C5-C3	2.76	1.57	1.51
9	L	303	BCL	C5-C3	2.80	1.57	1.51
9	X	102	BCL	C3C-C4C	2.81	1.55	1.51
12	t	303	PEF	O3-C30	2.82	1.47	1.33
9	5	102	BCL	C3C-C4C	2.82	1.55	1.51
12	M	408	PEF	O3-C30	2.84	1.47	1.33
14	y	403	MQ8	C37-C38	2.85	1.40	1.33
12	y	408	PEF	O3-C30	2.86	1.47	1.33
9	d	101	BCL	C5-C3	2.88	1.57	1.51
12	t	301	PEF	O3-C30	2.88	1.47	1.33
9	W	101	BCL	C3C-C4C	2.88	1.55	1.51
12	M	406	PEF	O3-C30	2.89	1.47	1.33
12	M	407	PEF	O3-C30	2.90	1.47	1.33
9	x	301	BCL	C3B-CAB	2.92	1.56	1.49
9	w	101	BCL	O2D-CED	2.94	1.52	1.45
9	k	102	BCL	O2D-CED	2.94	1.52	1.45
9	D	101	BCL	O2D-CED	2.95	1.52	1.45
9	x	303	BCL	O2D-CED	2.96	1.52	1.45
9	x	301	BCL	C5-C3	2.98	1.57	1.51
9	AH	101	BCL	O2D-CED	2.98	1.52	1.45
9	K	101	BCL	O2D-CED	2.98	1.52	1.45
17	AE	101	PGW	O01-C1	2.99	1.42	1.35
9	AK	101	BCL	O2D-CED	3.00	1.52	1.45
12	H	304	PEF	O3-C30	3.01	1.48	1.33
9	s	102	BCL	C5-C3	3.03	1.57	1.51
12	A	101	PEF	O3-C30	3.03	1.48	1.33
9	P	101	BCL	O2D-CED	3.05	1.52	1.45
9	AC	102	BCL	O2D-CED	3.05	1.52	1.45
9	Q	101	BCL	O2D-CED	3.06	1.52	1.45
9	h	101	BCL	C3C-C4C	3.06	1.55	1.51
11	x	304	UQ8	C4-C3	3.06	1.48	1.35
9	r	101	BCL	C3C-C4C	3.09	1.55	1.51
9	T	102	BCL	O2D-CED	3.11	1.52	1.45
9	AH	103	BCL	O2D-CED	3.11	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	102	BCL	CHB-C4A	3.11	1.37	1.33
9	Z	102	BCL	O2D-CED	3.14	1.52	1.45
9	AD	101	BCL	O2D-CED	3.14	1.52	1.45
9	AI	101	BCL	O2D-CED	3.15	1.52	1.45
9	L	303	BCL	O2D-CED	3.16	1.52	1.45
9	v	102	BCL	O2D-CED	3.17	1.52	1.45
9	L	305	BCL	O2D-CED	3.18	1.53	1.45
9	L	301	BCL	O2D-CED	3.18	1.53	1.45
9	AB	101	BCL	O2D-CED	3.18	1.53	1.45
9	B	101	BCL	O2D-CED	3.19	1.53	1.45
9	L	301	BCL	CHB-C4A	3.19	1.37	1.33
9	4	102	BCL	O2D-CED	3.19	1.53	1.45
9	P	101	BCL	C3C-C4C	3.20	1.55	1.51
9	D	102	BCL	O2D-CED	3.20	1.53	1.45
9	F	101	BCL	CHB-C4A	3.21	1.37	1.33
9	X	102	BCL	O2D-CED	3.21	1.53	1.45
9	g	101	BCL	O2D-CED	3.22	1.53	1.45
9	A	102	BCL	O2D-CED	3.24	1.53	1.45
9	w	101	BCL	CHB-C4A	3.24	1.37	1.33
9	I	101	BCL	CHB-C4A	3.26	1.37	1.33
9	AA	101	BCL	O2D-CED	3.26	1.53	1.45
9	u	101	BCL	C5-C3	3.26	1.58	1.51
9	z	102	BCL	O2D-CED	3.26	1.53	1.45
9	G	102	BCL	O2D-CED	3.28	1.53	1.45
9	I	101	BCL	O2D-CED	3.29	1.53	1.45
9	l	102	BCL	O2D-CED	3.29	1.53	1.45
9	h	101	BCL	O2D-CED	3.30	1.53	1.45
9	AL	102	BCL	O2D-CED	3.31	1.53	1.45
9	j	101	BCL	O2D-CED	3.31	1.53	1.45
9	e	102	BCL	O2D-CED	3.31	1.53	1.45
9	J	102	BCL	O2D-CED	3.31	1.53	1.45
9	d	101	BCL	O2D-CED	3.31	1.53	1.45
9	V	101	BCL	O2D-CED	3.31	1.53	1.45
9	L	301	BCL	C3C-C4C	3.33	1.55	1.51
9	p	104	BCL	O2D-CED	3.33	1.53	1.45
9	p	102	BCL	O2D-CED	3.34	1.53	1.45
9	S	102	BCL	O2D-CED	3.35	1.53	1.45
9	5	102	BCL	O2D-CED	3.37	1.53	1.45
9	i	102	BCL	O2D-CED	3.37	1.53	1.45
9	s	102	BCL	CHB-C4A	3.37	1.37	1.33
9	5	101	BCL	O2D-CED	3.38	1.53	1.45
9	AE	104	BCL	O2D-CED	3.39	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	l	101	BCL	O2D-CED	3.39	1.53	1.45
9	AJ	102	BCL	O2D-CED	3.40	1.53	1.45
9	u	101	BCL	O2D-CED	3.40	1.53	1.45
9	7	101	BCL	O2D-CED	3.41	1.53	1.45
9	r	101	BCL	O2D-CED	3.41	1.53	1.45
9	F	101	BCL	O2D-CED	3.41	1.53	1.45
9	AE	102	BCL	O2D-CED	3.42	1.53	1.45
9	R	102	BCL	O2D-CED	3.43	1.53	1.45
9	4	102	BCL	CHB-C4A	3.44	1.37	1.33
9	AB	101	BCL	CHB-C4A	3.44	1.37	1.33
9	4	102	BCL	C3C-C4C	3.44	1.56	1.51
9	f	101	BCL	O2D-CED	3.44	1.53	1.45
9	0	101	BCL	O2D-CED	3.45	1.53	1.45
9	N	102	BCL	O2D-CED	3.45	1.53	1.45
9	M	401	BCL	O2D-CED	3.47	1.53	1.45
9	O	101	BCL	CHB-C4A	3.47	1.38	1.33
9	8	102	BCL	CHB-C4A	3.48	1.38	1.33
9	9	103	BCL	O2D-CED	3.48	1.53	1.45
9	m	102	BCL	O2D-CED	3.49	1.53	1.45
9	P	101	BCL	CHB-C4A	3.51	1.38	1.33
9	W	101	BCL	O2D-CED	3.51	1.53	1.45
9	m	103	BCL	O2D-CED	3.51	1.53	1.45
9	c	102	BCL	O2D-CED	3.51	1.53	1.45
9	0	101	BCL	CHB-C4A	3.52	1.38	1.33
9	e	102	BCL	CHB-C4A	3.53	1.38	1.33
9	1	101	BCL	CHB-C4A	3.58	1.38	1.33
9	3	101	BCL	O2D-CED	3.58	1.53	1.45
12	y	407	PEF	O3-C30	3.60	1.51	1.33
9	Y	101	BCL	O2D-CED	3.60	1.54	1.45
9	AH	101	BCL	CHB-C4A	3.61	1.38	1.33
9	AK	101	BCL	CHB-C4A	3.62	1.38	1.33
9	x	305	BCL	O2D-CED	3.63	1.54	1.45
9	r	101	BCL	CHB-C4A	3.63	1.38	1.33
9	8	102	BCL	O2D-CED	3.64	1.54	1.45
9	1	101	BCL	O2D-CED	3.64	1.54	1.45
9	B	101	BCL	CHB-C4A	3.64	1.38	1.33
9	O	101	BCL	O2D-CED	3.64	1.54	1.45
9	y	401	BCL	C3C-C4C	3.65	1.56	1.51
9	j	101	BCL	CHB-C4A	3.65	1.38	1.33
9	L	305	BCL	CHB-C4A	3.69	1.38	1.33
9	y	401	BCL	CHB-C4A	3.70	1.38	1.33
9	3	101	BCL	CHB-C4A	3.72	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AE	104	BCL	CHB-C4A	3.73	1.38	1.33
9	x	301	BCL	O2D-CED	3.73	1.54	1.45
9	G	102	BCL	CHB-C4A	3.75	1.38	1.33
9	u	101	BCL	CHB-C4A	3.76	1.38	1.33
9	y	401	BCL	O2D-CED	3.78	1.54	1.45
9	v	102	BCL	CHB-C4A	3.79	1.38	1.33
9	l	102	BCL	CHB-C4A	3.80	1.38	1.33
9	f	101	BCL	CHB-C4A	3.82	1.38	1.33
9	T	102	BCL	CHB-C4A	3.87	1.38	1.33
9	L	303	BCL	CHB-C4A	3.88	1.38	1.33
9	N	102	BCL	CHB-C4A	3.89	1.38	1.33
9	D	101	BCL	CHB-C4A	3.91	1.38	1.33
9	K	101	BCL	CHB-C4A	3.96	1.38	1.33
9	M	401	BCL	C3C-C4C	3.96	1.56	1.51
9	x	301	BCL	CHB-C4A	3.96	1.38	1.33
9	AC	102	BCL	CHB-C4A	3.97	1.38	1.33
9	9	103	BCL	CHB-C4A	3.97	1.38	1.33
9	AI	101	BCL	CHB-C4A	4.01	1.38	1.33
9	Y	101	BCL	C3C-C4C	4.02	1.56	1.51
9	R	102	BCL	CHB-C4A	4.04	1.38	1.33
9	U	101	BCL	CHB-C4A	4.09	1.38	1.33
9	l	101	BCL	CHB-C4A	4.12	1.38	1.33
9	c	102	BCL	CHB-C4A	4.12	1.38	1.33
9	J	102	BCL	CHB-C4A	4.23	1.38	1.33
7	C	502	HEM	C4C-NC	4.25	1.41	1.36
7	o	502	HEM	C4C-NC	4.25	1.41	1.36
9	AL	102	BCL	CHB-C4A	4.30	1.39	1.33
9	x	305	BCL	CHB-C4A	4.34	1.39	1.33
9	5	101	BCL	CHB-C4A	4.34	1.39	1.33
9	m	103	BCL	CHB-C4A	4.35	1.39	1.33
9	AD	101	BCL	CHB-C4A	4.36	1.39	1.33
9	V	101	BCL	CHB-C4A	4.37	1.39	1.33
9	7	101	BCL	CHB-C4A	4.38	1.39	1.33
9	Z	102	BCL	CHB-C4A	4.43	1.39	1.33
9	g	101	BCL	CHB-C4A	4.44	1.39	1.33
9	Y	101	BCL	CHB-C4A	4.44	1.39	1.33
9	Q	101	BCL	CHB-C4A	4.44	1.39	1.33
9	S	102	BCL	CHB-C4A	4.50	1.39	1.33
9	d	101	BCL	CHB-C4A	4.51	1.39	1.33
12	M	406	PEF	O2-C10	4.51	1.45	1.35
9	p	102	BCL	CHB-C4A	4.52	1.39	1.33
9	X	102	BCL	CHB-C4A	4.53	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	x	301	BCL	C3C-C4C	4.56	1.57	1.51
12	A	101	PEF	O2-C10	4.56	1.45	1.35
9	AE	102	BCL	CHB-C4A	4.57	1.39	1.33
9	k	102	BCL	CHB-C4A	4.57	1.39	1.33
9	M	401	BCL	CHB-C4A	4.61	1.39	1.33
9	AA	101	BCL	CHB-C4A	4.61	1.39	1.33
12	t	301	PEF	O2-C10	4.65	1.45	1.35
9	AJ	102	BCL	CHB-C4A	4.65	1.39	1.33
9	i	102	BCL	CHB-C4A	4.68	1.39	1.33
12	t	303	PEF	O2-C10	4.71	1.46	1.35
12	y	406	PEF	O2-C10	4.76	1.46	1.35
9	z	102	BCL	CHB-C4A	4.81	1.39	1.33
9	m	102	BCL	CHB-C4A	4.86	1.39	1.33
9	p	102	BCL	OBD-CAD	4.90	1.29	1.22
9	S	102	BCL	CHC-C1C	4.93	1.39	1.33
9	3	101	BCL	CHC-C1C	4.98	1.39	1.33
9	5	101	BCL	CHC-C1C	5.00	1.39	1.33
12	H	304	PEF	O2-C10	5.03	1.46	1.35
9	5	102	BCL	CHB-C4A	5.05	1.40	1.33
12	H	303	PEF	O2-C10	5.06	1.46	1.35
9	W	101	BCL	CHB-C4A	5.13	1.40	1.33
12	m	101	PEF	O2-C10	5.23	1.47	1.35
9	A	102	BCL	CHB-C4A	5.24	1.40	1.33
9	d	101	BCL	CHC-C1C	5.24	1.40	1.33
9	p	102	BCL	CHC-C1C	5.25	1.40	1.33
9	9	103	BCL	OBD-CAD	5.26	1.29	1.22
12	y	408	PEF	O2-C10	5.29	1.47	1.35
9	f	101	BCL	OBD-CAD	5.32	1.30	1.22
9	L	303	BCL	OBD-CAD	5.33	1.30	1.22
9	e	102	BCL	OBD-CAD	5.35	1.30	1.22
12	M	408	PEF	O2-C10	5.41	1.47	1.35
9	x	301	BCL	OBD-CAD	5.41	1.30	1.22
9	AL	102	BCL	OBD-CAD	5.42	1.30	1.22
9	x	303	BCL	OBD-CAD	5.43	1.30	1.22
9	s	102	BCL	OBD-CAD	5.44	1.30	1.22
9	1	102	BCL	OBD-CAD	5.45	1.30	1.22
9	9	103	BCL	CHC-C1C	5.45	1.40	1.33
9	8	102	BCL	OBD-CAD	5.46	1.30	1.22
9	4	102	BCL	OBD-CAD	5.47	1.30	1.22
9	z	102	BCL	OBD-CAD	5.48	1.30	1.22
9	0	101	BCL	OBD-CAD	5.49	1.30	1.22
9	f	101	BCL	CHC-C1C	5.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Y	101	BCL	CHC-C1C	5.51	1.40	1.33
9	AC	102	BCL	OBD-CAD	5.52	1.30	1.22
9	h	101	BCL	CHB-C4A	5.52	1.40	1.33
9	F	101	BCL	OBD-CAD	5.53	1.30	1.22
9	v	102	BCL	OBD-CAD	5.54	1.30	1.22
9	y	401	BCL	OBD-CAD	5.57	1.30	1.22
9	AJ	102	BCL	OBD-CAD	5.57	1.30	1.22
9	B	101	BCL	OBD-CAD	5.57	1.30	1.22
9	K	101	BCL	OBD-CAD	5.58	1.30	1.22
9	3	101	BCL	OBD-CAD	5.58	1.30	1.22
12	y	407	PEF	O2-C10	5.60	1.48	1.35
9	J	102	BCL	OBD-CAD	5.64	1.30	1.22
9	AE	102	BCL	CHC-C1C	5.65	1.40	1.33
9	S	102	BCL	OBD-CAD	5.65	1.30	1.22
12	H	301	PEF	O2-C10	5.65	1.48	1.35
9	I	101	BCL	OBD-CAD	5.67	1.30	1.22
9	P	101	BCL	OBD-CAD	5.68	1.30	1.22
9	AI	101	BCL	OBD-CAD	5.70	1.30	1.22
9	h	101	BCL	OBD-CAD	5.71	1.30	1.22
9	L	305	BCL	OBD-CAD	5.71	1.30	1.22
9	u	101	BCL	OBD-CAD	5.71	1.30	1.22
12	x	306	PEF	O2-C10	5.72	1.48	1.35
9	A	102	BCL	OBD-CAD	5.72	1.30	1.22
9	g	101	BCL	OBD-CAD	5.72	1.30	1.22
9	D	101	BCL	CHC-C1C	5.72	1.40	1.33
9	Z	102	BCL	OBD-CAD	5.73	1.30	1.22
9	AH	103	BCL	CHB-C4A	5.73	1.40	1.33
9	D	102	BCL	OBD-CAD	5.74	1.30	1.22
9	G	102	BCL	OBD-CAD	5.74	1.30	1.22
9	O	101	BCL	OBD-CAD	5.75	1.30	1.22
9	X	102	BCL	OBD-CAD	5.75	1.30	1.22
9	4	102	BCL	CHC-C1C	5.76	1.40	1.33
9	j	101	BCL	OBD-CAD	5.78	1.30	1.22
9	m	102	BCL	OBD-CAD	5.78	1.30	1.22
9	U	101	BCL	OBD-CAD	5.79	1.30	1.22
9	7	101	BCL	OBD-CAD	5.79	1.30	1.22
9	d	101	BCL	OBD-CAD	5.80	1.30	1.22
9	AK	101	BCL	OBD-CAD	5.82	1.30	1.22
9	5	102	BCL	CHC-C1C	5.84	1.40	1.33
9	AE	102	BCL	OBD-CAD	5.85	1.30	1.22
9	l	101	BCL	OBD-CAD	5.85	1.30	1.22
9	5	101	BCL	OBD-CAD	5.85	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	k	102	BCL	OBD-CAD	5.86	1.30	1.22
9	c	102	BCL	OBD-CAD	5.87	1.30	1.22
9	AA	101	BCL	OBD-CAD	5.87	1.30	1.22
9	h	101	BCL	CHC-C1C	5.87	1.41	1.33
9	m	103	BCL	CHC-C1C	5.88	1.41	1.33
9	l	101	BCL	OBD-CAD	5.90	1.30	1.22
9	c	102	BCL	CHC-C1C	5.91	1.41	1.33
9	AE	104	BCL	OBD-CAD	5.92	1.30	1.22
9	R	102	BCL	OBD-CAD	5.92	1.30	1.22
9	i	102	BCL	OBD-CAD	5.93	1.30	1.22
9	V	101	BCL	OBD-CAD	5.94	1.30	1.22
9	l	101	BCL	CHC-C1C	5.94	1.41	1.33
9	AD	101	BCL	OBD-CAD	5.96	1.31	1.22
9	r	101	BCL	OBD-CAD	5.96	1.31	1.22
9	D	101	BCL	OBD-CAD	5.97	1.31	1.22
9	AA	101	BCL	CHC-C1C	5.98	1.41	1.33
9	AH	101	BCL	OBD-CAD	5.99	1.31	1.22
9	N	102	BCL	OBD-CAD	6.00	1.31	1.22
9	5	102	BCL	OBD-CAD	6.01	1.31	1.22
9	m	102	BCL	CHC-C1C	6.01	1.41	1.33
9	L	305	BCL	CHC-C1C	6.01	1.41	1.33
9	I	101	BCL	CHC-C1C	6.02	1.41	1.33
9	m	103	BCL	OBD-CAD	6.02	1.31	1.22
9	AI	101	BCL	CHC-C1C	6.04	1.41	1.33
9	x	305	BCL	OBD-CAD	6.06	1.31	1.22
9	J	102	BCL	CHC-C1C	6.07	1.41	1.33
9	O	101	BCL	CHC-C1C	6.07	1.41	1.33
9	W	101	BCL	OBD-CAD	6.08	1.31	1.22
9	k	102	BCL	CHC-C1C	6.10	1.41	1.33
9	K	101	BCL	CHC-C1C	6.10	1.41	1.33
9	0	101	BCL	CHC-C1C	6.11	1.41	1.33
9	Y	101	BCL	OBD-CAD	6.11	1.31	1.22
9	W	101	BCL	CHC-C1C	6.11	1.41	1.33
9	w	101	BCL	OBD-CAD	6.12	1.31	1.22
9	Q	101	BCL	CHC-C1C	6.12	1.41	1.33
9	p	104	BCL	OBD-CAD	6.13	1.31	1.22
9	N	102	BCL	CHC-C1C	6.13	1.41	1.33
9	Q	101	BCL	OBD-CAD	6.13	1.31	1.22
9	A	102	BCL	CHC-C1C	6.14	1.41	1.33
9	z	102	BCL	CHC-C1C	6.18	1.41	1.33
9	y	401	BCL	CHC-C1C	6.19	1.41	1.33
9	i	102	BCL	CHC-C1C	6.20	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AJ	102	BCL	CHC-C1C	6.24	1.41	1.33
9	AH	103	BCL	OBD-CAD	6.26	1.31	1.22
9	v	102	BCL	CHC-C1C	6.27	1.41	1.33
9	AB	101	BCL	OBD-CAD	6.27	1.31	1.22
9	AE	104	BCL	CHC-C1C	6.27	1.41	1.33
9	l	102	BCL	CHC-C1C	6.28	1.41	1.33
9	AD	101	BCL	CHC-C1C	6.29	1.41	1.33
9	r	101	BCL	CHC-C1C	6.31	1.41	1.33
9	AB	101	BCL	CHC-C1C	6.31	1.41	1.33
9	s	102	BCL	CHC-C1C	6.34	1.41	1.33
9	B	101	BCL	CHC-C1C	6.38	1.41	1.33
9	Z	102	BCL	CHC-C1C	6.40	1.41	1.33
9	x	305	BCL	CHC-C1C	6.41	1.41	1.33
9	P	101	BCL	CHC-C1C	6.42	1.41	1.33
9	M	401	BCL	OBD-CAD	6.43	1.31	1.22
9	AH	103	BCL	CHC-C1C	6.45	1.41	1.33
9	x	303	BCL	CHC-C1C	6.45	1.41	1.33
9	l	101	BCL	CHC-C1C	6.45	1.41	1.33
9	T	102	BCL	OBD-CAD	6.47	1.31	1.22
9	g	101	BCL	CHC-C1C	6.47	1.41	1.33
11	L	304	UQ8	C6-C1	6.47	1.49	1.35
9	T	102	BCL	CHC-C1C	6.48	1.41	1.33
9	G	102	BCL	CHC-C1C	6.48	1.41	1.33
9	AH	101	BCL	CHC-C1C	6.48	1.41	1.33
9	F	101	BCL	CHC-C1C	6.54	1.41	1.33
11	x	304	UQ8	C6-C1	6.54	1.49	1.35
9	7	101	BCL	CHC-C1C	6.58	1.41	1.33
9	AC	102	BCL	CHC-C1C	6.59	1.41	1.33
9	U	101	BCL	CHC-C1C	6.61	1.41	1.33
9	u	101	BCL	CHC-C1C	6.64	1.42	1.33
9	w	101	BCL	CHC-C1C	6.66	1.42	1.33
9	j	101	BCL	CHC-C1C	6.67	1.42	1.33
9	R	102	BCL	CHC-C1C	6.71	1.42	1.33
9	L	303	BCL	CHC-C1C	6.73	1.42	1.33
9	M	401	BCL	CHC-C1C	6.76	1.42	1.33
9	AK	101	BCL	CHC-C1C	6.84	1.42	1.33
9	p	104	BCL	CHC-C1C	6.86	1.42	1.33
9	8	102	BCL	CHC-C1C	6.87	1.42	1.33
9	e	102	BCL	CHC-C1C	6.94	1.42	1.33
9	V	101	BCL	CHC-C1C	6.96	1.42	1.33
9	AL	102	BCL	CHC-C1C	6.97	1.42	1.33
9	D	102	BCL	CHC-C1C	7.04	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	301	BCL	CHC-C1C	7.10	1.42	1.33
9	X	102	BCL	CHC-C1C	7.17	1.42	1.33
9	L	301	BCL	OBD-CAD	7.51	1.33	1.22
9	x	301	BCL	CHC-C1C	7.89	1.43	1.33

All (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
15	N	101	CRT	C3-C1-C4	-15.37	84.77	110.90
15	G	101	CRT	C2-C1-C4	-15.35	84.81	110.90
15	p	103	CRT	C2-C1-C4	-15.30	84.89	110.90
15	z	101	CRT	C2-C1-C4	-15.23	85.00	110.90
15	J	101	CRT	C3-C1-C4	-15.18	85.10	110.90
15	y	404	CRT	C3-C1-C4	-15.05	85.31	110.90
15	n	101	CRT	C3-C1-C4	-14.89	85.59	110.90
15	8	101	CRT	C2-C1-C4	-14.88	85.60	110.90
15	f	102	CRT	C3-C1-C4	-14.78	85.77	110.90
15	AH	102	CRT	C2-C1-C4	-14.77	85.79	110.90
15	v	101	CRT	C3-C1-C4	-14.75	85.82	110.90
15	AE	103	CRT	C3-C1-C4	-14.71	85.90	110.90
15	n	101	CRT	C2-C1-C4	-14.68	85.94	110.90
15	U	102	CRT	C2-C1-C4	-14.65	86.00	110.90
15	N	101	CRT	C2-C1-C4	-14.62	86.05	110.90
15	6	101	CRT	C2-C1-C4	-14.52	86.22	110.90
15	E	101	CRT	C2-C1-C4	-14.46	86.31	110.90
15	T	101	CRT	C2-C1-C4	-14.40	86.41	110.90
15	4	101	CRT	C2-C1-C4	-14.40	86.42	110.90
15	9	102	CRT	C2-C1-C4	-14.36	86.49	110.90
15	8	101	CRT	C3-C1-C4	-14.35	86.50	110.90
15	f	102	CRT	C2-C1-C4	-14.35	86.51	110.90
15	i	101	CRT	C2-C1-C4	-14.29	86.60	110.90
15	k	101	CRT	C2-C1-C4	-13.99	87.11	110.90
15	AE	103	CRT	C2-C1-C4	-13.90	87.27	110.90
15	c	101	CRT	C2-C1-C4	-13.86	87.34	110.90
15	k	101	CRT	C3-C1-C4	-13.84	87.37	110.90
15	p	103	CRT	C3-C1-C4	-13.54	87.88	110.90
15	z	101	CRT	C3-C1-C4	-13.54	87.88	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	101	CRT	C3-C1-C4	-13.18	88.50	110.90
15	AD	102	CRT	C2-C1-C4	-13.16	88.52	110.90
15	i	101	CRT	C3-C1-C4	-13.15	88.55	110.90
15	9	102	CRT	C3-C1-C4	-13.05	88.72	110.90
15	AD	102	CRT	C3-C1-C4	-12.88	89.01	110.90
15	y	404	CRT	C2-C1-C4	-12.74	89.24	110.90
15	R	101	CRT	C2-C1-C4	-12.31	89.97	110.90
15	c	101	CRT	C3-C1-C4	-12.29	90.00	110.90
15	R	101	CRT	C3-C1-C4	-12.18	90.19	110.90
15	6	101	CRT	C3-C1-C4	-11.84	90.77	110.90
15	J	101	CRT	C2-C1-C4	-11.82	90.80	110.90
15	E	101	CRT	C3-C1-C4	-11.73	90.96	110.90
15	v	101	CRT	C2-C1-C4	-11.66	91.08	110.90
15	M	404	CRT	C3-C1-C4	-11.43	91.46	110.90
15	AH	102	CRT	C3-C1-C4	-10.88	92.40	110.90
15	A	103	CRT	C3-C1-C4	-10.83	92.49	110.90
15	s	101	CRT	C3-C1-C4	-9.98	93.93	110.90
15	U	102	CRT	O1-C1-C4	-9.25	81.48	106.29
15	f	102	CRT	C31-C32-C33	-9.01	114.45	127.31
15	s	101	CRT	C37-C36-C35	-8.84	111.87	124.57
9	L	301	BCL	CAC-C3C-C2C	-8.58	92.68	114.24
15	AJ	101	CRT	C37-C36-C35	-8.24	112.72	124.57
15	y	404	CRT	C37-C36-C35	-8.00	113.07	124.57
15	U	102	CRT	C3-C1-C4	-7.99	97.31	110.90
15	AH	102	CRT	O1-C1-C4	-7.96	84.94	106.29
15	J	101	CRT	C37-C36-C35	-7.86	113.28	124.57
15	R	101	CRT	O1-C1-C4	-7.73	85.54	106.29
9	O	101	BCL	CMB-C2B-C1B	-7.70	116.62	128.46
15	E	101	CRT	O1-C1-C4	-7.65	85.76	106.29
9	AH	101	BCL	CMB-C2B-C1B	-7.63	116.74	128.46
15	s	101	CRT	O1-C1-C4	-7.60	85.90	106.29
15	i	101	CRT	O1-C1-C4	-7.59	85.91	106.29
15	c	101	CRT	O1-C1-C4	-7.57	85.99	106.29
15	N	101	CRT	C37-C36-C35	-7.49	113.82	124.57
9	j	101	BCL	CMB-C2B-C1B	-7.48	116.96	128.46
15	p	103	CRT	C37-C36-C35	-7.47	113.84	124.57
15	9	102	CRT	O1-C1-C4	-7.47	86.25	106.29
15	AD	102	CRT	O1-C1-C4	-7.46	86.27	106.29
7	C	501	HEM	CBD-CAD-C3D	-7.45	98.25	112.47
15	v	101	CRT	O1-C1-C4	-7.41	86.40	106.29
9	AB	101	BCL	CMB-C2B-C1B	-7.36	117.15	128.46
9	D	102	BCL	CMB-C2B-C1B	-7.33	117.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	v	101	CRT	C21-C22-C23	-7.26	116.95	127.31
15	6	101	CRT	O1-C1-C4	-7.21	86.94	106.29
9	1	101	BCL	CMB-C2B-C1B	-7.19	117.42	128.46
9	P	101	BCL	CMB-C2B-C1B	-7.08	117.58	128.46
9	f	101	BCL	CMB-C2B-C1B	-7.01	117.69	128.46
9	AE	104	BCL	CMB-C2B-C1B	-6.91	117.85	128.46
9	p	104	BCL	CMB-C2B-C1B	-6.89	117.88	128.46
15	N	101	CRT	C21-C22-C23	-6.86	117.52	127.31
9	N	102	BCL	CMB-C2B-C1B	-6.84	117.94	128.46
9	3	101	BCL	CMB-C2B-C1B	-6.84	117.95	128.46
9	5	101	BCL	CMB-C2B-C1B	-6.75	118.09	128.46
15	J	101	CRT	O1-C1-C4	-6.75	88.17	106.29
15	p	103	CRT	O1-C1-C4	-6.75	88.19	106.29
9	m	102	BCL	CMB-C2B-C1B	-6.68	118.19	128.46
15	J	101	CRT	C21-C22-C23	-6.68	117.78	127.31
15	z	101	CRT	O1-C1-C4	-6.67	88.39	106.29
15	G	101	CRT	C37-C36-C35	-6.65	115.01	124.57
9	e	102	BCL	CMB-C2B-C1B	-6.65	118.25	128.46
15	AE	103	CRT	O1-C1-C4	-6.65	88.45	106.29
9	s	102	BCL	CMB-C2B-C1B	-6.56	118.38	128.46
9	S	102	BCL	CMB-C2B-C1B	-6.56	118.38	128.46
9	I	101	BCL	CMB-C2B-C1B	-6.54	118.41	128.46
9	Y	101	BCL	CAC-C3C-C2C	-6.49	97.92	114.24
9	R	102	BCL	CMB-C2B-C1B	-6.49	118.50	128.46
15	G	101	CRT	O1-C1-C4	-6.48	88.91	106.29
9	B	101	BCL	CMB-C2B-C1B	-6.47	118.52	128.46
9	AI	101	BCL	CMB-C2B-C1B	-6.46	118.54	128.46
9	V	101	BCL	CMB-C2B-C1B	-6.44	118.56	128.46
9	M	401	BCL	CAC-C3C-C2C	-6.44	98.05	114.24
15	N	101	CRT	C4-C5-C6	-6.39	115.39	124.57
15	k	101	CRT	O1-C1-C4	-6.35	89.24	106.29
9	0	101	BCL	CMB-C2B-C1B	-6.35	118.70	128.46
9	AJ	102	BCL	CMB-C2B-C1B	-6.35	118.71	128.46
9	G	102	BCL	CMB-C2B-C1B	-6.34	118.72	128.46
15	A	103	CRT	C37-C36-C35	-6.33	115.48	124.57
9	m	103	BCL	CMB-C2B-C1B	-6.31	118.76	128.46
15	9	102	CRT	C21-C22-C23	-6.31	118.31	127.31
9	l	101	BCL	CMB-C2B-C1B	-6.30	118.78	128.46
9	F	101	BCL	CMB-C2B-C1B	-6.28	118.81	128.46
9	x	303	BCL	CMB-C2B-C1B	-6.26	118.84	128.46
15	X	101	CRT	C10-C9-C7	-6.26	118.38	127.31
9	w	101	BCL	CMB-C2B-C1B	-6.20	118.93	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	101	BCL	CMB-C2B-C1B	-6.20	118.94	128.46
15	T	101	CRT	C37-C36-C35	-6.17	115.70	124.57
15	AE	103	CRT	C37-C36-C35	-6.17	115.70	124.57
15	AC	101	CRT	C37-C36-C35	-6.16	115.72	124.57
9	v	102	BCL	CMB-C2B-C1B	-6.14	119.02	128.46
9	8	102	BCL	CMB-C2B-C1B	-6.13	119.04	128.46
9	x	303	BCL	C2C-C3C-C4C	-6.12	92.17	101.34
9	Y	101	BCL	CHD-C4C-NC	-6.12	118.28	125.08
15	U	102	CRT	C4-C5-C6	-6.11	115.79	124.57
15	AE	103	CRT	C21-C22-C23	-6.11	118.59	127.31
9	AK	101	BCL	CMB-C2B-C1B	-6.08	119.11	128.46
9	x	303	BCL	CAC-C3C-C2C	-6.08	98.97	114.24
9	AC	102	BCL	CMB-C2B-C1B	-6.06	119.15	128.46
9	g	101	BCL	CMB-C2B-C1B	-6.06	119.15	128.46
9	AE	102	BCL	CMB-C2B-C1B	-6.04	119.18	128.46
9	Y	101	BCL	CMB-C2B-C1B	-6.02	119.21	128.46
9	L	303	BCL	CMA-C3A-C4A	-6.01	95.62	111.77
15	4	101	CRT	O1-C1-C4	-6.00	90.18	106.29
9	p	102	BCL	CMB-C2B-C1B	-5.98	119.27	128.46
15	U	102	CRT	C37-C36-C35	-5.96	116.00	124.57
15	G	101	CRT	C21-C22-C23	-5.96	118.80	127.31
9	c	102	BCL	CMB-C2B-C1B	-5.96	119.31	128.46
9	A	102	BCL	CMB-C2B-C1B	-5.95	119.31	128.46
9	m	103	BCL	OBD-CAD-CBD	-5.95	116.96	125.94
12	M	408	PEF	C2-O2-C10	-5.94	106.46	117.94
9	Z	102	BCL	O2D-CGD-O1D	-5.93	111.89	123.82
15	M	404	CRT	C4-C5-C6	-5.93	116.05	124.57
9	AA	101	BCL	CMB-C2B-C1B	-5.89	119.41	128.46
15	R	101	CRT	C37-C36-C35	-5.89	116.10	124.57
9	y	401	BCL	CAC-C3C-C2C	-5.89	99.43	114.24
15	A	103	CRT	O1-C1-C4	-5.88	90.51	106.29
15	4	101	CRT	C36-C35-C33	-5.85	117.06	125.89
9	K	101	BCL	CMB-C2B-C1B	-5.84	119.48	128.46
9	M	401	BCL	CMB-C2B-C1B	-5.84	119.48	128.46
15	M	404	CRT	O1-C1-C4	-5.83	90.66	106.29
9	d	101	BCL	CMB-C2B-C1B	-5.81	119.53	128.46
15	M	404	CRT	C10-C9-C7	-5.81	119.02	127.31
7	o	501	HEM	CBD-CAD-C3D	-5.79	101.42	112.47
15	c	101	CRT	C37-C36-C35	-5.74	116.32	124.57
9	U	101	BCL	CMB-C2B-C1B	-5.73	119.66	128.46
9	AL	102	BCL	CMB-C2B-C1B	-5.72	119.67	128.46
15	AH	102	CRT	C37-C36-C35	-5.72	116.35	124.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	n	101	CRT	O1-C1-C4	-5.70	91.01	106.29
9	z	102	BCL	CMB-C2B-C1B	-5.69	119.71	128.46
9	J	102	BCL	CMB-C2B-C1B	-5.69	119.72	128.46
9	D	101	BCL	CMB-C2B-C1B	-5.67	119.75	128.46
9	u	101	BCL	CMB-C2B-C1B	-5.66	119.76	128.46
15	8	101	CRT	O1-C1-C4	-5.65	91.12	106.29
9	AJ	102	BCL	O2D-CGD-O1D	-5.64	112.48	123.82
15	9	102	CRT	C37-C36-C35	-5.63	116.49	124.57
9	5	102	BCL	O2D-CGD-O1D	-5.59	112.57	123.82
9	5	102	BCL	CMB-C2B-C1B	-5.56	119.91	128.46
9	M	401	BCL	O2D-CGD-O1D	-5.55	112.66	123.82
15	v	101	CRT	C37-C36-C35	-5.54	116.61	124.57
15	6	101	CRT	C26-C27-C28	-5.53	119.41	127.31
9	L	305	BCL	CMB-C2B-C1B	-5.52	119.99	128.46
9	X	102	BCL	CMB-C2B-C1B	-5.51	119.99	128.46
9	k	102	BCL	CMB-C2B-C1B	-5.51	120.00	128.46
9	4	102	BCL	CMB-C2B-C1B	-5.50	120.01	128.46
9	Z	102	BCL	CMB-C2B-C1B	-5.50	120.01	128.46
15	AD	102	CRT	C5-C6-C7	-5.47	117.62	125.89
15	Z	101	CRT	C37-C36-C35	-5.46	116.73	124.57
9	y	401	BCL	CMB-C2B-C1B	-5.45	120.08	128.46
9	x	301	BCL	CAC-C3C-C2C	-5.45	100.55	114.24
9	3	101	BCL	CAC-C3C-C2C	-5.43	100.59	114.24
15	E	101	CRT	C37-C36-C35	-5.43	116.77	124.57
9	1	102	BCL	CMB-C2B-C1B	-5.41	120.15	128.46
9	9	103	BCL	CMB-C2B-C1B	-5.39	120.18	128.46
15	AJ	101	CRT	C5-C6-C7	-5.38	117.76	125.89
15	AJ	101	CRT	C10-C9-C7	-5.38	119.64	127.31
9	d	101	BCL	O2D-CGD-O1D	-5.37	113.01	123.82
9	p	104	BCL	CAC-C3C-C2C	-5.36	100.76	114.24
7	C	501	HEM	CBA-CAA-C2A	-5.35	102.25	112.48
15	f	102	CRT	O1-C1-C4	-5.35	91.93	106.29
15	6	101	CRT	C37-C36-C35	-5.35	116.89	124.57
15	P	102	CRT	C37-C36-C35	-5.34	116.91	124.57
9	AD	101	BCL	CMB-C2B-C1B	-5.33	120.27	128.46
9	Q	101	BCL	CMB-C2B-C1B	-5.33	120.27	128.46
9	T	102	BCL	CMB-C2B-C1B	-5.33	120.28	128.46
9	s	102	BCL	O2D-CGD-O1D	-5.32	113.12	123.82
9	x	301	BCL	CHB-C4A-NA	-5.32	117.16	124.51
9	y	401	BCL	CHD-C4C-NC	-5.32	119.17	125.08
9	M	401	BCL	C3D-CAD-CBD	-5.31	100.08	107.60
9	D	101	BCL	O2D-CGD-O1D	-5.29	113.17	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	102	BCL	CMB-C2B-C1B	-5.28	120.35	128.46
9	l	102	BCL	O2D-CGD-O1D	-5.27	113.21	123.82
9	x	301	BCL	O2D-CGD-O1D	-5.25	113.26	123.82
15	M	404	CRT	C37-C36-C35	-5.25	117.03	124.57
9	l	102	BCL	CAC-C3C-C2C	-5.23	101.09	114.24
7	C	503	HEM	CBD-CAD-C3D	-5.22	102.52	112.47
9	S	102	BCL	O2D-CGD-O1D	-5.20	113.37	123.82
9	V	101	BCL	O2D-CGD-O1D	-5.19	113.39	123.82
15	AC	101	CRT	C4-C5-C6	-5.18	117.12	124.57
9	AH	103	BCL	O2D-CGD-O1D	-5.18	113.41	123.82
9	4	102	BCL	CAC-C3C-C2C	-5.16	101.27	114.24
9	5	102	BCL	CAC-C3C-C2C	-5.14	101.33	114.24
9	7	101	BCL	CMB-C2B-C1B	-5.12	120.59	128.46
15	AD	102	CRT	C37-C36-C35	-5.12	117.21	124.57
9	4	102	BCL	O2D-CGD-O1D	-5.12	113.52	123.82
15	P	102	CRT	C21-C22-C23	-5.11	120.02	127.31
9	AH	103	BCL	CMB-C2B-C1B	-5.10	120.63	128.46
15	G	101	CRT	C31-C32-C33	-5.10	120.04	127.31
15	9	102	CRT	C5-C6-C7	-5.09	118.20	125.89
9	T	102	BCL	O2D-CGD-O1D	-5.07	113.62	123.82
15	R	101	CRT	C15-C14-C12	-5.07	120.08	127.31
9	x	303	BCL	O2D-CGD-O1D	-5.06	113.64	123.82
9	AJ	102	BCL	CHD-C4C-NC	-5.04	119.47	125.08
9	8	102	BCL	OBD-CAD-CBD	-5.03	118.34	125.94
9	i	102	BCL	O2D-CGD-O1D	-5.01	113.74	123.82
9	e	102	BCL	O2D-CGD-O1D	-5.01	113.74	123.82
9	l	101	BCL	CAC-C3C-C2C	-5.01	101.65	114.24
9	l	101	BCL	O2D-CGD-O1D	-5.00	113.75	123.82
15	AL	101	CRT	C4-C5-C6	-5.00	117.39	124.57
15	v	101	CRT	C6-C7-C9	-5.00	111.27	118.94
9	h	101	BCL	CAC-C3C-C2C	-4.99	101.69	114.24
15	z	101	CRT	C4-C5-C6	-4.95	117.45	124.57
15	n	101	CRT	C37-C36-C35	-4.95	117.46	124.57
15	y	404	CRT	O1-C1-C4	-4.95	93.01	106.29
9	A	102	BCL	O2D-CGD-O1D	-4.95	113.87	123.82
12	t	303	PEF	C2-O2-C10	-4.94	108.39	117.94
15	N	101	CRT	O1-C1-C4	-4.93	93.07	106.29
9	4	102	BCL	CMA-C3A-C4A	-4.93	98.53	111.77
9	f	101	BCL	O2D-CGD-O1D	-4.92	113.92	123.82
15	AH	102	CRT	C26-C27-C28	-4.92	120.29	127.31
9	N	102	BCL	O2D-CGD-O1D	-4.92	113.93	123.82
15	k	101	CRT	C37-C36-C35	-4.91	117.52	124.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	101	CRT	C21-C22-C23	-4.91	120.31	127.31
9	M	401	BCL	CMA-C3A-C4A	-4.90	98.60	111.77
11	x	304	UQ8	C27-C28-C29	-4.89	115.39	127.68
9	AC	102	BCL	O2D-CGD-O1D	-4.88	114.00	123.82
9	Y	101	BCL	O2D-CGD-O1D	-4.88	114.00	123.82
9	v	102	BCL	O2D-CGD-O1D	-4.88	114.00	123.82
9	L	301	BCL	OBb-CAB-CBB	-4.88	109.03	120.16
12	M	406	PEF	C2-O2-C10	-4.87	108.52	117.94
9	j	101	BCL	O2D-CGD-O1D	-4.85	114.06	123.82
9	AH	101	BCL	O2D-CGD-O1D	-4.85	114.06	123.82
9	p	102	BCL	CAC-C3C-C2C	-4.84	102.06	114.24
9	9	103	BCL	CAC-C3C-C2C	-4.84	102.08	114.24
9	D	102	BCL	O2D-CGD-O1D	-4.83	114.10	123.82
9	h	101	BCL	O2D-CGD-O1D	-4.83	114.11	123.82
9	AH	103	BCL	CAC-C3C-C2C	-4.80	102.19	114.24
9	y	401	BCL	O2D-CGD-O1D	-4.79	114.18	123.82
9	3	101	BCL	C4B-CHC-C1C	-4.79	120.63	130.12
9	AE	104	BCL	O2D-CGD-O1D	-4.78	114.20	123.82
9	z	102	BCL	CAC-C3C-C2C	-4.78	102.23	114.24
15	i	101	CRT	C37-C36-C35	-4.78	117.71	124.57
9	w	101	BCL	CMA-C3A-C4A	-4.77	98.96	111.77
9	Q	101	BCL	O2D-CGD-O1D	-4.76	114.23	123.82
9	AB	101	BCL	CAC-C3C-C2C	-4.76	102.27	114.24
9	L	305	BCL	O2D-CGD-O1D	-4.75	114.27	123.82
9	AK	101	BCL	O2D-CGD-O1D	-4.74	114.28	123.82
9	W	101	BCL	CMB-C2B-C1B	-4.74	121.18	128.46
9	i	102	BCL	CAC-C3C-C2C	-4.73	102.34	114.24
9	f	101	BCL	CAC-C3C-C2C	-4.72	102.37	114.24
9	w	101	BCL	O2D-CGD-O1D	-4.72	114.33	123.82
9	p	104	BCL	O2D-CGD-O1D	-4.72	114.33	123.82
9	L	301	BCL	CMB-C2B-C1B	-4.72	121.22	128.46
9	x	305	BCL	CAC-C3C-C2C	-4.72	102.39	114.24
9	Q	101	BCL	C7-C6-C5	-4.71	100.01	113.11
15	P	102	CRT	C20-C19-C17	-4.70	120.60	127.31
9	AC	102	BCL	CAC-C3C-C2C	-4.70	102.42	114.24
9	AD	101	BCL	O2D-CGD-O1D	-4.70	114.37	123.82
9	X	102	BCL	O2D-CGD-O1D	-4.69	114.39	123.82
9	z	102	BCL	O2D-CGD-O1D	-4.68	114.40	123.82
9	3	101	BCL	O2D-CGD-O1D	-4.68	114.40	123.82
9	X	102	BCL	CAC-C3C-C2C	-4.68	102.48	114.24
15	T	101	CRT	C4-C5-C6	-4.68	117.85	124.57
15	X	101	CRT	C5-C6-C7	-4.66	118.85	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	101	BCL	O2D-CGD-O1D	-4.66	114.45	123.82
7	o	501	HEM	CAA-CBA-CGA	-4.66	104.70	112.66
9	AD	101	BCL	CAC-C3C-C2C	-4.65	102.54	114.24
9	AE	104	BCL	CAC-C3C-C2C	-4.65	102.56	114.24
9	f	101	BCL	CHD-C4C-NC	-4.64	119.92	125.08
9	s	102	BCL	CAC-C3C-C2C	-4.64	102.58	114.24
9	U	101	BCL	CAC-C3C-C2C	-4.64	102.58	114.24
9	f	101	BCL	C4B-CHC-C1C	-4.63	120.94	130.12
15	p	103	CRT	C4-C5-C6	-4.63	117.92	124.57
9	m	103	BCL	O2D-CGD-O1D	-4.62	114.52	123.82
9	AB	101	BCL	O2D-CGD-O1D	-4.62	114.53	123.82
9	L	303	BCL	CMB-C2B-C1B	-4.61	121.38	128.46
9	5	101	BCL	CAC-C3C-C2C	-4.60	102.68	114.24
15	c	101	CRT	C31-C32-C33	-4.60	120.75	127.31
9	x	301	BCL	OBB-CAB-CBB	-4.59	109.69	120.16
9	m	102	BCL	CAC-C3C-C2C	-4.58	102.72	114.24
15	T	101	CRT	C26-C27-C28	-4.58	120.78	127.31
10	M	402	BPH	O1D-CGD-CBD	-4.57	116.40	124.60
9	l	101	BCL	CAC-C3C-C2C	-4.56	102.79	114.24
9	5	101	BCL	O2D-CGD-O1D	-4.54	114.69	123.82
9	AL	102	BCL	CAC-C3C-C2C	-4.51	102.89	114.24
9	AH	101	BCL	CAC-C3C-C2C	-4.51	102.90	114.24
9	5	102	BCL	CHD-C4C-NC	-4.51	120.07	125.08
9	M	401	BCL	O2A-CGA-O1A	-4.50	112.38	123.55
15	e	101	CRT	C32-C31-C30	-4.50	109.44	123.23
9	AI	101	BCL	O2D-CGD-O1D	-4.48	114.81	123.82
9	AJ	102	BCL	C4B-CHC-C1C	-4.48	121.25	130.12
9	V	101	BCL	CAC-C3C-C2C	-4.48	102.99	114.24
9	r	101	BCL	C4B-CHC-C1C	-4.48	121.25	130.12
9	AK	101	BCL	CHB-C4A-NA	-4.47	118.33	124.51
9	u	101	BCL	O2D-CGD-O1D	-4.46	114.85	123.82
9	L	303	BCL	CAC-C3C-C4C	-4.45	102.71	112.58
9	d	101	BCL	CAC-C3C-C2C	-4.44	103.08	114.24
9	F	101	BCL	O2D-CGD-O1D	-4.44	114.89	123.82
9	I	101	BCL	CAC-C3C-C2C	-4.42	103.12	114.24
15	s	101	CRT	C4-C5-C6	-4.41	118.24	124.57
9	8	102	BCL	O2D-CGD-O1D	-4.41	114.95	123.82
9	P	101	BCL	O2D-CGD-O1D	-4.40	114.96	123.82
15	AD	102	CRT	C15-C14-C12	-4.39	121.05	127.31
9	AL	102	BCL	O2D-CGD-O1D	-4.39	114.99	123.82
9	Y	101	BCL	C4B-CHC-C1C	-4.39	121.43	130.12
9	m	102	BCL	O2D-CGD-O1D	-4.38	115.00	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	p	102	BCL	O2D-CGD-O1D	-4.38	115.02	123.82
9	AH	101	BCL	CHA-C1A-NA	-4.36	116.06	126.18
15	z	101	CRT	C21-C22-C23	-4.35	121.10	127.31
9	5	102	BCL	CHA-C1A-NA	-4.35	116.08	126.18
9	9	103	BCL	O2D-CGD-O1D	-4.33	115.11	123.82
7	o	503	HEM	CBD-CAD-C3D	-4.32	104.22	112.47
9	AE	102	BCL	CAC-C3C-C2C	-4.32	103.37	114.24
9	0	101	BCL	CAC-C3C-C2C	-4.32	103.37	114.24
9	K	101	BCL	O2D-CGD-O1D	-4.32	115.13	123.82
15	n	101	CRT	C5-C6-C7	-4.32	119.37	125.89
9	8	102	BCL	CAC-C3C-C2C	-4.31	103.40	114.24
15	p	103	CRT	C21-C22-C23	-4.31	121.16	127.31
9	h	101	BCL	CMB-C2B-C1B	-4.31	121.84	128.46
9	y	401	BCL	C3D-CAD-CBD	-4.30	101.52	107.60
15	AC	101	CRT	C31-C32-C33	-4.30	121.18	127.31
7	C	501	HEM	CAA-CBA-CGA	-4.30	105.32	112.66
9	AA	101	BCL	C4B-CHC-C1C	-4.29	121.62	130.12
15	N	101	CRT	C26-C27-C28	-4.29	121.18	127.31
15	9	102	CRT	C15-C14-C12	-4.29	121.18	127.31
14	y	403	MQ8	C11-C3-C4	-4.28	113.72	118.50
15	T	101	CRT	C31-C32-C33	-4.28	121.20	127.31
15	z	101	CRT	C37-C36-C35	-4.28	118.42	124.57
9	w	101	BCL	CAC-C3C-C2C	-4.28	103.48	114.24
9	AH	101	BCL	OBD-CAD-CBD	-4.27	119.49	125.94
9	g	101	BCL	O2D-CGD-O1D	-4.27	115.23	123.82
9	AA	101	BCL	O2D-CGD-O1D	-4.26	115.25	123.82
15	p	103	CRT	C5-C6-C7	-4.26	119.45	125.89
9	L	305	BCL	CMA-C3A-C4A	-4.26	100.33	111.77
15	k	101	CRT	C20-C19-C17	-4.24	121.25	127.31
15	8	101	CRT	C37-C36-C35	-4.24	118.48	124.57
9	Z	102	BCL	CHB-C4A-NA	-4.23	118.67	124.51
15	Z	101	CRT	C21-C20-C19	-4.22	114.46	123.46
9	r	101	BCL	CAC-C3C-C2C	-4.21	103.65	114.24
9	0	101	BCL	O2D-CGD-O1D	-4.21	115.36	123.82
15	P	102	CRT	C4-C5-C6	-4.19	118.56	124.57
9	h	101	BCL	CHA-C1A-NA	-4.18	116.48	126.18
11	x	304	UQ8	O5-C5-C6	-4.17	114.14	121.82
9	p	104	BCL	OBD-CAD-CBD	-4.17	119.64	125.94
9	r	101	BCL	O2D-CGD-O1D	-4.16	115.45	123.82
9	L	305	BCL	CAC-C3C-C2C	-4.15	103.82	114.24
9	c	102	BCL	O2D-CGD-O1D	-4.14	115.48	123.82
9	O	101	BCL	O2D-CGD-O1D	-4.14	115.49	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	101	CRT	C21-C22-C23	-4.12	121.42	127.31
9	S	102	BCL	CAC-C3C-C2C	-4.12	103.89	114.24
15	4	101	CRT	C4-C5-C6	-4.11	118.66	124.57
9	L	301	BCL	O2A-CGA-O1A	-4.10	113.37	123.55
15	p	103	CRT	C9-C10-C11	-4.10	110.65	123.23
9	W	101	BCL	OBD-CAD-CBD	-4.09	119.76	125.94
9	Q	101	BCL	CHA-C1A-NA	-4.08	116.70	126.18
9	k	102	BCL	CGD-CBD-CAD	-4.08	97.04	110.71
15	s	101	CRT	C20-C19-C17	-4.08	121.49	127.31
9	x	303	BCL	O2A-CGA-O1A	-4.08	113.42	123.55
9	T	102	BCL	CAC-C3C-C2C	-4.06	104.03	114.24
15	z	101	CRT	C31-C32-C33	-4.06	121.52	127.31
9	L	301	BCL	CMA-C3A-C4A	-4.06	100.87	111.77
9	l	101	BCL	OBB-CAB-CBB	-4.05	110.92	120.16
15	v	101	CRT	C31-C32-C33	-4.05	121.53	127.31
9	L	303	BCL	C3D-CAD-CBD	-4.05	101.88	107.60
9	R	102	BCL	O2D-CGD-O1D	-4.05	115.68	123.82
9	P	101	BCL	CHA-C1A-NA	-4.04	116.80	126.18
9	J	102	BCL	O2D-CGD-O1D	-4.04	115.69	123.82
15	J	101	CRT	C26-C27-C28	-4.03	121.56	127.31
12	M	406	PEF	O2-C10-O4	-4.03	114.79	122.94
9	s	102	BCL	OBB-CAB-CBB	-4.02	111.00	120.16
15	2	101	CRT	C21-C22-C23	-4.01	121.58	127.31
15	6	101	CRT	C32-C31-C30	-4.01	110.92	123.23
15	v	101	CRT	C21-C20-C19	-4.01	114.90	123.46
9	h	101	BCL	CHD-C4C-NC	-4.01	120.62	125.08
9	B	101	BCL	CAC-C3C-C2C	-4.00	104.17	114.24
15	e	101	CRT	C20-C19-C17	-4.00	121.60	127.31
9	AH	103	BCL	OBB-CAB-CBB	-4.00	111.04	120.16
9	k	102	BCL	CAC-C3C-C2C	-4.00	104.19	114.24
9	AH	101	BCL	OBB-CAB-CBB	-3.99	111.06	120.16
9	F	101	BCL	CAC-C3C-C2C	-3.99	104.22	114.24
9	AL	102	BCL	CHA-C1A-NA	-3.99	116.92	126.18
9	L	301	BCL	C12-C11-C10	-3.98	93.99	113.25
9	l	101	BCL	O2D-CGD-O1D	-3.98	115.81	123.82
9	W	101	BCL	O2D-CGD-O1D	-3.98	115.81	123.82
9	R	102	BCL	CAC-C3C-C2C	-3.98	104.24	114.24
9	D	101	BCL	CAC-C3C-C2C	-3.98	104.24	114.24
9	N	102	BCL	CAC-C3C-C2C	-3.97	104.25	114.24
9	x	303	BCL	CMA-C3A-C4A	-3.97	101.09	111.77
9	L	305	BCL	CMC-C2C-C1C	-3.97	101.11	111.77
15	AC	101	CRT	C21-C22-C23	-3.97	121.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	102	BCL	CAC-C3C-C2C	-3.96	104.30	114.24
9	K	101	BCL	CAC-C3C-C2C	-3.95	104.31	114.24
15	U	102	CRT	C26-C27-C28	-3.94	121.68	127.31
9	m	103	BCL	CAC-C3C-C2C	-3.94	104.33	114.24
15	n	101	CRT	C15-C14-C12	-3.94	121.68	127.31
15	A	103	CRT	C21-C22-C23	-3.94	121.68	127.31
9	m	102	BCL	OBB-CAB-CBB	-3.93	111.19	120.16
7	o	502	HEM	CAA-CBA-CGA	-3.93	105.94	112.66
15	R	101	CRT	C10-C9-C7	-3.93	121.70	127.31
9	p	102	BCL	CHA-C1A-NA	-3.93	117.05	126.18
15	G	101	CRT	C20-C19-C17	-3.93	121.71	127.31
15	R	101	CRT	C5-C6-C7	-3.92	119.96	125.89
15	e	101	CRT	C37-C36-C35	-3.92	118.94	124.57
9	I	101	BCL	C4B-CHC-C1C	-3.92	122.35	130.12
9	S	102	BCL	CHA-C1A-NA	-3.92	117.08	126.18
9	k	102	BCL	O2D-CGD-O1D	-3.92	115.94	123.82
9	M	401	BCL	CHA-C1A-NA	-3.91	117.10	126.18
9	AE	102	BCL	O2D-CGD-O1D	-3.91	115.95	123.82
9	G	102	BCL	O2D-CGD-O1D	-3.91	115.95	123.82
15	4	101	CRT	C31-C32-C33	-3.91	121.73	127.31
15	n	101	CRT	C4-C5-C6	-3.91	118.96	124.57
9	AJ	102	BCL	CAC-C3C-C2C	-3.90	104.43	114.24
9	AB	101	BCL	C4B-CHC-C1C	-3.90	122.39	130.12
15	AL	101	CRT	C37-C36-C35	-3.90	118.97	124.57
15	T	101	CRT	O1-C1-C4	-3.90	95.83	106.29
9	c	102	BCL	CAC-C3C-C2C	-3.88	104.48	114.24
9	x	305	BCL	CMB-C2B-C1B	-3.88	122.50	128.46
9	U	101	BCL	CHA-C1A-NA	-3.88	117.17	126.18
9	z	102	BCL	OBB-CAB-CBB	-3.88	111.31	120.16
9	d	101	BCL	C4B-CHC-C1C	-3.88	122.44	130.12
9	O	101	BCL	CAC-C3C-C2C	-3.88	104.49	114.24
15	N	101	CRT	C20-C19-C17	-3.87	121.78	127.31
9	U	101	BCL	OBD-CAD-CBD	-3.87	120.10	125.94
9	AI	101	BCL	C4B-CHC-C1C	-3.86	122.47	130.12
15	p	103	CRT	C26-C27-C28	-3.86	121.81	127.31
9	L	303	BCL	CHA-C1A-NA	-3.85	117.23	126.18
9	A	102	BCL	CAC-C3C-C2C	-3.85	104.55	114.24
15	6	101	CRT	C4-C5-C6	-3.85	119.04	124.57
9	x	301	BCL	C1B-CHB-C4A	-3.85	122.50	130.12
15	c	101	CRT	C4-C5-C6	-3.85	119.05	124.57
9	Z	102	BCL	CAC-C3C-C2C	-3.84	104.58	114.24
9	A	102	BCL	C4B-CHC-C1C	-3.84	122.52	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	101	CRT	C16-C17-C19	-3.83	113.06	118.94
9	5	102	BCL	OBB-CAB-CBB	-3.83	111.42	120.16
15	AC	101	CRT	C20-C19-C17	-3.83	121.84	127.31
9	K	101	BCL	CED-O2D-CGD	-3.83	107.00	115.97
9	U	101	BCL	O2A-CGA-O1A	-3.82	114.06	123.55
9	AA	101	BCL	CHA-C1A-NA	-3.81	117.33	126.18
15	c	101	CRT	C10-C9-C7	-3.81	121.87	127.31
9	L	305	BCL	C1D-CHD-C4C	-3.81	120.24	125.92
9	0	101	BCL	C4B-CHC-C1C	-3.80	122.59	130.12
9	R	102	BCL	OBB-CAB-CBB	-3.80	111.49	120.16
9	9	103	BCL	C4B-CHC-C1C	-3.79	122.60	130.12
9	W	101	BCL	CHB-C4A-NA	-3.78	119.28	124.51
9	4	102	BCL	C4B-CHC-C1C	-3.78	122.63	130.12
15	e	101	CRT	C21-C22-C23	-3.77	121.93	127.31
9	W	101	BCL	C7-C6-C5	-3.77	102.64	113.11
9	x	301	BCL	CMB-C2B-C1B	-3.77	122.68	128.46
15	y	404	CRT	C13-C12-C14	-3.77	117.65	122.92
15	AD	102	CRT	C21-C22-C23	-3.76	121.94	127.31
9	B	101	BCL	C1D-CHD-C4C	-3.76	120.31	125.92
15	U	102	CRT	C21-C22-C23	-3.76	121.94	127.31
9	O	101	BCL	C4B-CHC-C1C	-3.76	122.67	130.12
9	J	102	BCL	CAC-C3C-C2C	-3.76	104.80	114.24
9	L	303	BCL	C4B-CHC-C1C	-3.76	122.68	130.12
15	J	101	CRT	C15-C14-C12	-3.75	121.96	127.31
9	AE	102	BCL	OBB-CAB-CBB	-3.74	111.63	120.16
9	7	101	BCL	O2D-CGD-O1D	-3.73	116.31	123.82
9	N	102	BCL	OBB-CAB-CBB	-3.73	111.65	120.16
15	v	101	CRT	C9-C10-C11	-3.73	111.79	123.23
9	D	101	BCL	C16-C15-C13	-3.73	103.49	115.73
9	Q	101	BCL	OBB-CAB-CBB	-3.73	111.66	120.16
7	C	504	HEM	CAA-CBA-CGA	-3.72	106.31	112.66
9	T	102	BCL	C4B-CHC-C1C	-3.72	122.76	130.12
10	y	402	BPH	CGD-CBD-CAD	-3.71	98.28	110.71
9	r	101	BCL	CHA-C1A-NA	-3.70	117.60	126.18
7	C	503	HEM	C3B-C4B-NB	-3.69	104.44	109.21
9	1	102	BCL	CHA-C1A-NA	-3.69	117.62	126.18
15	n	101	CRT	C10-C11-C12	-3.69	116.06	126.42
9	0	101	BCL	OBB-CAB-CBB	-3.68	111.76	120.16
9	L	305	BCL	C4B-CHC-C1C	-3.68	122.83	130.12
9	L	301	BCL	CHA-C1A-NA	-3.67	117.66	126.18
15	E	101	CRT	C10-C9-C7	-3.67	122.07	127.31
9	s	102	BCL	CHA-C1A-NA	-3.67	117.66	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	y	403	MQ8	O4-C4-C3	-3.67	115.07	120.63
9	AE	104	BCL	CHA-C1A-NA	-3.67	117.66	126.18
9	L	303	BCL	C1D-CHD-C4C	-3.67	120.46	125.92
9	I	101	BCL	CHA-C1A-NA	-3.66	117.69	126.18
9	J	102	BCL	CMA-C3A-C4A	-3.65	101.96	111.77
9	j	101	BCL	OBB-CAB-CBB	-3.65	111.83	120.16
9	3	101	BCL	CMC-C2C-C3C	-3.64	98.99	113.77
9	3	101	BCL	CHD-C4C-NC	-3.64	121.03	125.08
9	D	101	BCL	C4B-CHC-C1C	-3.64	122.92	130.12
9	F	101	BCL	CMA-C3A-C4A	-3.64	102.00	111.77
9	k	102	BCL	C7-C6-C5	-3.63	103.02	113.11
9	W	101	BCL	CAC-C3C-C2C	-3.63	105.12	114.24
9	Z	102	BCL	CHA-C1A-NA	-3.63	117.76	126.18
9	Z	102	BCL	OBB-CAB-CBB	-3.62	111.90	120.16
10	M	402	BPH	C3A-C4A-NA	-3.62	106.81	113.06
15	i	101	CRT	C10-C9-C7	-3.62	122.14	127.31
9	G	102	BCL	CAC-C3C-C2C	-3.62	105.15	114.24
9	J	102	BCL	OBB-CAB-CBB	-3.61	111.93	120.16
9	AA	101	BCL	CAC-C3C-C2C	-3.61	105.17	114.24
9	AI	101	BCL	O2A-CGA-O1A	-3.61	114.59	123.55
9	F	101	BCL	OBB-CAB-CBB	-3.61	111.94	120.16
9	Y	101	BCL	OBB-CAB-CBB	-3.60	111.94	120.16
9	7	101	BCL	OBB-CAB-CBB	-3.60	111.95	120.16
15	AH	102	CRT	C21-C22-C23	-3.60	122.18	127.31
9	z	102	BCL	C4B-CHC-C1C	-3.60	123.00	130.12
15	9	102	CRT	C21-C20-C19	-3.59	115.79	123.46
15	f	102	CRT	C37-C36-C35	-3.59	119.41	124.57
9	x	305	BCL	O2D-CGD-O1D	-3.59	116.60	123.82
9	AJ	102	BCL	C1D-CHD-C4C	-3.59	120.58	125.92
9	0	101	BCL	CHA-C1A-NA	-3.59	117.85	126.18
15	E	101	CRT	C21-C20-C19	-3.59	115.81	123.46
9	i	102	BCL	C1D-CHD-C4C	-3.58	120.58	125.92
9	Y	101	BCL	OBD-CAD-CBD	-3.57	120.54	125.94
15	T	101	CRT	C21-C22-C23	-3.57	122.21	127.31
9	W	101	BCL	OBB-CAB-CBB	-3.57	112.02	120.16
9	L	305	BCL	OBB-CAB-CBB	-3.57	112.02	120.16
9	l	101	BCL	C11-C10-C8	-3.57	104.01	115.73
9	U	101	BCL	OBB-CAB-CBB	-3.57	112.02	120.16
9	AK	101	BCL	CED-O2D-CGD	-3.57	107.61	115.97
9	g	101	BCL	CHA-C1A-NA	-3.57	117.90	126.18
15	J	101	CRT	C9-C10-C11	-3.56	112.30	123.23
9	AD	101	BCL	C16-C15-C13	-3.56	104.03	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	u	101	BCL	CAC-C3C-C2C	-3.56	105.28	114.24
9	AI	101	BCL	OBB-CAB-CBB	-3.56	112.03	120.16
9	g	101	BCL	C4B-CHC-C1C	-3.56	123.07	130.12
9	5	101	BCL	OBB-CAB-CBB	-3.56	112.04	120.16
12	A	101	PEF	C2-O2-C10	-3.56	111.06	117.94
9	AI	101	BCL	CAC-C3C-C2C	-3.55	105.31	114.24
9	V	101	BCL	C16-C15-C13	-3.55	104.07	115.73
9	e	102	BCL	CHA-C1A-NA	-3.55	117.93	126.18
15	AD	102	CRT	C10-C9-C7	-3.55	122.24	127.31
9	S	102	BCL	C4B-CHC-C1C	-3.54	123.10	130.12
9	L	303	BCL	O2D-CGD-O1D	-3.54	116.69	123.82
9	B	101	BCL	CHA-C1A-NA	-3.54	117.96	126.18
9	W	101	BCL	CHA-C1A-NA	-3.54	117.97	126.18
9	h	101	BCL	C4B-CHC-C1C	-3.53	123.12	130.12
9	y	401	BCL	O2A-CGA-O1A	-3.53	114.78	123.55
7	C	503	HEM	CAA-CBA-CGA	-3.53	106.63	112.66
9	u	101	BCL	CMC-C2C-C3C	-3.53	99.45	113.77
15	4	101	CRT	C25-C23-C22	-3.52	113.54	118.94
9	G	102	BCL	C4B-CHC-C1C	-3.52	123.15	130.12
9	AL	102	BCL	CHB-C4A-NA	-3.52	119.65	124.51
9	r	101	BCL	CHD-C4C-NC	-3.51	121.17	125.08
15	2	101	CRT	C37-C36-C35	-3.51	119.53	124.57
9	K	101	BCL	C16-C15-C13	-3.51	104.21	115.73
9	v	102	BCL	OBB-CAB-CBB	-3.51	112.16	120.16
9	K	101	BCL	CMA-C3A-C4A	-3.51	102.34	111.77
9	AD	101	BCL	CHA-C1A-NA	-3.51	118.03	126.18
9	e	102	BCL	OBB-CAB-CBB	-3.51	112.16	120.16
9	R	102	BCL	C4B-CHC-C1C	-3.51	123.17	130.12
9	x	301	BCL	CHA-C1A-NA	-3.51	118.04	126.18
9	M	401	BCL	C4B-CHC-C1C	-3.50	123.18	130.12
9	z	102	BCL	C1D-CHD-C4C	-3.50	120.70	125.92
15	y	404	CRT	C20-C19-C17	-3.50	122.32	127.31
12	t	303	PEF	O2-C10-O4	-3.49	115.86	122.94
9	p	102	BCL	C4B-CHC-C1C	-3.49	123.20	130.12
9	L	305	BCL	C7-C6-C5	-3.49	103.40	113.11
9	A	102	BCL	OBB-CAB-CBB	-3.49	112.21	120.16
9	p	104	BCL	CHA-C1A-NA	-3.48	118.09	126.18
9	5	101	BCL	CHA-C1A-NA	-3.48	118.09	126.18
9	5	102	BCL	C16-C15-C13	-3.48	104.31	115.73
15	n	101	CRT	C13-C12-C14	-3.48	118.05	122.92
9	9	103	BCL	C11-C10-C8	-3.48	104.31	115.73
9	x	305	BCL	C1D-CHD-C4C	-3.48	120.73	125.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	m	103	BCL	OBB-CAB-CBB	-3.48	112.23	120.16
15	T	101	CRT	C10-C9-C7	-3.48	122.35	127.31
9	N	102	BCL	C7-C6-C5	-3.47	103.45	113.11
9	I	101	BCL	C1D-CHD-C4C	-3.47	120.75	125.92
9	u	101	BCL	CMA-C3A-C4A	-3.47	102.45	111.77
9	O	101	BCL	C11-C10-C8	-3.47	104.35	115.73
9	v	102	BCL	C11-C10-C8	-3.47	104.36	115.73
9	m	102	BCL	OBD-CAD-CBD	-3.46	120.72	125.94
15	U	102	CRT	C9-C10-C11	-3.46	112.62	123.23
11	L	304	UQ8	C27-C28-C29	-3.45	119.01	127.68
9	7	101	BCL	C4B-CHC-C1C	-3.45	123.28	130.12
15	6	101	CRT	C35-C33-C32	-3.45	113.65	118.94
9	k	102	BCL	C4B-CHC-C1C	-3.44	123.30	130.12
9	AK	101	BCL	CMC-C2C-C3C	-3.44	99.80	113.77
15	e	101	CRT	C4-C5-C6	-3.44	119.63	124.57
9	8	102	BCL	OBB-CAB-CBB	-3.44	112.32	120.16
9	p	104	BCL	CGD-CBD-CAD	-3.44	99.19	110.71
9	k	102	BCL	OBB-CAB-CBB	-3.44	112.32	120.16
15	J	101	CRT	C20-C19-C17	-3.44	122.41	127.31
15	2	101	CRT	C14-C15-C16	-3.43	112.70	123.23
9	v	102	BCL	CAC-C3C-C2C	-3.43	105.61	114.24
9	AE	102	BCL	C7-C6-C5	-3.43	103.58	113.11
9	4	102	BCL	CHD-C4C-NC	-3.43	121.27	125.08
9	y	401	BCL	C3C-C4C-CHD	-3.43	116.13	123.34
9	D	101	BCL	CED-O2D-CGD	-3.42	107.94	115.97
15	6	101	CRT	C21-C22-C23	-3.42	122.42	127.31
9	K	101	BCL	OBB-CAB-CBB	-3.42	112.36	120.16
9	x	301	BCL	C12-C11-C10	-3.42	96.72	113.25
9	AL	102	BCL	C16-C15-C13	-3.42	104.51	115.73
9	4	102	BCL	CHA-C1A-NA	-3.42	118.25	126.18
9	AC	102	BCL	C4B-CHC-C1C	-3.42	123.35	130.12
9	AJ	102	BCL	C3C-C4C-CHD	-3.42	116.15	123.34
9	k	102	BCL	CHA-C1A-NA	-3.42	118.25	126.18
9	AB	101	BCL	CHA-C1A-NA	-3.41	118.25	126.18
9	AL	102	BCL	OBB-CAB-CBB	-3.41	112.38	120.16
9	x	303	BCL	C1D-CHD-C4C	-3.41	120.84	125.92
9	8	102	BCL	C1D-CHD-C4C	-3.41	120.84	125.92
9	I	101	BCL	O2D-CGD-O1D	-3.40	116.97	123.82
15	AD	102	CRT	C10-C11-C12	-3.40	116.86	126.42
9	X	102	BCL	CMA-C3A-C4A	-3.40	102.65	111.77
9	e	102	BCL	CAC-C3C-C2C	-3.38	105.75	114.24
14	M	403	MQ8	C35-C33-C32	-3.38	114.19	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	303	BCL	CHD-C4C-NC	-3.38	121.32	125.08
14	y	403	MQ8	C26-C27-C28	-3.38	119.19	127.68
9	j	101	BCL	CAC-C3C-C2C	-3.38	105.75	114.24
9	P	101	BCL	CHB-C4A-NA	-3.37	119.85	124.51
9	g	101	BCL	CAC-C3C-C2C	-3.37	105.76	114.24
7	o	502	HEM	CAD-CBD-CGD	-3.37	106.90	112.66
15	AL	101	CRT	C21-C20-C19	-3.37	116.27	123.46
15	U	102	CRT	C35-C33-C32	-3.37	113.78	118.94
9	D	101	BCL	CHA-C1A-NA	-3.36	118.37	126.18
9	l	101	BCL	C4B-CHC-C1C	-3.36	123.46	130.12
9	x	305	BCL	CHA-C1A-NA	-3.36	118.38	126.18
9	L	305	BCL	C11-C10-C8	-3.36	104.70	115.73
9	c	102	BCL	C4B-CHC-C1C	-3.36	123.47	130.12
10	L	302	BPH	C3A-C4A-NA	-3.36	107.27	113.06
9	i	102	BCL	CHA-C1A-NA	-3.35	118.40	126.18
9	c	102	BCL	C16-C15-C13	-3.35	104.74	115.73
9	M	401	BCL	C12-C11-C10	-3.35	97.07	113.25
9	N	102	BCL	C16-C15-C13	-3.33	104.79	115.73
9	w	101	BCL	CHA-C1A-NA	-3.33	118.44	126.18
15	G	101	CRT	C4-C5-C6	-3.33	119.78	124.57
9	e	102	BCL	C11-C12-C13	-3.33	104.79	115.73
9	x	303	BCL	CHA-C1A-NA	-3.33	118.45	126.18
15	2	101	CRT	C20-C19-C17	-3.33	122.56	127.31
15	k	101	CRT	C26-C25-C23	-3.33	117.07	126.42
9	c	102	BCL	OBB-CAB-CBB	-3.33	112.57	120.16
9	P	101	BCL	C4B-CHC-C1C	-3.33	123.53	130.12
15	Z	101	CRT	C4-C5-C6	-3.33	119.79	124.57
9	AK	101	BCL	CHA-C1A-NA	-3.32	118.46	126.18
9	D	102	BCL	C1D-CHD-C4C	-3.32	120.97	125.92
9	M	401	BCL	C16-C15-C13	-3.32	104.83	115.73
9	G	102	BCL	C2C-C3C-C4C	-3.32	96.37	101.34
9	D	102	BCL	CHA-C1A-NA	-3.31	118.49	126.18
9	B	101	BCL	O2D-CGD-O1D	-3.31	117.16	123.82
9	z	102	BCL	C16-C15-C13	-3.31	104.87	115.73
9	Y	101	BCL	CHA-C1A-NA	-3.31	118.50	126.18
9	m	103	BCL	CHA-C1A-NA	-3.30	118.50	126.18
9	l	101	BCL	C4B-CHC-C1C	-3.30	123.58	130.12
15	c	101	CRT	C27-C26-C25	-3.30	113.11	123.23
15	6	101	CRT	C21-C20-C19	-3.30	116.42	123.46
9	O	101	BCL	CHA-C1A-NA	-3.30	118.53	126.18
15	AL	101	CRT	C32-C31-C30	-3.29	113.13	123.23
9	AL	102	BCL	C1-C2-C3	-3.29	119.89	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	102	BCL	OBB-CAB-CBB	-3.29	112.65	120.16
7	C	502	HEM	CAA-CBA-CGA	-3.29	107.04	112.66
9	y	401	BCL	CMC-C2C-C3C	-3.29	100.42	113.77
9	K	101	BCL	CHA-C1A-NA	-3.29	118.55	126.18
9	V	101	BCL	CHA-C1A-NA	-3.28	118.56	126.18
9	AD	101	BCL	C4B-CHC-C1C	-3.28	123.62	130.12
9	V	101	BCL	OBB-CAB-CBB	-3.28	112.68	120.16
15	n	101	CRT	C20-C19-C17	-3.28	122.63	127.31
9	w	101	BCL	C4B-CHC-C1C	-3.28	123.62	130.12
9	D	101	BCL	O2A-CGA-O1A	-3.28	115.41	123.55
15	c	101	CRT	C14-C15-C16	-3.28	113.19	123.23
15	9	102	CRT	C10-C11-C12	-3.27	117.22	126.42
9	AA	101	BCL	OBD-CAD-CBD	-3.27	121.00	125.94
9	K	101	BCL	O2A-CGA-O1A	-3.27	115.43	123.55
9	y	401	BCL	CHA-C1A-NA	-3.27	118.58	126.18
9	i	102	BCL	OBB-CAB-CBB	-3.27	112.71	120.16
9	AI	101	BCL	OBD-CAD-CBD	-3.26	121.01	125.94
9	m	102	BCL	C4B-CHC-C1C	-3.26	123.66	130.12
9	5	101	BCL	O2A-CGA-O1A	-3.26	115.46	123.55
9	1	101	BCL	OBB-CAB-CBB	-3.26	112.74	120.16
9	R	102	BCL	C11-C10-C8	-3.26	105.05	115.73
15	Z	101	CRT	C16-C17-C19	-3.25	113.95	118.94
9	y	401	BCL	C11-C10-C8	-3.25	105.07	115.73
15	s	101	CRT	C21-C22-C23	-3.25	122.67	127.31
9	O	101	BCL	C3C-C4C-CHD	-3.25	116.51	123.34
9	p	104	BCL	CMA-C3A-C4A	-3.25	103.05	111.77
15	AJ	101	CRT	C20-C21-C22	-3.24	116.54	123.46
11	x	304	UQ8	C32-C33-C34	-3.24	119.53	127.68
9	L	303	BCL	CGD-CBD-CAD	-3.24	99.85	110.71
9	s	102	BCL	C1D-CHD-C4C	-3.24	121.09	125.92
9	d	101	BCL	CHA-C1A-NA	-3.24	118.66	126.18
14	M	403	MQ8	C26-C27-C28	-3.24	119.55	127.68
9	8	102	BCL	CMA-C3A-C4A	-3.24	103.08	111.77
9	8	102	BCL	C16-C15-C13	-3.23	105.13	115.73
9	AE	104	BCL	C4B-CHC-C1C	-3.23	123.72	130.12
9	G	102	BCL	CHA-C1A-NA	-3.23	118.68	126.18
9	X	102	BCL	CHA-C1A-NA	-3.23	118.69	126.18
9	D	102	BCL	OBB-CAB-CBB	-3.22	112.81	120.16
9	V	101	BCL	C2C-C3C-C4C	-3.22	96.52	101.34
9	A	102	BCL	C1D-CHD-C4C	-3.22	121.12	125.92
9	P	101	BCL	OBB-CAB-CBB	-3.22	112.82	120.16
9	m	102	BCL	CHA-C1A-NA	-3.21	118.72	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	403	MQ8	C20-C18-C17	-3.21	114.54	121.10
9	k	102	BCL	CHB-C4A-NA	-3.21	120.08	124.51
11	x	304	UQ8	C40-C39-C38	-3.20	115.14	123.69
9	5	101	BCL	CHB-C4A-NA	-3.20	120.08	124.51
9	V	101	BCL	OBD-CAD-CBD	-3.20	121.11	125.94
9	X	102	BCL	C4B-CHC-C1C	-3.19	123.79	130.12
15	A	103	CRT	C21-C20-C19	-3.19	116.65	123.46
9	m	103	BCL	CHB-C4A-NA	-3.19	120.10	124.51
9	u	101	BCL	C4B-CHC-C1C	-3.19	123.81	130.12
9	T	102	BCL	C7-C6-C5	-3.19	104.26	113.11
9	p	102	BCL	O2A-CGA-O1A	-3.18	115.64	123.55
9	c	102	BCL	CHA-C1A-NA	-3.18	118.79	126.18
9	AK	101	BCL	C1D-CHD-C4C	-3.18	121.18	125.92
9	AB	101	BCL	CMC-C2C-C3C	-3.18	100.86	113.77
15	z	101	CRT	C21-C20-C19	-3.18	116.67	123.46
9	S	102	BCL	CMA-C3A-C4A	-3.18	103.24	111.77
9	P	101	BCL	C2C-C3C-C4C	-3.17	96.58	101.34
9	j	101	BCL	CHA-C1A-NA	-3.17	118.81	126.18
9	P	101	BCL	O2A-CGA-O1A	-3.17	115.69	123.55
9	U	101	BCL	C1D-CHD-C4C	-3.16	121.20	125.92
9	r	101	BCL	O2A-CGA-O1A	-3.16	115.70	123.55
9	p	104	BCL	O2A-CGA-O1A	-3.16	115.70	123.55
9	T	102	BCL	C2C-C3C-C4C	-3.16	96.60	101.34
9	9	103	BCL	CHA-C1A-NA	-3.16	118.84	126.18
15	J	101	CRT	C21-C20-C19	-3.16	116.72	123.46
12	t	301	PEF	O4P-C4-C5	-3.16	97.28	109.10
9	X	102	BCL	C1D-CHD-C4C	-3.16	121.22	125.92
9	v	102	BCL	CHA-C1A-NA	-3.16	118.85	126.18
15	P	102	CRT	C32-C31-C30	-3.16	113.55	123.23
9	X	102	BCL	OBB-CAB-CBB	-3.15	112.97	120.16
9	d	101	BCL	OBB-CAB-CBB	-3.15	112.97	120.16
9	l	101	BCL	OBD-CAD-CBD	-3.15	121.18	125.94
9	AE	102	BCL	OBD-CAD-CBD	-3.15	121.18	125.94
15	A	103	CRT	C10-C9-C7	-3.15	122.81	127.31
9	M	401	BCL	C6-C5-C3	-3.15	105.52	112.66
9	l	101	BCL	CAA-CBA-CGA	-3.15	103.86	113.35
9	Q	101	BCL	CED-O2D-CGD	-3.15	108.59	115.97
9	L	303	BCL	C3C-C4C-CHD	-3.15	116.72	123.34
9	Q	101	BCL	C16-C15-C13	-3.15	105.40	115.73
9	AE	104	BCL	CMC-C2C-C3C	-3.15	101.00	113.77
9	x	301	BCL	CAA-CBA-CGA	-3.15	103.87	113.35
9	x	305	BCL	C7-C6-C5	-3.14	104.37	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	101	BCL	C4B-CHC-C1C	-3.14	123.90	130.12
9	K	101	BCL	C11-C10-C8	-3.13	105.45	115.73
9	7	101	BCL	CAC-C3C-C2C	-3.13	106.37	114.24
15	2	101	CRT	C26-C27-C28	-3.13	122.84	127.31
9	T	102	BCL	CHA-C1A-NA	-3.13	118.91	126.18
9	AI	101	BCL	CHA-C1A-NA	-3.13	118.91	126.18
9	AE	102	BCL	C4B-CHC-C1C	-3.13	123.92	130.12
9	AI	101	BCL	C1D-CHD-C4C	-3.13	121.26	125.92
15	k	101	CRT	C15-C14-C12	-3.13	122.85	127.31
9	r	101	BCL	OBB-CAB-CBB	-3.13	113.03	120.16
9	AJ	102	BCL	OBB-CAB-CBB	-3.12	113.03	120.16
9	D	101	BCL	C3C-C4C-CHD	-3.12	116.77	123.34
14	y	403	MQ8	C15-C13-C12	-3.12	114.71	121.10
15	f	102	CRT	C14-C15-C16	-3.12	113.65	123.23
9	AE	102	BCL	CHA-C1A-NA	-3.12	118.93	126.18
9	u	101	BCL	OBB-CAB-CBB	-3.12	113.05	120.16
9	f	101	BCL	CHA-C1A-NA	-3.12	118.94	126.18
9	e	102	BCL	C16-C15-C13	-3.12	105.49	115.73
9	N	102	BCL	C4B-CHC-C1C	-3.12	123.94	130.12
9	z	102	BCL	CHA-C1A-NA	-3.12	118.94	126.18
9	O	101	BCL	CHD-C4C-NC	-3.11	121.62	125.08
9	AH	103	BCL	OBD-CAD-CBD	-3.11	121.24	125.94
15	AL	101	CRT	C26-C27-C28	-3.11	122.87	127.31
9	AA	101	BCL	OBB-CAB-CBB	-3.11	113.06	120.16
15	i	101	CRT	C21-C22-C23	-3.11	122.87	127.31
9	D	102	BCL	OBD-CAD-CBD	-3.11	121.24	125.94
9	AE	104	BCL	OBB-CAB-CBB	-3.11	113.07	120.16
9	8	102	BCL	CGD-CBD-CAD	-3.11	100.30	110.71
9	Q	101	BCL	CAC-C3C-C2C	-3.11	106.43	114.24
15	Z	101	CRT	C25-C23-C22	-3.10	114.18	118.94
9	9	103	BCL	C7-C6-C5	-3.10	104.49	113.11
9	N	102	BCL	CHA-C1A-NA	-3.10	118.98	126.18
9	3	101	BCL	CHA-C1A-NA	-3.10	118.98	126.18
9	D	102	BCL	C16-C15-C13	-3.10	105.56	115.73
9	w	101	BCL	CED-O2D-CGD	-3.10	108.71	115.97
9	I	101	BCL	OBD-CAD-CBD	-3.10	121.27	125.94
15	A	103	CRT	C31-C32-C33	-3.09	122.89	127.31
9	AH	103	BCL	CHA-C1A-NA	-3.09	119.00	126.18
9	l	101	BCL	CMC-C2C-C3C	-3.09	101.23	113.77
9	l	101	BCL	O2A-CGA-O1A	-3.09	115.88	123.55
9	A	102	BCL	CHA-C1A-NA	-3.09	119.01	126.18
9	T	102	BCL	CMC-C2C-C3C	-3.09	101.24	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	102	BCL	C11-C12-C13	-3.09	105.60	115.73
9	AJ	102	BCL	CHA-C1A-NA	-3.09	119.01	126.18
9	w	101	BCL	OBB-CAB-CBB	-3.09	113.12	120.16
15	X	101	CRT	C37-C36-C35	-3.08	120.14	124.57
9	AA	101	BCL	C1D-CHD-C4C	-3.08	121.33	125.92
9	AD	101	BCL	OBB-CAB-CBB	-3.08	113.14	120.16
9	u	101	BCL	OBD-CAD-CBD	-3.08	121.29	125.94
15	U	102	CRT	C24-C23-C22	-3.08	118.61	122.92
9	AH	103	BCL	CED-O2D-CGD	-3.07	108.76	115.97
9	h	101	BCL	O2A-CGA-O1A	-3.07	115.92	123.55
12	H	301	PEF	C3-C2-C1	-3.07	104.92	111.86
9	AA	101	BCL	O2A-CGA-O1A	-3.07	115.93	123.55
9	A	102	BCL	CMC-C2C-C3C	-3.07	101.31	113.77
9	y	401	BCL	CMA-C3A-C4A	-3.07	103.52	111.77
15	p	103	CRT	C20-C19-C17	-3.07	122.93	127.31
9	c	102	BCL	C7-C6-C5	-3.07	104.58	113.11
9	e	102	BCL	C1D-CHD-C4C	-3.06	121.35	125.92
9	AH	101	BCL	O2A-CGA-O1A	-3.06	115.94	123.55
9	l	101	BCL	C16-C15-C13	-3.06	105.68	115.73
9	p	102	BCL	C16-C15-C13	-3.06	105.68	115.73
9	AB	101	BCL	C1-C2-C3	-3.06	120.32	125.96
9	8	102	BCL	C4B-CHC-C1C	-3.06	124.06	130.12
15	P	102	CRT	C31-C32-C33	-3.06	122.95	127.31
9	v	102	BCL	CHB-C4A-NA	-3.06	120.28	124.51
15	AJ	101	CRT	C26-C27-C28	-3.06	122.95	127.31
9	AD	101	BCL	C1D-CHD-C4C	-3.06	121.37	125.92
9	4	102	BCL	C16-C15-C13	-3.06	105.70	115.73
9	AK	101	BCL	CGD-CBD-CAD	-3.06	100.47	110.71
9	u	101	BCL	CHD-C4C-NC	-3.05	121.68	125.08
9	x	305	BCL	C12-C11-C10	-3.05	98.49	113.25
9	T	102	BCL	OBD-CAD-CBD	-3.05	121.33	125.94
11	x	304	UQ8	C26-C24-C23	-3.05	114.87	121.10
10	x	302	BPH	CMC-C2C-C1C	-3.04	103.58	112.09
9	9	103	BCL	CMC-C2C-C3C	-3.04	101.43	113.77
9	4	102	BCL	OBD-CAD-CBD	-3.04	121.35	125.94
9	O	101	BCL	CMA-C3A-C4A	-3.04	103.61	111.77
9	AH	101	BCL	C4B-CHC-C1C	-3.04	124.10	130.12
9	1	102	BCL	C4B-CHC-C1C	-3.04	124.10	130.12
9	AH	103	BCL	C16-C15-C13	-3.04	105.77	115.73
9	W	101	BCL	O2A-CGA-O1A	-3.03	116.02	123.55
9	0	101	BCL	OBD-CAD-CBD	-3.03	121.36	125.94
7	o	503	HEM	CMA-C3A-C4A	-3.03	123.81	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	102	BCL	CMC-C2C-C3C	-3.03	101.48	113.77
9	F	101	BCL	C4B-CHC-C1C	-3.03	124.12	130.12
15	M	404	CRT	C15-C14-C12	-3.03	122.99	127.31
15	z	101	CRT	C9-C10-C11	-3.03	113.95	123.23
9	O	101	BCL	O2A-CGA-O1A	-3.02	116.04	123.55
9	4	102	BCL	OBB-CAB-CBB	-3.02	113.26	120.16
9	S	102	BCL	OBB-CAB-CBB	-3.02	113.27	120.16
9	L	305	BCL	O2A-CGA-O1A	-3.02	116.05	123.55
9	X	102	BCL	O2A-CGA-O1A	-3.02	116.05	123.55
9	V	101	BCL	C4B-CHC-C1C	-3.02	124.14	130.12
10	x	302	BPH	C2A-C1A-NA	-3.02	108.24	111.91
15	E	101	CRT	C4-C5-C6	-3.02	120.24	124.57
9	AK	101	BCL	OBB-CAB-CBB	-3.02	113.28	120.16
9	AB	101	BCL	OBB-CAB-CBB	-3.01	113.29	120.16
9	0	101	BCL	CMC-C2C-C3C	-3.01	101.55	113.77
15	U	102	CRT	C6-C7-C9	-3.01	114.32	118.94
9	5	102	BCL	C1D-CHD-C4C	-3.01	121.44	125.92
9	P	101	BCL	CMA-C3A-C4A	-3.01	103.69	111.77
9	Y	101	BCL	CHB-C4A-NA	-3.00	120.36	124.51
9	Q	101	BCL	C4B-CHC-C1C	-3.00	124.17	130.12
9	AE	104	BCL	C7-C6-C5	-3.00	104.77	113.11
9	I	101	BCL	O2A-CGA-O1A	-3.00	116.11	123.55
9	z	102	BCL	C11-C10-C8	-2.99	105.90	115.73
15	X	101	CRT	C15-C14-C12	-2.99	123.04	127.31
15	AD	102	CRT	C21-C20-C19	-2.99	117.09	123.46
15	P	102	CRT	C14-C15-C16	-2.98	114.08	123.23
9	L	305	BCL	C6-C5-C3	-2.98	105.91	112.66
15	6	101	CRT	C14-C15-C16	-2.98	114.10	123.23
9	J	102	BCL	CHA-C1A-NA	-2.97	119.29	126.18
9	L	301	BCL	O2D-CGD-O1D	-2.97	117.85	123.82
10	x	302	BPH	C3A-C4A-NA	-2.97	107.95	113.06
9	g	101	BCL	C1D-CHD-C4C	-2.96	121.50	125.92
15	4	101	CRT	C27-C26-C25	-2.96	114.14	123.23
9	h	101	BCL	OBD-CAD-CBD	-2.96	121.47	125.94
15	k	101	CRT	C32-C31-C30	-2.96	114.14	123.23
9	F	101	BCL	C1D-CHD-C4C	-2.96	121.51	125.92
9	m	103	BCL	C11-C10-C8	-2.96	106.02	115.73
9	X	102	BCL	OBD-CAD-CBD	-2.96	121.47	125.94
9	h	101	BCL	CHB-C4A-NA	-2.96	120.42	124.51
9	I	101	BCL	CMA-C3A-C4A	-2.96	103.83	111.77
9	3	101	BCL	CHB-C4A-NA	-2.96	120.42	124.51
15	8	101	CRT	C24-C23-C22	-2.96	118.78	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	9	103	BCL	OBB-CAB-CBB	-2.95	113.42	120.16
11	x	304	UQ8	C37-C38-C39	-2.95	120.26	127.68
9	p	102	BCL	C7-C6-C5	-2.95	104.90	113.11
9	1	102	BCL	C16-C15-C13	-2.95	106.04	115.73
9	B	101	BCL	OBB-CAB-CBB	-2.95	113.43	120.16
9	D	101	BCL	C7-C6-C5	-2.95	104.91	113.11
7	C	501	HEM	CMD-C2D-C1D	-2.95	123.93	128.46
9	AH	103	BCL	CMC-C2C-C3C	-2.94	101.82	113.77
15	N	101	CRT	C32-C31-C30	-2.94	114.20	123.23
15	6	101	CRT	C10-C9-C7	-2.94	123.11	127.31
15	AE	103	CRT	C20-C19-C17	-2.94	123.11	127.31
9	x	305	BCL	CMC-C2C-C1C	-2.94	103.88	111.77
9	O	101	BCL	C7-C6-C5	-2.94	104.95	113.11
9	O	101	BCL	OBB-CAB-CBB	-2.93	113.47	120.16
15	N	101	CRT	C15-C14-C12	-2.93	123.12	127.31
9	v	102	BCL	C7-C6-C5	-2.93	104.96	113.11
9	I	101	BCL	CMC-C2C-C3C	-2.93	101.88	113.77
9	x	305	BCL	C16-C15-C13	-2.93	106.11	115.73
9	K	101	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
9	v	102	BCL	C1B-CHB-C4A	-2.93	124.31	130.12
9	AC	102	BCL	C16-C15-C13	-2.93	106.12	115.73
15	i	101	CRT	C14-C15-C16	-2.93	114.25	123.23
9	h	101	BCL	OBB-CAB-CBB	-2.93	113.48	120.16
9	l	101	BCL	CHA-C1A-NA	-2.93	119.38	126.18
9	p	102	BCL	OBB-CAB-CBB	-2.93	113.48	120.16
9	x	305	BCL	OBB-CAB-CBB	-2.93	113.49	120.16
9	x	303	BCL	CGD-CBD-CAD	-2.92	100.91	110.71
9	P	101	BCL	CAC-C3C-C2C	-2.92	106.89	114.24
9	W	101	BCL	CGD-CBD-CAD	-2.92	100.92	110.71
9	M	401	BCL	C1-C2-C3	-2.92	120.57	125.96
9	5	101	BCL	CMC-C2C-C3C	-2.92	101.92	113.77
9	p	102	BCL	C1D-CHD-C4C	-2.92	121.57	125.92
9	O	101	BCL	CMC-C2C-C3C	-2.92	101.92	113.77
9	AH	103	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
9	Z	102	BCL	CMC-C2C-C3C	-2.91	101.95	113.77
9	G	102	BCL	CGD-CBD-CAD	-2.91	100.96	110.71
9	g	101	BCL	CGD-CBD-CAD	-2.91	100.97	110.71
9	u	101	BCL	CHA-C1A-NA	-2.91	119.43	126.18
9	m	102	BCL	O2A-CGA-O1A	-2.91	116.33	123.55
9	J	102	BCL	C11-C10-C8	-2.91	106.19	115.73
9	Z	102	BCL	C4B-CHC-C1C	-2.90	124.37	130.12
15	9	102	CRT	C20-C19-C17	-2.90	123.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	101	CRT	C21-C20-C19	-2.90	117.27	123.46
9	k	102	BCL	C16-C15-C13	-2.90	106.21	115.73
15	y	404	CRT	C15-C14-C12	-2.90	123.17	127.31
9	k	102	BCL	OBD-CAD-CBD	-2.90	121.56	125.94
9	p	104	BCL	C4B-CHC-C1C	-2.90	124.38	130.12
9	U	101	BCL	C16-C15-C13	-2.89	106.23	115.73
9	D	101	BCL	CHD-C4C-NC	-2.89	121.86	125.08
9	AK	101	BCL	O2A-CGA-O1A	-2.89	116.37	123.55
9	I	101	BCL	C11-C10-C8	-2.89	106.24	115.73
9	j	101	BCL	C4B-CHC-C1C	-2.89	124.39	130.12
15	f	102	CRT	C8-C7-C9	-2.89	118.87	122.92
9	l	101	BCL	CMA-C3A-C4A	-2.89	104.00	111.77
15	y	404	CRT	C21-C22-C23	-2.89	123.19	127.31
9	m	102	BCL	CMC-C2C-C3C	-2.89	102.04	113.77
9	g	101	BCL	C3C-C4C-CHD	-2.89	117.27	123.34
9	X	102	BCL	C16-C15-C13	-2.89	106.25	115.73
9	AE	104	BCL	C3C-C4C-CHD	-2.89	117.27	123.34
9	U	101	BCL	C7-C6-C5	-2.88	105.09	113.11
9	AH	101	BCL	CED-O2D-CGD	-2.88	109.21	115.97
9	D	101	BCL	OBD-CAD-CBD	-2.88	121.59	125.94
9	5	101	BCL	C11-C12-C13	-2.88	106.27	115.73
15	X	101	CRT	C20-C21-C22	-2.88	117.31	123.46
9	w	101	BCL	CMC-C2C-C3C	-2.88	102.08	113.77
15	AJ	101	CRT	C4-C5-C6	-2.88	120.43	124.57
9	0	101	BCL	C1D-CHD-C4C	-2.88	121.63	125.92
9	AC	102	BCL	CHA-C1A-NA	-2.88	119.50	126.18
9	4	102	BCL	C7-C6-C5	-2.88	105.11	113.11
9	AJ	102	BCL	CMC-C2C-C3C	-2.88	102.11	113.77
10	L	302	BPH	C2A-C1A-NA	-2.87	108.41	111.91
9	M	401	BCL	OBB-CAB-CBB	-2.87	113.61	120.16
9	4	102	BCL	O2A-CGA-O1A	-2.87	116.42	123.55
15	AL	101	CRT	C14-C15-C16	-2.87	114.42	123.23
15	s	101	CRT	C31-C32-C33	-2.87	123.21	127.31
7	C	504	HEM	CMD-C2D-C1D	-2.87	124.06	128.46
9	k	102	BCL	C1D-CHD-C4C	-2.87	121.65	125.92
15	z	101	CRT	C27-C26-C25	-2.87	114.44	123.23
15	v	101	CRT	C20-C19-C17	-2.86	123.22	127.31
9	I	101	BCL	OBB-CAB-CBB	-2.86	113.63	120.16
9	z	102	BCL	C3C-C4C-CHD	-2.86	117.33	123.34
9	M	401	BCL	CGD-CBD-CAD	-2.86	101.13	110.71
9	AA	101	BCL	C7-C6-C5	-2.86	105.17	113.11
9	8	102	BCL	CMC-C2C-C3C	-2.86	102.18	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AC	102	BCL	CMC-C2C-C3C	-2.86	102.18	113.77
9	5	101	BCL	C3C-C4C-CHD	-2.86	117.33	123.34
9	8	102	BCL	C7-C6-C5	-2.85	105.19	113.11
9	0	101	BCL	CMA-C3A-C4A	-2.85	104.12	111.77
9	Z	102	BCL	C16-C15-C13	-2.84	106.40	115.73
9	AC	102	BCL	OBB-CAB-CBB	-2.84	113.68	120.16
9	Y	101	BCL	O2A-CGA-O1A	-2.84	116.51	123.55
15	v	101	CRT	C15-C14-C12	-2.83	123.26	127.31
9	AH	103	BCL	C1D-CHD-C4C	-2.83	121.70	125.92
9	p	104	BCL	CHB-C4A-NA	-2.83	120.60	124.51
15	2	101	CRT	C10-C9-C7	-2.83	123.27	127.31
15	A	103	CRT	C4-C5-C6	-2.83	120.51	124.57
15	AC	101	CRT	C27-C26-C25	-2.83	114.56	123.23
9	V	101	BCL	CMC-C2C-C3C	-2.82	102.31	113.77
9	S	102	BCL	O2A-CGA-O1A	-2.82	116.55	123.55
9	F	101	BCL	CHA-C1A-NA	-2.82	119.63	126.18
15	y	404	CRT	C14-C15-C16	-2.82	114.58	123.23
9	0	101	BCL	C2C-C3C-C4C	-2.82	97.12	101.34
15	AE	103	CRT	C14-C15-C16	-2.82	114.60	123.23
9	7	101	BCL	CHA-C1A-NA	-2.81	119.64	126.18
15	M	404	CRT	C36-C35-C33	-2.81	121.64	125.89
15	y	404	CRT	C29-C28-C27	-2.81	118.99	122.92
9	D	102	BCL	C11-C12-C13	-2.81	106.52	115.73
15	P	102	CRT	C26-C25-C23	-2.81	118.53	126.42
9	3	101	BCL	OBB-CAB-CBB	-2.81	113.76	120.16
9	h	101	BCL	CMC-C2C-C3C	-2.80	102.39	113.77
15	A	103	CRT	C26-C27-C28	-2.80	123.31	127.31
9	p	104	BCL	OBB-CAB-CBB	-2.80	113.77	120.16
9	G	102	BCL	OBD-CAD-CBD	-2.80	121.71	125.94
9	G	102	BCL	C1D-CHD-C4C	-2.80	121.75	125.92
15	T	101	CRT	C21-C20-C19	-2.80	117.49	123.46
9	m	103	BCL	C4B-CHC-C1C	-2.80	124.58	130.12
9	r	101	BCL	CHB-C4A-NA	-2.80	120.64	124.51
9	V	101	BCL	CHD-C4C-NC	-2.80	121.97	125.08
15	Z	101	CRT	C32-C31-C30	-2.80	114.65	123.23
9	j	101	BCL	C1D-CHD-C4C	-2.80	121.75	125.92
9	J	102	BCL	C4B-CHC-C1C	-2.80	124.58	130.12
7	o	504	HEM	CAA-CBA-CGA	-2.80	107.88	112.66
9	l	101	BCL	C7-C6-C5	-2.79	105.35	113.11
15	M	404	CRT	C20-C19-C17	-2.79	123.33	127.31
9	j	101	BCL	C7-C6-C5	-2.79	105.35	113.11
9	f	101	BCL	C1D-CHD-C4C	-2.79	121.76	125.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	102	BCL	CMA-C3A-C4A	-2.79	104.28	111.77
12	H	301	PEF	O3-C3-C2	-2.79	101.65	108.66
9	5	101	BCL	C6-C5-C3	-2.79	106.34	112.66
9	G	102	BCL	C16-C15-C13	-2.79	106.59	115.73
9	v	102	BCL	C4B-CHC-C1C	-2.78	124.61	130.12
9	i	102	BCL	C16-C15-C13	-2.78	106.60	115.73
9	s	102	BCL	CMA-C3A-C4A	-2.78	104.30	111.77
9	AA	101	BCL	C16-C15-C13	-2.78	106.61	115.73
10	x	302	BPH	O1D-CGD-CBD	-2.77	119.62	124.60
9	S	102	BCL	C1D-CHD-C4C	-2.77	121.79	125.92
15	v	101	CRT	C27-C26-C25	-2.77	114.73	123.23
15	T	101	CRT	C27-C26-C25	-2.77	114.73	123.23
9	x	303	BCL	C4B-CHC-C1C	-2.77	124.63	130.12
9	AB	101	BCL	CHD-C4C-NC	-2.77	122.00	125.08
15	c	101	CRT	C21-C22-C23	-2.77	123.36	127.31
9	s	102	BCL	C16-C15-C13	-2.77	106.64	115.73
9	L	301	BCL	CGD-CBD-CAD	-2.77	101.44	110.71
10	y	402	BPH	CBB-CAB-C3B	-2.76	114.60	120.52
9	S	102	BCL	OBD-CAD-CBD	-2.76	121.77	125.94
15	8	101	CRT	C5-C6-C7	-2.76	121.72	125.89
9	d	101	BCL	C2A-C3A-C4A	-2.76	97.40	101.87
9	g	101	BCL	OBB-CAB-CBB	-2.76	113.86	120.16
15	E	101	CRT	C35-C33-C32	-2.76	114.70	118.94
15	U	102	CRT	C32-C31-C30	-2.76	114.76	123.23
9	0	101	BCL	C7-C6-C5	-2.76	105.44	113.11
9	e	102	BCL	CMC-C2C-C3C	-2.76	102.57	113.77
9	x	301	BCL	C11-C10-C8	-2.76	106.67	115.73
9	g	101	BCL	OBD-CAD-CBD	-2.76	121.77	125.94
10	M	402	BPH	OBB-CAB-CBB	-2.76	113.49	119.71
9	X	102	BCL	CHD-C4C-NC	-2.76	122.01	125.08
15	c	101	CRT	C21-C20-C19	-2.76	117.58	123.46
15	2	101	CRT	C31-C32-C33	-2.75	123.38	127.31
15	s	101	CRT	C35-C33-C32	-2.75	114.72	118.94
9	T	102	BCL	C16-C15-C13	-2.75	106.71	115.73
9	e	102	BCL	O2A-CGA-O1A	-2.75	116.73	123.55
9	R	102	BCL	CHA-C1A-NA	-2.75	119.80	126.18
15	e	101	CRT	C15-C14-C12	-2.74	123.40	127.31
9	z	102	BCL	CMC-C2C-C3C	-2.74	102.66	113.77
15	s	101	CRT	C26-C25-C23	-2.74	118.73	126.42
9	5	102	BCL	OBD-CAD-CBD	-2.73	121.81	125.94
9	x	305	BCL	C6-C5-C3	-2.73	106.46	112.66
15	AC	101	CRT	C21-C20-C19	-2.73	117.63	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	102	BCL	C11-C10-C8	-2.73	106.76	115.73
15	T	101	CRT	C9-C10-C11	-2.73	114.85	123.23
9	J	102	BCL	C3C-C4C-CHD	-2.73	117.60	123.34
9	M	401	BCL	CAA-CBA-CGA	-2.73	105.12	113.35
9	l	102	BCL	OBD-CAD-CBD	-2.73	121.82	125.94
11	x	304	UQ8	C30-C29-C28	-2.73	116.41	123.69
9	j	101	BCL	O2A-CGA-O1A	-2.73	116.78	123.55
9	AB	101	BCL	C11-C10-C8	-2.73	106.78	115.73
9	F	101	BCL	C16-C15-C13	-2.73	106.78	115.73
10	x	302	BPH	C4D-CHA-C1A	-2.73	123.28	130.23
9	AL	102	BCL	C4B-CHC-C1C	-2.73	124.72	130.12
15	AC	101	CRT	C26-C27-C28	-2.72	123.42	127.31
9	x	305	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
9	u	101	BCL	CGD-CBD-CAD	-2.72	101.59	110.71
9	p	104	BCL	C16-C15-C13	-2.72	106.80	115.73
9	B	101	BCL	CMC-C2C-C3C	-2.72	102.73	113.77
9	5	101	BCL	C4B-CHC-C1C	-2.72	124.73	130.12
9	R	102	BCL	CMC-C2C-C3C	-2.72	102.74	113.77
9	m	103	BCL	O2A-CGA-O1A	-2.72	116.80	123.55
9	p	104	BCL	C11-C12-C13	-2.72	106.81	115.73
9	D	101	BCL	C1D-CHD-C4C	-2.72	121.87	125.92
15	6	101	CRT	C8-C7-C9	-2.72	119.12	122.92
15	R	101	CRT	C21-C20-C19	-2.71	117.67	123.46
15	U	102	CRT	C15-C14-C12	-2.71	123.44	127.31
9	K	101	BCL	C1D-CHD-C4C	-2.71	121.88	125.92
9	F	101	BCL	CMC-C2C-C3C	-2.71	102.77	113.77
9	j	101	BCL	CMC-C2C-C3C	-2.71	102.78	113.77
9	z	102	BCL	C7-C6-C5	-2.71	105.58	113.11
15	2	101	CRT	C11-C12-C14	-2.71	114.78	118.94
15	k	101	CRT	C24-C23-C22	-2.71	119.13	122.92
9	f	101	BCL	OBB-CAB-CBB	-2.71	113.99	120.16
15	T	101	CRT	C34-C33-C32	-2.71	119.13	122.92
15	9	102	CRT	C27-C26-C25	-2.70	114.94	123.23
9	A	102	BCL	CHD-C4C-NC	-2.70	122.07	125.08
15	R	101	CRT	C13-C12-C14	-2.70	119.14	122.92
9	G	102	BCL	C7-C6-C5	-2.70	105.60	113.11
9	AA	101	BCL	C2C-C3C-C4C	-2.70	97.29	101.34
15	4	101	CRT	C10-C9-C7	-2.70	123.46	127.31
9	O	101	BCL	C16-C15-C13	-2.70	106.87	115.73
9	5	102	BCL	CMC-C2C-C3C	-2.70	102.82	113.77
9	j	101	BCL	CMA-C3A-C4A	-2.70	104.52	111.77
10	L	302	BPH	O1D-CGD-CBD	-2.69	119.76	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	102	BCL	CMA-C3A-C4A	-2.69	104.53	111.77
9	x	301	BCL	CMC-C2C-C3C	-2.69	102.84	113.77
9	x	301	BCL	OBD-CAD-CBD	-2.69	121.88	125.94
10	L	302	BPH	C4D-CHA-C1A	-2.69	123.37	130.23
9	y	401	BCL	OBB-CAB-CBB	-2.69	114.02	120.16
12	t	303	PEF	O5-C30-C31	-2.69	114.95	124.82
7	o	502	HEM	CBD-CAD-C3D	-2.68	107.35	112.47
9	3	101	BCL	CAA-CBA-CGA	-2.68	105.26	113.35
9	AK	101	BCL	C11-C10-C8	-2.68	106.92	115.73
9	7	101	BCL	CMA-C3A-C4A	-2.68	104.56	111.77
15	Z	101	CRT	C26-C27-C28	-2.68	123.48	127.31
9	L	305	BCL	OBD-CAD-CBD	-2.68	121.89	125.94
15	n	101	CRT	C26-C27-C28	-2.68	123.49	127.31
15	AH	102	CRT	C5-C6-C7	-2.68	121.84	125.89
9	j	101	BCL	CED-O2D-CGD	-2.68	109.69	115.97
9	x	305	BCL	C11-C10-C8	-2.68	106.94	115.73
9	5	101	BCL	OBD-CAD-CBD	-2.68	121.90	125.94
9	N	102	BCL	CMC-C2C-C3C	-2.68	102.91	113.77
9	F	101	BCL	C11-C12-C13	-2.68	106.95	115.73
9	P	101	BCL	C1D-CHD-C4C	-2.67	121.94	125.92
9	s	102	BCL	C4B-CHC-C1C	-2.67	124.82	130.12
9	f	101	BCL	C16-C15-C13	-2.67	106.96	115.73
9	7	101	BCL	C1D-CHD-C4C	-2.67	121.94	125.92
9	k	102	BCL	CMC-C2C-C3C	-2.67	102.94	113.77
9	i	102	BCL	C4B-CHC-C1C	-2.67	124.83	130.12
12	y	406	PEF	C2-O2-C10	-2.67	112.78	117.94
9	AC	102	BCL	C1-C2-C3	-2.67	121.04	125.96
11	x	304	UQ8	O4-C4-C3	-2.67	113.37	123.62
9	AH	103	BCL	C7-C6-C5	-2.67	105.69	113.11
15	AH	102	CRT	C9-C10-C11	-2.67	115.05	123.23
9	R	102	BCL	C2C-C3C-C4C	-2.67	97.35	101.34
9	Y	101	BCL	C1D-CHD-C4C	-2.66	121.95	125.92
9	l	101	BCL	CGD-CBD-CAD	-2.66	101.79	110.71
9	AL	102	BCL	CAA-CBA-CGA	-2.66	105.34	113.35
9	5	102	BCL	C4B-CHC-C1C	-2.65	124.86	130.12
9	G	102	BCL	C11-C10-C8	-2.65	107.02	115.73
9	5	102	BCL	CAA-CBA-CGA	-2.65	105.35	113.35
9	r	101	BCL	C7-C6-C5	-2.65	105.73	113.11
15	G	101	CRT	C9-C10-C11	-2.65	115.09	123.23
9	s	102	BCL	C11-C12-C13	-2.65	107.03	115.73
9	L	305	BCL	CHA-C1A-NA	-2.65	120.02	126.18
11	x	304	UQ8	C12-C13-C14	-2.65	121.02	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	c	102	BCL	OBD-CAD-CBD	-2.65	121.94	125.94
15	G	101	CRT	C31-C30-C28	-2.65	118.97	126.42
7	o	503	HEM	C3B-C4B-NB	-2.65	105.79	109.21
9	L	301	BCL	C3D-CAD-CBD	-2.64	103.86	107.60
9	u	101	BCL	C3C-C4C-CHD	-2.64	117.78	123.34
15	k	101	CRT	C10-C9-C7	-2.64	123.54	127.31
9	AK	101	BCL	C4B-CHC-C1C	-2.64	124.89	130.12
9	Q	101	BCL	C2C-C3C-C4C	-2.64	97.38	101.34
9	AC	102	BCL	C11-C10-C8	-2.64	107.06	115.73
9	AB	101	BCL	OBD-CAD-CBD	-2.64	121.96	125.94
9	K	101	BCL	C11-C12-C13	-2.64	107.08	115.73
9	y	401	BCL	C7-C6-C5	-2.64	105.78	113.11
15	U	102	CRT	C20-C19-C17	-2.63	123.55	127.31
9	7	101	BCL	CMC-C2C-C3C	-2.63	103.09	113.77
9	R	102	BCL	CMA-C3A-C4A	-2.63	104.70	111.77
9	W	101	BCL	C4B-CHC-C1C	-2.63	124.91	130.12
9	R	102	BCL	C16-C15-C13	-2.63	107.09	115.73
9	x	303	BCL	C1B-CHB-C4A	-2.63	124.91	130.12
15	J	101	CRT	C32-C31-C30	-2.63	115.17	123.23
9	J	102	BCL	C16-C15-C13	-2.63	107.11	115.73
7	C	504	HEM	C3B-C4B-NB	-2.63	105.81	109.21
9	O	101	BCL	C1D-CHD-C4C	-2.63	122.01	125.92
9	AK	101	BCL	C3C-C4C-CHD	-2.63	117.82	123.34
15	AC	101	CRT	C14-C15-C16	-2.62	115.19	123.23
9	3	101	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
9	c	102	BCL	C11-C12-C13	-2.62	107.14	115.73
9	3	101	BCL	C7-C6-C5	-2.62	105.84	113.11
9	g	101	BCL	C16-C15-C13	-2.62	107.15	115.73
9	w	101	BCL	C3C-C4C-CHD	-2.61	117.84	123.34
9	w	101	BCL	CHD-C4C-NC	-2.61	122.17	125.08
9	T	102	BCL	C1-C2-C3	-2.61	121.14	125.96
9	D	101	BCL	OBB-CAB-CBB	-2.61	114.20	120.16
9	y	401	BCL	CAA-CBA-CGA	-2.61	105.48	113.35
9	8	102	BCL	CHA-C1A-NA	-2.61	120.12	126.18
9	AJ	102	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
9	AI	101	BCL	CMC-C2C-C3C	-2.61	103.19	113.77
9	w	101	BCL	C16-C15-C13	-2.61	107.17	115.73
9	AL	102	BCL	CMC-C2C-C3C	-2.61	103.20	113.77
15	N	101	CRT	C24-C23-C22	-2.61	119.27	122.92
9	D	101	BCL	C11-C12-C13	-2.60	107.18	115.73
10	y	402	BPH	C2A-C1A-NA	-2.60	108.74	111.91
9	AE	102	BCL	C1D-CHD-C4C	-2.60	122.04	125.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	102	BCL	C3C-C4C-CHD	-2.60	117.87	123.34
9	1	102	BCL	CMC-C2C-C3C	-2.60	103.22	113.77
15	AE	103	CRT	C9-C10-C11	-2.60	115.26	123.23
15	y	404	CRT	C26-C27-C28	-2.60	123.60	127.31
9	Z	102	BCL	C11-C10-C8	-2.60	107.20	115.73
9	f	101	BCL	OBD-CAD-CBD	-2.60	122.02	125.94
9	D	101	BCL	CMC-C2C-C3C	-2.59	103.25	113.77
9	g	101	BCL	O2A-CGA-O1A	-2.59	117.12	123.55
11	L	304	UQ8	C45-C44-C43	-2.59	114.83	122.65
15	6	101	CRT	C20-C19-C17	-2.59	123.61	127.31
7	C	502	HEM	C4C-C3C-C2C	-2.59	105.09	106.90
14	y	403	MQ8	C21-C22-C23	-2.59	121.18	127.68
15	G	101	CRT	C21-C20-C19	-2.59	117.94	123.46
9	O	101	BCL	C11-C12-C13	-2.59	107.24	115.73
7	o	502	HEM	C3B-C4B-NB	-2.58	105.87	109.21
15	i	101	CRT	C21-C20-C19	-2.58	117.95	123.46
9	1	101	BCL	C11-C10-C8	-2.58	107.25	115.73
9	M	401	BCL	CHD-C4C-NC	-2.58	122.21	125.08
12	H	304	PEF	O2-C10-O4	-2.58	117.72	122.94
9	M	401	BCL	C10-C8-C7	-2.58	99.72	112.10
9	AH	101	BCL	C7-C6-C5	-2.58	105.95	113.11
15	v	101	CRT	C26-C25-C23	-2.58	119.18	126.42
7	o	502	HEM	CMD-C2D-C1D	-2.58	124.50	128.46
9	h	101	BCL	C11-C10-C8	-2.57	107.28	115.73
15	f	102	CRT	C5-C6-C7	-2.57	122.00	125.89
15	J	101	CRT	C6-C7-C9	-2.57	114.99	118.94
10	M	402	BPH	C4D-CHA-C1A	-2.57	123.67	130.23
9	e	102	BCL	C4B-CHC-C1C	-2.57	125.02	130.12
9	c	102	BCL	C1D-CHD-C4C	-2.57	122.09	125.92
9	F	101	BCL	CHD-C4C-NC	-2.57	122.22	125.08
15	v	101	CRT	C30-C28-C27	-2.57	115.00	118.94
7	o	503	HEM	CAA-CBA-CGA	-2.57	108.27	112.66
9	I	101	BCL	CGD-CBD-CAD	-2.57	102.10	110.71
9	AD	101	BCL	C3C-C4C-CHD	-2.57	117.94	123.34
15	N	101	CRT	C21-C20-C19	-2.57	117.98	123.46
9	A	102	BCL	C7-C6-C5	-2.57	105.98	113.11
12	y	408	PEF	C2-O2-C10	-2.57	112.98	117.94
15	k	101	CRT	C8-C7-C9	-2.57	119.33	122.92
9	r	101	BCL	OBD-CAD-CBD	-2.57	122.07	125.94
10	M	402	BPH	C2A-C1A-NA	-2.57	108.79	111.91
9	z	102	BCL	CMA-C3A-C4A	-2.56	104.89	111.77
15	AJ	101	CRT	C35-C33-C32	-2.56	115.02	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	101	CRT	C32-C31-C30	-2.56	115.39	123.23
9	x	303	BCL	OBB-CAB-CBB	-2.56	114.33	120.16
9	W	101	BCL	C1D-CHD-C4C	-2.56	122.11	125.92
9	0	101	BCL	O2A-CGA-O1A	-2.55	117.21	123.55
15	AE	103	CRT	C5-C6-C7	-2.55	122.04	125.89
15	i	101	CRT	C32-C31-C30	-2.55	115.41	123.23
9	L	301	BCL	C11-C10-C8	-2.55	107.36	115.73
9	e	102	BCL	OBD-CAD-CBD	-2.55	122.09	125.94
9	x	305	BCL	O2A-CGA-O1A	-2.55	117.22	123.55
9	v	102	BCL	CMA-C3A-C4A	-2.55	104.93	111.77
9	m	103	BCL	C3C-C4C-CHD	-2.55	117.98	123.34
15	f	102	CRT	C4-C5-C6	-2.55	120.91	124.57
15	AH	102	CRT	C29-C28-C27	-2.55	119.36	122.92
9	l	101	BCL	CMC-C2C-C3C	-2.54	103.45	113.77
15	Z	101	CRT	C21-C22-C23	-2.54	123.68	127.31
9	P	101	BCL	C16-C15-C13	-2.54	107.38	115.73
15	s	101	CRT	C26-C27-C28	-2.54	123.68	127.31
9	J	102	BCL	C7-C6-C5	-2.54	106.05	113.11
9	k	102	BCL	CAA-CBA-CGA	-2.54	105.70	113.35
9	S	102	BCL	C7-C6-C5	-2.54	106.06	113.11
9	K	101	BCL	C3C-C4C-CHD	-2.54	118.00	123.34
9	J	102	BCL	C11-C12-C13	-2.54	107.41	115.73
7	C	502	HEM	C3B-C4B-NB	-2.53	105.93	109.21
15	f	102	CRT	C10-C9-C7	-2.53	123.70	127.31
9	G	102	BCL	C12-C11-C10	-2.53	101.02	113.25
10	M	402	BPH	CBA-CAA-C2A	-2.53	106.23	113.80
10	x	302	BPH	CBA-CAA-C2A	-2.53	106.23	113.80
15	p	103	CRT	C35-C33-C32	-2.53	115.06	118.94
15	k	101	CRT	C21-C22-C23	-2.53	123.70	127.31
9	f	101	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
9	X	102	BCL	C7-C6-C5	-2.53	106.09	113.11
15	e	101	CRT	C26-C25-C23	-2.53	119.32	126.42
9	G	102	BCL	CMC-C2C-C3C	-2.53	103.53	113.77
9	Z	102	BCL	C7-C6-C5	-2.53	106.09	113.11
9	W	101	BCL	CMC-C2C-C3C	-2.52	103.54	113.77
9	Z	102	BCL	C1D-CHD-C4C	-2.52	122.16	125.92
9	A	102	BCL	CHB-C4A-NA	-2.52	121.03	124.51
15	z	101	CRT	C30-C28-C27	-2.52	115.07	118.94
15	G	101	CRT	C26-C25-C23	-2.52	119.34	126.42
15	p	103	CRT	C14-C15-C16	-2.52	115.50	123.23
11	L	304	UQ8	C40-C39-C38	-2.52	116.97	123.69
15	c	101	CRT	C34-C33-C32	-2.51	119.40	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	102	BCL	C16-C15-C13	-2.51	107.48	115.73
9	g	101	BCL	C12-C11-C10	-2.51	101.09	113.25
14	y	403	MQ8	C7-C8-C9	-2.51	116.75	120.21
15	AE	103	CRT	C36-C35-C33	-2.51	122.10	125.89
9	F	101	BCL	C11-C10-C8	-2.51	107.50	115.73
15	AC	101	CRT	C9-C10-C11	-2.51	115.54	123.23
15	k	101	CRT	C13-C12-C14	-2.51	119.41	122.92
9	v	102	BCL	C1D-CHD-C4C	-2.51	122.18	125.92
9	r	101	BCL	CMC-C2C-C3C	-2.51	103.60	113.77
15	AL	101	CRT	C10-C9-C7	-2.51	123.73	127.31
9	e	102	BCL	CMA-C3A-C4A	-2.51	105.03	111.77
15	AH	102	CRT	C4-C5-C6	-2.51	120.97	124.57
9	J	102	BCL	CHD-C4C-NC	-2.51	122.29	125.08
15	U	102	CRT	C20-C21-C22	-2.50	118.12	123.46
15	Z	101	CRT	C29-C28-C27	-2.50	119.42	122.92
15	N	101	CRT	C29-C28-C27	-2.50	119.42	122.92
15	P	102	CRT	C9-C10-C11	-2.50	115.56	123.23
15	f	102	CRT	C30-C28-C27	-2.50	115.11	118.94
9	B	101	BCL	O2A-CGA-O1A	-2.50	117.34	123.55
9	4	102	BCL	CED-O2D-CGD	-2.50	110.11	115.97
9	7	101	BCL	C11-C12-C13	-2.50	107.53	115.73
9	1	101	BCL	CHA-C1A-NA	-2.50	120.38	126.18
9	p	104	BCL	C7-C6-C5	-2.50	106.17	113.11
10	y	402	BPH	C3A-C4A-NA	-2.50	108.76	113.06
15	AH	102	CRT	C35-C33-C32	-2.50	115.11	118.94
9	v	102	BCL	CED-O2D-CGD	-2.49	110.13	115.97
9	AH	101	BCL	C1D-CHD-C4C	-2.49	122.20	125.92
15	v	101	CRT	C15-C16-C17	-2.49	119.42	126.42
9	P	101	BCL	CED-O2D-CGD	-2.49	110.13	115.97
15	p	103	CRT	C6-C7-C9	-2.49	115.12	118.94
9	w	101	BCL	C1D-CHD-C4C	-2.49	122.21	125.92
9	7	101	BCL	C11-C10-C8	-2.49	107.57	115.73
9	x	301	BCL	CMA-C3A-C4A	-2.49	105.09	111.77
9	x	303	BCL	C16-C15-C13	-2.48	107.58	115.73
9	AD	101	BCL	C11-C12-C13	-2.48	107.58	115.73
15	e	101	CRT	C35-C33-C32	-2.48	115.13	118.94
9	g	101	BCL	CMC-C2C-C3C	-2.48	103.71	113.77
15	2	101	CRT	C4-C5-C6	-2.48	121.01	124.57
9	AC	102	BCL	C3C-C4C-CHD	-2.48	118.12	123.34
15	AJ	101	CRT	C15-C14-C12	-2.48	123.77	127.31
9	s	102	BCL	CMC-C2C-C3C	-2.48	103.73	113.77
9	c	102	BCL	C3C-C4C-CHD	-2.47	118.14	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	4	102	BCL	C12-C11-C10	-2.47	101.30	113.25
9	AJ	102	BCL	C11-C10-C8	-2.47	107.63	115.73
9	7	101	BCL	C16-C15-C13	-2.47	107.63	115.73
15	4	101	CRT	C14-C15-C16	-2.47	115.67	123.23
9	U	101	BCL	C11-C12-C13	-2.47	107.64	115.73
14	M	403	MQ8	C21-C22-C23	-2.46	121.49	127.68
9	AI	101	BCL	C3C-C4C-CHD	-2.46	118.16	123.34
15	4	101	CRT	C20-C21-C22	-2.46	118.20	123.46
15	6	101	CRT	C9-C10-C11	-2.46	115.67	123.23
9	Q	101	BCL	C1D-CHD-C4C	-2.46	122.25	125.92
9	L	305	BCL	CED-O2D-CGD	-2.46	110.20	115.97
9	5	102	BCL	C6-C5-C3	-2.46	107.08	112.66
9	T	102	BCL	C11-C12-C13	-2.46	107.66	115.73
9	AE	102	BCL	CMC-C2C-C3C	-2.46	103.80	113.77
9	G	102	BCL	O2A-CGA-O1A	-2.46	117.45	123.55
15	p	103	CRT	C24-C23-C22	-2.46	119.48	122.92
15	R	101	CRT	C16-C17-C19	-2.46	115.17	118.94
9	7	101	BCL	C2C-C3C-C4C	-2.46	97.66	101.34
9	0	101	BCL	C1-C2-C3	-2.45	121.44	125.96
9	x	303	BCL	CED-O2D-CGD	-2.45	110.22	115.97
15	z	101	CRT	C14-C15-C16	-2.45	115.72	123.23
15	i	101	CRT	C4-C5-C6	-2.45	121.05	124.57
9	X	102	BCL	CMC-C2C-C3C	-2.45	103.84	113.77
16	t	302	PO4	O4-P-O1	-2.45	100.55	110.97
9	Y	101	BCL	C7-C6-C5	-2.45	106.31	113.11
9	l	101	BCL	C11-C12-C13	-2.44	107.71	115.73
9	Z	102	BCL	C2C-C3C-C4C	-2.44	97.68	101.34
9	N	102	BCL	C1D-CHD-C4C	-2.44	122.28	125.92
9	Z	102	BCL	O2A-CGA-O1A	-2.44	117.49	123.55
9	i	102	BCL	O2A-CGA-O1A	-2.44	117.50	123.55
9	z	102	BCL	CHD-C4C-NC	-2.44	122.37	125.08
9	L	301	BCL	C2A-C3A-C4A	-2.44	97.93	101.87
9	R	102	BCL	C7-C6-C5	-2.44	106.34	113.11
9	AD	101	BCL	CMC-C2C-C3C	-2.44	103.89	113.77
9	T	102	BCL	CED-O2D-CGD	-2.43	110.26	115.97
9	g	101	BCL	CAA-CBA-CGA	-2.43	106.02	113.35
9	AH	103	BCL	C11-C10-C8	-2.43	107.75	115.73
9	p	104	BCL	CMC-C2C-C3C	-2.43	103.91	113.77
15	P	102	CRT	C10-C9-C7	-2.43	123.84	127.31
9	AB	101	BCL	CGD-CBD-CAD	-2.43	102.58	110.71
9	v	102	BCL	CHD-C4C-NC	-2.43	122.38	125.08
15	n	101	CRT	C18-C17-C19	-2.42	119.53	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AE	103	CRT	C32-C31-C30	-2.42	115.81	123.23
9	R	102	BCL	OBD-CAD-CBD	-2.42	122.29	125.94
15	T	101	CRT	C16-C17-C19	-2.42	115.23	118.94
9	f	101	BCL	CMC-C2C-C3C	-2.42	103.96	113.77
9	x	305	BCL	C4B-CHC-C1C	-2.42	125.33	130.12
9	T	102	BCL	C3C-C4C-CHD	-2.42	118.26	123.34
9	A	102	BCL	O2A-CGA-O1A	-2.41	117.56	123.55
11	x	304	UQ8	C7-C6-C5	-2.41	115.38	118.47
7	o	502	HEM	C4C-C3C-C2C	-2.41	105.21	106.90
9	AE	104	BCL	C11-C12-C13	-2.41	107.81	115.73
9	T	102	BCL	OBB-CAB-CBB	-2.41	114.67	120.16
15	e	101	CRT	C26-C27-C28	-2.41	123.88	127.31
9	d	101	BCL	CMC-C2C-C1C	-2.41	105.31	111.77
9	Y	101	BCL	CMC-C2C-C1C	-2.41	105.31	111.77
15	2	101	CRT	C21-C20-C19	-2.41	118.33	123.46
9	L	303	BCL	OBB-CAB-CBB	-2.41	114.67	120.16
9	P	101	BCL	C1B-CHB-C4A	-2.40	125.36	130.12
15	T	101	CRT	C29-C28-C27	-2.40	119.56	122.92
9	G	102	BCL	CMA-C3A-C4A	-2.40	105.32	111.77
15	AD	102	CRT	C26-C25-C23	-2.40	119.67	126.42
9	AI	101	BCL	CMA-C3A-C4A	-2.40	105.33	111.77
9	B	101	BCL	CMA-C3A-C4A	-2.39	105.34	111.77
9	L	301	BCL	C1B-CHB-C4A	-2.39	125.38	130.12
9	U	101	BCL	CMC-C2C-C3C	-2.39	104.07	113.77
9	d	101	BCL	CMC-C2C-C3C	-2.39	104.08	113.77
9	p	102	BCL	CHB-C4A-NA	-2.39	121.21	124.51
15	s	101	CRT	C6-C7-C9	-2.39	115.28	118.94
12	m	101	PEF	C3-C2-C1	-2.39	106.47	111.86
9	h	101	BCL	C7-C6-C5	-2.39	106.47	113.11
15	A	103	CRT	C16-C17-C19	-2.39	115.28	118.94
9	p	104	BCL	C1B-CHB-C4A	-2.38	125.39	130.12
15	U	102	CRT	C14-C15-C16	-2.38	115.92	123.23
9	AE	104	BCL	OBD-CAD-CBD	-2.38	122.34	125.94
9	N	102	BCL	C3C-C4C-CHD	-2.38	118.33	123.34
15	A	103	CRT	C14-C15-C16	-2.38	115.94	123.23
15	f	102	CRT	C11-C12-C14	-2.38	115.29	118.94
9	r	101	BCL	C11-C12-C13	-2.38	107.93	115.73
9	D	102	BCL	C11-C10-C8	-2.38	107.93	115.73
9	S	102	BCL	CMA-C3A-C2A	-2.38	104.13	113.77
9	AH	101	BCL	C16-C15-C13	-2.37	107.94	115.73
9	c	102	BCL	CGD-CBD-CAD	-2.37	102.76	110.71
9	p	104	BCL	C11-C10-C8	-2.37	107.94	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AH	101	BCL	CHB-C4A-NA	-2.37	121.23	124.51
9	h	101	BCL	C3C-C4C-CHD	-2.37	118.35	123.34
9	D	101	BCL	CMA-C3A-C4A	-2.37	105.40	111.77
9	I	101	BCL	C7-C6-C5	-2.37	106.52	113.11
9	l	101	BCL	C6-C5-C3	-2.37	107.28	112.66
9	3	101	BCL	C11-C12-C13	-2.37	107.95	115.73
12	t	303	PEF	O3P-P-O1P	-2.37	99.69	109.25
15	2	101	CRT	C32-C31-C30	-2.36	115.98	123.23
15	E	101	CRT	C32-C31-C30	-2.36	115.98	123.23
9	AL	102	BCL	C11-C12-C13	-2.36	107.97	115.73
9	AD	101	BCL	C11-C10-C8	-2.36	107.98	115.73
9	T	102	BCL	O2A-CGA-O1A	-2.36	117.69	123.55
9	Q	101	BCL	CHD-C4C-NC	-2.36	122.45	125.08
9	L	303	BCL	CAC-C3C-C2C	-2.36	108.31	114.24
9	AE	104	BCL	C11-C10-C8	-2.36	108.00	115.73
9	F	101	BCL	CAA-CBA-CGA	-2.36	106.25	113.35
9	AH	101	BCL	C11-C10-C8	-2.36	108.00	115.73
9	AB	101	BCL	C16-C15-C13	-2.35	108.00	115.73
9	9	103	BCL	C3C-C4C-CHD	-2.35	118.39	123.34
9	AC	102	BCL	OBD-CAD-CBD	-2.35	122.39	125.94
9	AE	104	BCL	CMA-C3A-C4A	-2.35	105.46	111.77
15	i	101	CRT	C26-C27-C28	-2.35	123.96	127.31
15	4	101	CRT	C34-C33-C32	-2.34	119.64	122.92
9	w	101	BCL	C2A-C3A-C4A	-2.34	98.09	101.87
10	y	402	BPH	C4D-CHA-C1A	-2.34	124.26	130.23
9	AH	101	BCL	CMC-C2C-C3C	-2.34	104.28	113.77
11	x	304	UQ8	O3-C3-C4	-2.34	114.64	123.62
10	M	402	BPH	C6-C7-C8	-2.34	108.06	115.73
9	D	102	BCL	C4B-CHC-C1C	-2.33	125.49	130.12
9	J	102	BCL	C1D-CHD-C4C	-2.33	122.44	125.92
15	G	101	CRT	C27-C26-C25	-2.33	116.07	123.23
7	C	503	HEM	C4C-C3C-C2C	-2.33	105.27	106.90
9	G	102	BCL	CHD-C4C-NC	-2.33	122.49	125.08
9	5	102	BCL	C7-C6-C5	-2.33	106.64	113.11
9	9	103	BCL	C16-C15-C13	-2.33	108.09	115.73
9	AC	102	BCL	CMA-C3A-C4A	-2.33	105.52	111.77
9	s	102	BCL	OBD-CAD-CBD	-2.32	122.43	125.94
9	l	102	BCL	CHB-C4A-NA	-2.32	121.30	124.51
9	m	103	BCL	CMC-C2C-C3C	-2.32	104.34	113.77
9	R	102	BCL	C3C-C4C-CHD	-2.32	118.45	123.34
15	Z	101	CRT	C35-C33-C32	-2.32	115.38	118.94
9	AK	101	BCL	C6-C5-C3	-2.32	107.40	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	R	101	CRT	C26-C27-C28	-2.32	124.00	127.31
9	L	305	BCL	C16-C15-C13	-2.32	108.12	115.73
10	L	302	BPH	CBA-CAA-C2A	-2.32	106.86	113.80
15	s	101	CRT	C9-C10-C11	-2.32	116.12	123.23
9	g	101	BCL	C7-C6-C5	-2.32	106.67	113.11
9	AA	101	BCL	CMA-C3A-C4A	-2.32	105.55	111.77
9	AK	101	BCL	CMA-C3A-C4A	-2.32	105.55	111.77
9	w	101	BCL	C7-C6-C5	-2.32	106.67	113.11
10	y	402	BPH	O2A-CGA-O1A	-2.32	117.80	123.55
15	G	101	CRT	C18-C17-C19	-2.32	119.68	122.92
9	AH	101	BCL	CMA-C3A-C4A	-2.31	105.55	111.77
9	x	301	BCL	C16-C15-C13	-2.31	108.14	115.73
9	AD	101	BCL	C12-C11-C10	-2.31	102.08	113.25
9	AC	102	BCL	C7-C6-C5	-2.31	106.69	113.11
9	7	101	BCL	CMC-C2C-C1C	-2.31	105.56	111.77
9	AJ	102	BCL	C16-C15-C13	-2.31	108.15	115.73
9	J	102	BCL	CMC-C2C-C3C	-2.31	104.41	113.77
9	w	101	BCL	C11-C10-C8	-2.31	108.16	115.73
15	2	101	CRT	C5-C6-C7	-2.31	122.41	125.89
9	z	102	BCL	O2A-CGA-O1A	-2.31	117.82	123.55
9	K	101	BCL	CMC-C2C-C3C	-2.30	104.42	113.77
9	Z	102	BCL	CMA-C3A-C4A	-2.30	105.58	111.77
9	U	101	BCL	CED-O2D-CGD	-2.30	110.58	115.97
9	h	101	BCL	CMA-C3A-C2A	-2.30	104.44	113.77
15	E	101	CRT	C26-C27-C28	-2.30	124.03	127.31
15	J	101	CRT	C35-C33-C32	-2.30	115.42	118.94
15	e	101	CRT	C10-C11-C12	-2.30	119.97	126.42
9	5	102	BCL	C12-C11-C10	-2.30	102.15	113.25
10	L	302	BPH	C11-C10-C8	-2.29	108.20	115.73
9	AD	101	BCL	O2A-CGA-O1A	-2.29	117.86	123.55
9	h	101	BCL	C16-C15-C13	-2.29	108.20	115.73
9	z	102	BCL	C11-C12-C13	-2.29	108.21	115.73
9	AH	103	BCL	C12-C11-C10	-2.29	102.17	113.25
9	p	102	BCL	C11-C12-C13	-2.29	108.22	115.73
9	D	102	BCL	C3C-C4C-CHD	-2.29	118.53	123.34
9	0	101	BCL	C16-C15-C13	-2.28	108.23	115.73
9	AE	102	BCL	CMC-C2C-C1C	-2.28	105.64	111.77
9	p	102	BCL	CMC-C2C-C3C	-2.28	104.52	113.77
15	i	101	CRT	C9-C10-C11	-2.28	116.24	123.23
9	AI	101	BCL	C7-C6-C5	-2.28	106.78	113.11
9	AH	103	BCL	O2A-CGA-O1A	-2.28	117.89	123.55
9	V	101	BCL	CAA-CBA-CGA	-2.28	106.49	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	102	BCL	C2C-C3C-C4C	-2.28	97.93	101.34
9	s	102	BCL	CHD-C4C-NC	-2.27	122.55	125.08
9	S	102	BCL	CHB-C4A-NA	-2.27	121.37	124.51
9	AK	101	BCL	C7-C6-C5	-2.27	106.80	113.11
9	i	102	BCL	CMA-C3A-C4A	-2.27	105.67	111.77
9	d	101	BCL	CAA-CBA-CGA	-2.27	106.51	113.35
9	AE	102	BCL	O2A-CGA-O1A	-2.27	117.92	123.55
10	x	302	BPH	C1-C2-C3	-2.27	121.78	125.96
15	M	404	CRT	C29-C28-C27	-2.27	119.75	122.92
9	c	102	BCL	C11-C10-C8	-2.26	108.30	115.73
15	z	101	CRT	C36-C35-C33	-2.26	122.47	125.89
9	w	101	BCL	O2A-CGA-O1A	-2.26	117.94	123.55
9	AL	102	BCL	C3C-C4C-CHD	-2.26	118.58	123.34
9	AB	101	BCL	C6-C5-C3	-2.26	107.54	112.66
9	3	101	BCL	C11-C10-C8	-2.26	108.32	115.73
9	V	101	BCL	C3C-C4C-CHD	-2.26	118.59	123.34
15	e	101	CRT	C9-C10-C11	-2.26	116.31	123.23
9	AB	101	BCL	C1D-CHD-C4C	-2.25	122.56	125.92
15	AL	101	CRT	C9-C10-C11	-2.25	116.32	123.23
9	k	102	BCL	C11-C10-C8	-2.25	108.33	115.73
15	T	101	CRT	C14-C15-C16	-2.25	116.32	123.23
15	4	101	CRT	C30-C28-C27	-2.25	115.48	118.94
9	l	101	BCL	C1D-CHD-C4C	-2.25	122.57	125.92
9	v	102	BCL	C2C-C3C-C4C	-2.25	97.97	101.34
15	P	102	CRT	C8-C7-C9	-2.25	119.77	122.92
9	D	102	BCL	C12-C11-C10	-2.25	102.38	113.25
9	u	101	BCL	C11-C12-C13	-2.25	108.35	115.73
9	R	102	BCL	C1D-CHD-C4C	-2.25	122.57	125.92
9	c	102	BCL	C12-C11-C10	-2.25	102.39	113.25
9	f	101	BCL	O2A-CGA-O1A	-2.25	117.97	123.55
9	e	102	BCL	C11-C10-C8	-2.25	108.36	115.73
9	Y	101	BCL	C11-C10-C8	-2.25	108.36	115.73
9	AE	104	BCL	CHD-C4C-NC	-2.24	122.58	125.08
9	m	102	BCL	CHB-C4A-NA	-2.24	121.41	124.51
9	AA	101	BCL	CGD-CBD-CAD	-2.24	103.20	110.71
9	5	102	BCL	C11-C12-C13	-2.24	108.38	115.73
15	c	101	CRT	C8-C7-C9	-2.24	119.79	122.92
9	K	101	BCL	C7-C6-C5	-2.24	106.89	113.11
15	8	101	CRT	C4-C5-C6	-2.24	121.36	124.57
9	u	101	BCL	C14-C13-C12	-2.24	103.21	111.36
9	B	101	BCL	C3C-C4C-CHD	-2.24	118.64	123.34
7	o	504	HEM	C3B-C4B-NB	-2.24	106.32	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	x	305	BCL	OBD-CAD-CBD	-2.23	122.57	125.94
9	AB	101	BCL	C11-C12-C13	-2.23	108.41	115.73
9	R	102	BCL	CMA-C3A-C2A	-2.23	104.72	113.77
15	J	101	CRT	C14-C15-C16	-2.23	116.39	123.23
9	v	102	BCL	CMC-C2C-C3C	-2.23	104.73	113.77
10	L	302	BPH	C11-C12-C13	-2.23	108.42	115.73
12	x	306	PEF	O2P-P-O3P	-2.23	97.63	108.14
9	4	102	BCL	C6-C5-C3	-2.23	107.61	112.66
15	8	101	CRT	C20-C19-C17	-2.22	124.14	127.31
9	4	102	BCL	CMC-C2C-C3C	-2.22	104.75	113.77
9	c	102	BCL	CMC-C2C-C3C	-2.22	104.75	113.77
9	x	301	BCL	C10-C8-C7	-2.22	101.42	112.10
9	y	401	BCL	C16-C15-C13	-2.22	108.44	115.73
15	M	404	CRT	C8-C7-C9	-2.22	119.81	122.92
9	I	101	BCL	CED-O2D-CGD	-2.22	110.77	115.97
9	u	101	BCL	O2A-CGA-O1A	-2.22	118.04	123.55
9	7	101	BCL	CAA-CBA-CGA	-2.22	106.66	113.35
14	M	403	MQ8	C15-C13-C12	-2.22	116.56	121.10
9	m	102	BCL	C11-C10-C8	-2.22	108.45	115.73
9	G	102	BCL	C3C-C4C-CHD	-2.22	118.68	123.34
9	AE	102	BCL	CMA-C3A-C4A	-2.22	105.81	111.77
15	X	101	CRT	C32-C31-C30	-2.22	116.44	123.23
15	A	103	CRT	C10-C11-C12	-2.21	120.19	126.42
9	Q	101	BCL	OBD-CAD-CBD	-2.21	122.60	125.94
9	V	101	BCL	O2A-CGA-O1A	-2.21	118.05	123.55
9	AK	101	BCL	OBD-CAD-CBD	-2.21	122.60	125.94
15	T	101	CRT	C11-C12-C14	-2.21	115.55	118.94
9	S	102	BCL	CHD-C4C-NC	-2.21	122.62	125.08
15	AL	101	CRT	C21-C22-C23	-2.21	124.16	127.31
9	3	101	BCL	O2A-CGA-O1A	-2.21	118.07	123.55
9	U	101	BCL	C3C-C4C-CHD	-2.21	118.70	123.34
9	G	102	BCL	C11-C12-C13	-2.21	108.49	115.73
15	AJ	101	CRT	C32-C31-C30	-2.20	116.47	123.23
15	P	102	CRT	C27-C26-C25	-2.20	116.47	123.23
9	AH	101	BCL	C11-C12-C13	-2.20	108.50	115.73
15	9	102	CRT	C24-C23-C22	-2.20	119.84	122.92
9	AA	101	BCL	CMC-C2C-C3C	-2.20	104.84	113.77
15	AH	102	CRT	C27-C26-C25	-2.20	116.48	123.23
9	AI	101	BCL	CHB-C4A-NA	-2.20	121.47	124.51
9	AL	102	BCL	C11-C10-C8	-2.20	108.52	115.73
9	AK	101	BCL	CAC-C3C-C2C	-2.19	108.72	114.24
9	1	102	BCL	CMA-C3A-C4A	-2.19	105.88	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	101	BCL	CMC-C2C-C3C	-2.19	104.88	113.77
15	AH	102	CRT	C24-C23-C22	-2.19	119.85	122.92
9	R	102	BCL	C11-C12-C13	-2.19	108.54	115.73
9	N	102	BCL	C12-C11-C10	-2.19	102.66	113.25
15	T	101	CRT	C8-C7-C9	-2.19	119.86	122.92
15	s	101	CRT	C5-C6-C7	-2.19	122.58	125.89
9	4	102	BCL	C1D-CHD-C4C	-2.19	122.66	125.92
9	u	101	BCL	C11-C10-C8	-2.19	108.55	115.73
9	5	102	BCL	CHB-C4A-NA	-2.19	121.49	124.51
9	5	101	BCL	CMA-C3A-C2A	-2.19	104.90	113.77
15	4	101	CRT	C8-C7-C9	-2.19	119.86	122.92
15	z	101	CRT	C34-C33-C32	-2.19	119.86	122.92
15	N	101	CRT	C14-C15-C16	-2.18	116.53	123.23
15	AH	102	CRT	C14-C15-C16	-2.18	116.54	123.23
14	y	403	MQ8	C41-C42-C43	-2.18	122.20	127.68
9	D	102	BCL	C7-C6-C5	-2.18	107.05	113.11
9	f	101	BCL	CHB-C4A-NA	-2.18	121.50	124.51
15	c	101	CRT	C16-C17-C19	-2.18	115.60	118.94
15	A	103	CRT	C32-C31-C30	-2.18	116.55	123.23
15	4	101	CRT	C37-C36-C35	-2.18	121.45	124.57
9	k	102	BCL	CED-O2D-CGD	-2.17	110.87	115.97
15	N	101	CRT	C8-C7-C9	-2.17	119.88	122.92
9	x	305	BCL	CGD-CBD-CAD	-2.17	103.43	110.71
15	R	101	CRT	C24-C23-C22	-2.17	119.88	122.92
15	J	101	CRT	C29-C28-C27	-2.17	119.88	122.92
9	P	101	BCL	C11-C10-C8	-2.17	108.61	115.73
12	y	406	PEF	O2-C10-O4	-2.17	118.55	122.94
10	M	402	BPH	C5-C3-C2	-2.17	116.67	121.10
9	s	102	BCL	CHB-C4A-NA	-2.17	121.52	124.51
15	e	101	CRT	C6-C7-C9	-2.17	115.62	118.94
9	d	101	BCL	OBD-CAD-CBD	-2.17	122.67	125.94
15	T	101	CRT	C32-C31-C30	-2.16	116.59	123.23
15	M	404	CRT	C9-C10-C11	-2.16	116.59	123.23
9	e	102	BCL	C7-C6-C5	-2.16	107.10	113.11
9	B	101	BCL	C11-C10-C8	-2.16	108.64	115.73
12	H	304	PEF	C2-O2-C10	-2.16	113.76	117.94
14	M	403	MQ8	O1-C1-C2	-2.16	117.67	120.31
9	F	101	BCL	O2A-CGA-O1A	-2.16	118.19	123.55
9	AA	101	BCL	CED-O2D-CGD	-2.16	110.91	115.97
9	AE	104	BCL	C2C-C3C-C4C	-2.16	98.11	101.34
9	V	101	BCL	C1D-CHD-C4C	-2.15	122.71	125.92
9	7	101	BCL	OBD-CAD-CBD	-2.15	122.69	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	y	408	PEF	O5-C30-C31	-2.15	116.90	124.82
11	L	304	UQ8	C21-C22-C23	-2.15	104.58	111.97
9	W	101	BCL	C11-C10-C8	-2.15	108.67	115.73
9	AE	102	BCL	C12-C11-C10	-2.15	102.85	113.25
15	i	101	CRT	C27-C26-C25	-2.15	116.64	123.23
15	9	102	CRT	C18-C17-C19	-2.15	119.91	122.92
9	d	101	BCL	CHB-C4A-NA	-2.15	121.54	124.51
9	i	102	BCL	CMC-C2C-C3C	-2.15	105.07	113.77
15	E	101	CRT	C14-C15-C16	-2.14	116.65	123.23
9	O	101	BCL	C12-C11-C10	-2.14	102.88	113.25
7	C	501	HEM	CMA-C3A-C4A	-2.14	125.17	128.46
9	AD	101	BCL	CED-O2D-CGD	-2.14	110.94	115.97
9	AD	101	BCL	CAA-CBA-CGA	-2.14	106.89	113.35
15	2	101	CRT	C20-C21-C22	-2.14	118.89	123.46
9	p	104	BCL	CHD-C4C-NC	-2.14	122.69	125.08
9	Q	101	BCL	CMA-C3A-C4A	-2.14	106.02	111.77
9	T	102	BCL	C12-C11-C10	-2.14	102.91	113.25
9	AC	102	BCL	C12-C11-C10	-2.14	102.92	113.25
9	w	101	BCL	C11-C12-C13	-2.14	108.72	115.73
9	0	101	BCL	C11-C12-C13	-2.13	108.72	115.73
9	AA	101	BCL	CHB-C4A-NA	-2.13	121.56	124.51
9	B	101	BCL	C4B-CHC-C1C	-2.13	125.89	130.12
9	L	305	BCL	C1B-CHB-C4A	-2.13	125.89	130.12
10	L	302	BPH	CMC-C2C-C1C	-2.13	106.13	112.09
9	u	101	BCL	C1D-CHD-C4C	-2.13	122.74	125.92
9	j	101	BCL	C16-C15-C13	-2.13	108.74	115.73
9	1	101	BCL	CGD-CBD-CAD	-2.13	103.58	110.71
9	7	101	BCL	C6-C5-C3	-2.13	107.84	112.66
7	o	504	HEM	CMD-C2D-C1D	-2.13	125.19	128.46
11	L	304	UQ8	C37-C38-C39	-2.13	122.34	127.68
9	x	301	BCL	CHD-C4C-NC	-2.12	122.72	125.08
9	l	101	BCL	CHB-C4A-NA	-2.12	121.58	124.51
9	A	102	BCL	CED-O2D-CGD	-2.12	111.00	115.97
9	S	102	BCL	C16-C15-C13	-2.12	108.78	115.73
15	E	101	CRT	C9-C10-C11	-2.11	116.75	123.23
15	N	101	CRT	C27-C26-C25	-2.11	116.75	123.23
9	J	102	BCL	O2A-CGA-O1A	-2.11	118.30	123.55
9	p	104	BCL	C1D-CHD-C4C	-2.11	122.77	125.92
15	k	101	CRT	C4-C5-C6	-2.11	121.54	124.57
9	m	102	BCL	C3C-C4C-CHD	-2.11	118.91	123.34
9	P	101	BCL	C11-C12-C13	-2.11	108.81	115.73
7	o	504	HEM	CMA-C3A-C4A	-2.11	125.23	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	403	MQ8	C34-C33-C32	-2.11	118.07	123.69
15	y	404	CRT	C31-C30-C28	-2.11	120.50	126.42
15	p	103	CRT	C20-C21-C22	-2.11	118.97	123.46
15	R	101	CRT	C18-C17-C19	-2.11	119.97	122.92
9	x	301	BCL	C4B-CHC-C1C	-2.10	125.95	130.12
9	r	101	BCL	CMA-C3A-C4A	-2.10	106.12	111.77
9	L	301	BCL	C1D-CHD-C4C	-2.10	122.78	125.92
9	y	401	BCL	C11-C12-C13	-2.10	108.83	115.73
7	C	502	HEM	CBA-CAA-C2A	-2.10	108.46	112.48
9	O	101	BCL	C6-C5-C3	-2.10	107.89	112.66
9	K	101	BCL	CHB-C4A-NA	-2.10	121.61	124.51
15	AE	103	CRT	C4-C5-C6	-2.10	121.55	124.57
15	p	103	CRT	C21-C20-C19	-2.10	118.98	123.46
9	e	102	BCL	CGD-CBD-CAD	-2.10	103.67	110.71
14	y	403	MQ8	C29-C28-C27	-2.10	118.09	123.69
9	AC	102	BCL	CGD-CBD-CAD	-2.10	103.68	110.71
15	n	101	CRT	C21-C20-C19	-2.10	118.98	123.46
9	m	102	BCL	C1D-CHD-C4C	-2.10	122.79	125.92
9	S	102	BCL	CMC-C2C-C3C	-2.10	105.26	113.77
9	Q	101	BCL	C12-C11-C10	-2.10	103.10	113.25
15	R	101	CRT	C8-C7-C9	-2.10	119.98	122.92
9	AC	102	BCL	CHD-C4C-NC	-2.10	122.75	125.08
15	AL	101	CRT	C31-C32-C33	-2.10	124.32	127.31
15	A	103	CRT	C8-C7-C9	-2.09	119.99	122.92
9	F	101	BCL	C3C-C4C-CHD	-2.09	118.94	123.34
15	AE	103	CRT	C31-C32-C33	-2.09	124.32	127.31
9	T	102	BCL	CMA-C3A-C4A	-2.09	106.15	111.77
9	s	102	BCL	O2A-CGA-O1A	-2.09	118.36	123.55
9	u	101	BCL	CED-O2D-CGD	-2.09	111.07	115.97
9	l	101	BCL	CMA-C3A-C4A	-2.09	106.16	111.77
15	6	101	CRT	C20-C21-C22	-2.09	119.00	123.46
9	l	101	BCL	OBD-CAD-CBD	-2.09	122.79	125.94
9	F	101	BCL	C7-C6-C5	-2.09	107.31	113.11
9	v	102	BCL	CGD-CBD-CAD	-2.09	103.72	110.71
9	5	102	BCL	C2C-C3C-C4C	-2.08	98.22	101.34
9	m	102	BCL	C12-C11-C10	-2.08	103.17	113.25
9	A	102	BCL	CMA-C3A-C4A	-2.08	106.17	111.77
9	M	401	BCL	CMC-C2C-C3C	-2.08	105.32	113.77
9	Z	102	BCL	C11-C12-C13	-2.08	108.90	115.73
9	r	101	BCL	C16-C15-C13	-2.08	108.91	115.73
9	Q	101	BCL	CAA-CBA-CGA	-2.08	107.08	113.35
10	L	302	BPH	C6-C7-C8	-2.07	108.92	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	401	BCL	C7-C6-C5	-2.07	107.34	113.11
9	D	102	BCL	C1B-CHB-C4A	-2.07	126.01	130.12
9	g	101	BCL	C2A-C3A-C4A	-2.07	98.52	101.87
15	G	101	CRT	C26-C27-C28	-2.07	124.35	127.31
15	f	102	CRT	C24-C23-C22	-2.07	120.02	122.92
9	S	102	BCL	C6-C5-C3	-2.07	107.96	112.66
9	x	305	BCL	C10-C8-C7	-2.07	102.15	112.10
9	v	102	BCL	C11-C12-C13	-2.07	108.94	115.73
9	i	102	BCL	C12-C11-C10	-2.07	103.26	113.25
15	AE	103	CRT	C26-C25-C23	-2.06	120.62	126.42
14	M	403	MQ8	O4-C4-C5	-2.06	118.16	121.55
11	L	304	UQ8	C12-C13-C14	-2.06	122.50	127.68
9	d	101	BCL	CHD-C4C-NC	-2.06	122.78	125.08
15	AC	101	CRT	C32-C31-C30	-2.06	116.91	123.23
14	y	403	MQ8	C20-C18-C17	-2.06	116.88	121.10
9	AE	102	BCL	CHB-C4A-NA	-2.06	121.66	124.51
9	5	102	BCL	O2A-CGA-O1A	-2.06	118.43	123.55
9	AK	101	BCL	C1B-CHB-C4A	-2.06	126.04	130.12
9	B	101	BCL	CGD-CBD-CAD	-2.06	103.81	110.71
9	d	101	BCL	C14-C13-C12	-2.06	103.86	111.36
9	m	103	BCL	CHD-C4C-NC	-2.06	122.79	125.08
9	x	305	BCL	C4-C3-C5	-2.06	111.72	115.29
15	AL	101	CRT	C8-C7-C9	-2.06	120.04	122.92
9	AH	103	BCL	C10-C8-C7	-2.06	102.22	112.10
10	y	402	BPH	C6-C5-C3	-2.05	108.00	112.66
15	2	101	CRT	C27-C26-C25	-2.05	116.94	123.23
9	N	102	BCL	O2A-CGA-O1A	-2.05	118.47	123.55
15	9	102	CRT	C30-C28-C27	-2.04	115.80	118.94
9	AB	101	BCL	C3C-C4C-CHD	-2.04	119.04	123.34
9	9	103	BCL	O2A-CGA-O1A	-2.04	118.47	123.55
9	3	101	BCL	C1D-CHD-C4C	-2.04	122.87	125.92
9	S	102	BCL	CED-O2D-CGD	-2.04	111.18	115.97
9	L	301	BCL	CHD-C4C-NC	-2.04	122.81	125.08
9	e	102	BCL	CAC-C3C-C4C	-2.04	108.05	112.58
15	c	101	CRT	C36-C35-C33	-2.04	122.81	125.89
9	S	102	BCL	CMC-C2C-C1C	-2.04	106.28	111.77
9	4	102	BCL	C11-C10-C8	-2.04	109.03	115.73
9	T	102	BCL	C10-C8-C7	-2.04	102.30	112.10
9	c	102	BCL	C1-C2-C3	-2.04	122.20	125.96
9	y	401	BCL	C6-C5-C3	-2.04	108.03	112.66
15	p	103	CRT	C32-C31-C30	-2.04	116.97	123.23
9	G	102	BCL	C1B-CHB-C4A	-2.04	126.08	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	m	103	BCL	C11-C12-C13	-2.04	109.04	115.73
11	L	304	UQ8	C7-C6-C1	-2.04	119.46	123.47
9	g	101	BCL	C2C-C3C-C4C	-2.04	98.29	101.34
9	h	101	BCL	C12-C11-C10	-2.04	103.40	113.25
9	9	103	BCL	CED-O2D-CGD	-2.04	111.20	115.97
9	c	102	BCL	CHD-C4C-NC	-2.03	122.82	125.08
9	l	101	BCL	C3C-C4C-CHD	-2.03	119.07	123.34
11	x	304	UQ8	C15-C14-C13	-2.03	118.27	123.69
9	P	101	BCL	C12-C11-C10	-2.03	103.43	113.25
15	AD	102	CRT	C16-C17-C19	-2.03	115.83	118.94
12	H	303	PEF	C2-O2-C10	-2.03	114.01	117.94
11	L	304	UQ8	C17-C18-C19	-2.03	122.58	127.68
9	e	102	BCL	CHB-C4A-NA	-2.03	121.71	124.51
15	E	101	CRT	C16-C17-C19	-2.03	115.83	118.94
9	m	102	BCL	CHD-C4C-NC	-2.03	122.83	125.08
15	M	404	CRT	C21-C22-C23	-2.02	124.42	127.31
15	v	101	CRT	C14-C15-C16	-2.02	117.03	123.23
15	T	101	CRT	C40-C38-C39	-2.02	106.31	110.31
9	i	102	BCL	C11-C12-C13	-2.02	109.10	115.73
9	4	102	BCL	CGD-CBD-CAD	-2.02	103.94	110.71
15	AH	102	CRT	C32-C31-C30	-2.02	117.03	123.23
9	f	101	BCL	CED-O2D-CGD	-2.02	111.24	115.97
9	7	101	BCL	CGD-CBD-CAD	-2.02	103.95	110.71
9	9	103	BCL	C1D-CHD-C4C	-2.02	122.91	125.92
9	j	101	BCL	C6-C5-C3	-2.02	108.08	112.66
9	V	101	BCL	C11-C10-C8	-2.02	109.11	115.73
9	v	102	BCL	C3C-C4C-CHD	-2.02	119.10	123.34
9	Q	101	BCL	C3C-C4C-CHD	-2.02	119.10	123.34
9	e	102	BCL	C12-C11-C10	-2.01	103.52	113.25
15	M	404	CRT	C21-C20-C19	-2.01	119.17	123.46
9	5	101	BCL	CGD-CBD-CAD	-2.01	103.97	110.71
15	P	102	CRT	C30-C28-C27	-2.01	115.86	118.94
9	G	102	BCL	CHB-C4A-NA	-2.01	121.73	124.51
9	3	101	BCL	C12-C11-C10	-2.01	103.53	113.25
9	d	101	BCL	CMA-C3A-C4A	-2.01	106.37	111.77
9	v	102	BCL	O2A-CGA-O1A	-2.01	118.56	123.55
9	AE	102	BCL	C11-C10-C8	-2.01	109.14	115.73
15	f	102	CRT	C16-C17-C19	-2.01	115.86	118.94
9	V	101	BCL	C7-C6-C5	-2.01	107.53	113.11
15	c	101	CRT	C31-C30-C28	-2.01	120.78	126.42
9	A	102	BCL	C11-C12-C13	-2.01	109.15	115.73
9	X	102	BCL	C2C-C3C-C4C	-2.01	98.34	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	401	BCL	C1B-CHB-C4A	-2.00	126.15	130.12
15	X	101	CRT	C13-C12-C14	-2.00	120.11	122.92
10	M	402	BPH	O2A-CGA-O1A	-2.00	118.58	123.55
9	AH	103	BCL	CHB-C4A-NA	-2.00	121.74	124.51
9	AE	104	BCL	O2A-CGA-O1A	-2.00	118.58	123.55
9	X	102	BCL	C12-C11-C10	-2.00	103.57	113.25
9	i	102	BCL	C10-C8-C7	-2.00	102.49	112.10
9	5	102	BCL	CHC-C1C-NC	2.00	127.28	124.51
9	W	101	BCL	CBA-CAA-C2A	2.00	119.79	113.80
11	x	304	UQ8	O2-C2-C3	2.00	125.22	120.95
12	p	101	PEF	O3-C30-C31	2.01	121.47	112.44
9	4	102	BCL	O2A-CGA-CBA	2.01	117.74	111.90
9	u	101	BCL	C6-C5-C3	2.01	117.21	112.66
9	w	101	BCL	O2A-CGA-CBA	2.01	117.75	111.90
9	Y	101	BCL	C1-O2A-CGA	2.02	121.61	116.77
15	Z	101	CRT	O1-C1-C4	2.02	111.70	106.29
15	N	101	CRT	C24-C23-C25	2.02	121.31	118.10
9	g	101	BCL	OBD-CAD-C3D	2.02	131.75	128.03
9	h	101	BCL	C1-O2A-CGA	2.02	121.62	116.77
9	8	102	BCL	C3C-C2C-C1C	2.03	105.14	101.87
9	L	305	BCL	CHC-C1C-NC	2.03	127.32	124.51
9	x	301	BCL	O2A-CGA-CBA	2.03	117.82	111.90
9	5	101	BCL	OBD-CAD-C3D	2.03	131.77	128.03
12	t	301	PEF	O2-C10-C11	2.04	114.93	111.10
9	AK	101	BCL	CHC-C1C-NC	2.04	127.33	124.51
9	O	101	BCL	CBA-CAA-C2A	2.04	119.90	113.80
9	x	301	BCL	C2A-C1A-CHA	2.04	127.54	123.92
9	AH	103	BCL	C3C-C2C-C1C	2.04	105.17	101.87
9	AE	104	BCL	C3C-C2C-C1C	2.04	105.17	101.87
15	9	102	CRT	C9-C10-C11	2.04	129.50	123.23
12	M	408	PEF	O2P-P-O1P	2.04	122.86	112.28
15	i	101	CRT	C18-C17-C16	2.05	121.36	118.10
9	L	305	BCL	C3C-C2C-C1C	2.05	105.17	101.87
9	L	303	BCL	C4A-NA-C1A	2.05	109.00	106.45
9	AH	103	BCL	C1-O2A-CGA	2.05	121.69	116.77
15	AE	103	CRT	C8-C7-C6	2.05	121.37	118.10
9	AB	101	BCL	C2A-C1A-CHA	2.05	127.56	123.92
9	AL	102	BCL	C4A-NA-C1A	2.06	109.01	106.45
15	AJ	101	CRT	C6-C7-C9	2.06	122.10	118.94
15	2	101	CRT	C24-C23-C25	2.06	121.38	118.10
9	y	401	BCL	C5-C3-C2	2.06	125.32	121.10
9	8	102	BCL	CHC-C1C-NC	2.06	127.36	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	301	BCL	CAC-C3C-C4C	2.06	117.16	112.58
11	L	304	UQ8	C3M-O3-C3	2.06	123.82	116.44
9	D	101	BCL	C1-O2A-CGA	2.06	121.72	116.77
9	4	102	BCL	CBB-CAB-C3B	2.06	126.39	120.39
9	K	101	BCL	CHC-C1C-NC	2.07	127.37	124.51
9	B	101	BCL	CBB-CAB-C3B	2.07	126.41	120.39
9	j	101	BCL	C2A-C1A-CHA	2.07	127.59	123.92
15	G	101	CRT	C29-C28-C30	2.07	121.40	118.10
9	p	104	BCL	CBC-CAC-C3C	2.07	118.21	113.51
15	6	101	CRT	C24-C23-C25	2.07	121.40	118.10
9	c	102	BCL	C3C-C2C-C1C	2.07	105.22	101.87
9	L	305	BCL	OBD-CAD-C3D	2.07	131.85	128.03
9	AB	101	BCL	C5-C3-C2	2.07	125.35	121.10
9	5	102	BCL	C1-O2A-CGA	2.08	121.75	116.77
9	d	101	BCL	C5-C3-C2	2.08	125.35	121.10
9	l	101	BCL	C3C-C2C-C1C	2.08	105.23	101.87
9	z	102	BCL	C2A-C1A-CHA	2.08	127.60	123.92
15	AH	102	CRT	C13-C12-C11	2.08	121.41	118.10
15	R	101	CRT	C11-C12-C14	2.08	122.13	118.94
11	L	304	UQ8	C46-C44-C45	2.08	119.46	114.60
9	m	103	BCL	CBB-CAB-C3B	2.08	126.45	120.39
15	s	101	CRT	C29-C28-C30	2.09	121.42	118.10
15	X	101	CRT	O2-C38-C37	2.09	111.89	106.29
9	h	101	BCL	CHC-C1C-NC	2.09	127.40	124.51
9	R	102	BCL	CMD-C2D-C3D	2.10	128.78	124.89
12	x	306	PEF	O3-C30-C31	2.10	121.87	112.44
9	Y	101	BCL	C3C-C2C-C1C	2.10	105.25	101.87
9	AJ	102	BCL	C4A-NA-C1A	2.10	109.05	106.45
9	8	102	BCL	C1-C2-C3	2.10	129.82	125.96
14	M	403	MQ8	C9-C10-C1	2.10	123.24	120.11
9	y	401	BCL	CAA-C2A-C3A	2.10	118.57	112.81
11	L	304	UQ8	C41-C42-C43	2.11	119.19	111.97
9	Q	101	BCL	CBB-CAB-C3B	2.11	126.52	120.39
9	d	101	BCL	CBB-CAB-C3B	2.11	126.53	120.39
9	W	101	BCL	O2A-CGA-CBA	2.11	118.05	111.90
15	N	101	CRT	C18-C17-C16	2.11	121.47	118.10
15	9	102	CRT	C18-C17-C16	2.11	121.47	118.10
11	L	304	UQ8	O5-C5-C6	2.12	125.72	121.82
9	AB	101	BCL	CBB-CAB-C3B	2.12	126.55	120.39
9	x	305	BCL	C4A-NA-C1A	2.12	109.08	106.45
9	V	101	BCL	C2A-C1A-CHA	2.12	127.67	123.92
9	Z	102	BCL	O2A-CGA-CBA	2.12	118.07	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	304	PEF	O2-C2-C3	2.12	116.14	108.44
9	AE	104	BCL	CBB-CAB-C3B	2.12	126.56	120.39
9	k	102	BCL	CBB-CAB-C3B	2.12	126.56	120.39
15	G	101	CRT	C13-C12-C11	2.13	121.49	118.10
9	AJ	102	BCL	C1-O2A-CGA	2.13	121.88	116.77
9	z	102	BCL	C1-O2A-CGA	2.13	121.89	116.77
10	M	402	BPH	CMA-C3A-C4A	2.14	118.78	112.37
9	L	303	BCL	C6-C7-C8	2.14	122.75	115.73
9	v	102	BCL	CBB-CAB-C3B	2.14	126.61	120.39
9	h	101	BCL	CBB-CAB-C3B	2.14	126.62	120.39
11	x	304	UQ8	C42-C41-C39	2.14	120.19	112.93
9	5	102	BCL	O2A-CGA-CBA	2.15	118.15	111.90
9	D	102	BCL	OBD-CAD-C3D	2.15	131.99	128.03
9	M	401	BCL	CAC-C3C-C4C	2.15	117.36	112.58
9	u	101	BCL	CMD-C2D-C3D	2.15	128.88	124.89
9	I	101	BCL	O2A-CGA-CBA	2.15	118.16	111.90
9	F	101	BCL	C2A-C1A-CHA	2.15	127.73	123.92
9	Z	102	BCL	CHC-C1C-NC	2.15	127.49	124.51
15	k	101	CRT	C13-C12-C11	2.15	121.53	118.10
9	9	103	BCL	CBB-CAB-C3B	2.16	126.66	120.39
9	AA	101	BCL	O2A-CGA-CBA	2.16	118.18	111.90
9	O	101	BCL	CBB-CAB-C3B	2.16	126.67	120.39
9	3	101	BCL	CBB-CAB-C3B	2.16	126.67	120.39
9	m	103	BCL	C3C-C2C-C1C	2.16	105.36	101.87
9	j	101	BCL	CHC-C1C-NC	2.16	127.50	124.51
9	Y	101	BCL	CBB-CAB-C3B	2.16	126.68	120.39
9	W	101	BCL	CBB-CAB-C3B	2.16	126.68	120.39
15	4	101	CRT	C1-C4-C5	2.16	118.46	112.87
14	y	403	MQ8	C45-C43-C44	2.16	119.04	115.29
14	M	403	MQ8	C11-C3-C4	2.17	120.91	118.50
15	f	102	CRT	C29-C28-C30	2.17	121.55	118.10
9	AC	102	BCL	C1-O2A-CGA	2.17	121.97	116.77
9	B	101	BCL	CHC-C1C-NC	2.17	127.51	124.51
9	D	102	BCL	CBB-CAB-C3B	2.17	126.69	120.39
17	S	101	PGW	O01-C02-C03	2.17	116.32	108.44
15	f	102	CRT	C24-C23-C25	2.17	121.56	118.10
9	L	305	BCL	C2A-C1A-CHA	2.17	127.77	123.92
9	G	102	BCL	CBB-CAB-C3B	2.17	126.70	120.39
15	J	101	CRT	C13-C12-C11	2.18	121.57	118.10
9	p	104	BCL	O2A-CGA-CBA	2.18	118.25	111.90
15	k	101	CRT	C1-C4-C5	2.19	118.51	112.87
9	x	303	BCL	CBB-CAB-C3B	2.19	126.75	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	102	CRT	C18-C17-C16	2.19	121.59	118.10
15	4	101	CRT	C31-C30-C28	2.19	132.57	126.42
9	L	305	BCL	CAA-C2A-C3A	2.19	118.82	112.81
15	G	101	CRT	C18-C17-C16	2.19	121.59	118.10
15	E	101	CRT	C24-C23-C25	2.20	121.60	118.10
10	y	402	BPH	O2D-CGD-CBD	2.20	115.22	111.30
15	AJ	101	CRT	C24-C23-C25	2.20	121.61	118.10
9	F	101	BCL	O2A-CGA-CBA	2.20	118.31	111.90
9	g	101	BCL	O2A-CGA-CBA	2.20	118.31	111.90
9	g	101	BCL	C3C-C2C-C1C	2.21	105.43	101.87
10	L	302	BPH	CHB-C1B-NB	2.21	128.97	124.64
9	c	102	BCL	CBB-CAB-C3B	2.21	126.81	120.39
9	P	101	BCL	CHC-C1C-NC	2.21	127.56	124.51
12	t	303	PEF	O3-C3-C2	2.21	114.20	108.66
10	M	402	BPH	OBB-CAB-C3B	2.21	124.37	120.37
9	AI	101	BCL	CBB-CAB-C3B	2.21	126.82	120.39
9	5	102	BCL	CBB-CAB-C3B	2.21	126.82	120.39
9	P	101	BCL	CBB-CAB-C3B	2.21	126.82	120.39
9	V	101	BCL	CBB-CAB-C3B	2.21	126.83	120.39
9	5	101	BCL	C5-C3-C2	2.21	125.63	121.10
9	x	301	BCL	CMB-C2B-C3B	2.22	129.01	124.89
9	l	101	BCL	C3C-C2C-C1C	2.22	105.46	101.87
9	k	102	BCL	C4A-NA-C1A	2.22	109.21	106.45
15	G	101	CRT	C34-C33-C35	2.22	121.64	118.10
9	K	101	BCL	O2A-CGA-CBA	2.22	118.37	111.90
9	Q	101	BCL	CHC-C1C-NC	2.23	127.59	124.51
7	C	504	HEM	CMD-C2D-C3D	2.23	129.14	124.94
9	y	401	BCL	CBA-CAA-C2A	2.23	120.47	113.80
9	l	101	BCL	C2A-C1A-CHA	2.23	127.87	123.92
12	t	303	PEF	O2P-P-O1P	2.23	123.82	112.28
7	o	501	HEM	CMB-C2B-C3B	2.23	129.03	124.89
9	h	101	BCL	C3C-C2C-C1C	2.23	105.47	101.87
15	AL	101	CRT	C18-C17-C16	2.23	121.66	118.10
15	T	101	CRT	C36-C35-C33	2.23	129.27	125.89
9	D	101	BCL	OBD-CAD-C3D	2.23	132.14	128.03
9	p	102	BCL	C3C-C2C-C1C	2.23	105.48	101.87
15	c	101	CRT	C13-C12-C11	2.24	121.66	118.10
9	e	102	BCL	C3C-C2C-C1C	2.24	105.48	101.87
15	X	101	CRT	C10-C11-C12	2.24	132.70	126.42
15	R	101	CRT	C15-C16-C17	2.24	132.71	126.42
9	L	305	BCL	CBB-CAB-C3B	2.24	126.91	120.39
15	8	101	CRT	C1-C4-C5	2.24	118.66	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AL	101	CRT	C8-C7-C6	2.24	121.67	118.10
9	j	101	BCL	CBB-CAB-C3B	2.24	126.92	120.39
15	y	404	CRT	C40-C38-C39	2.25	114.75	110.31
9	f	101	BCL	CBB-CAB-C3B	2.25	126.93	120.39
9	S	102	BCL	CMD-C2D-C3D	2.25	129.07	124.89
9	l	101	BCL	OBD-CAD-C3D	2.25	132.17	128.03
11	x	304	UQ8	C41-C42-C43	2.25	119.69	111.97
15	y	404	CRT	C6-C7-C9	2.25	122.40	118.94
15	c	101	CRT	C34-C33-C35	2.25	121.69	118.10
11	L	304	UQ8	C7-C6-C5	2.26	121.36	118.47
9	J	102	BCL	CAA-C2A-C3A	2.26	119.00	112.81
9	d	101	BCL	CMD-C2D-C3D	2.26	129.09	124.89
12	t	301	PEF	O2P-P-O1P	2.27	124.00	112.28
9	4	102	BCL	CHC-C1C-NC	2.27	127.65	124.51
9	9	103	BCL	C3C-C2C-C1C	2.27	105.54	101.87
9	1	101	BCL	C1-O2A-CGA	2.27	122.22	116.77
9	K	101	BCL	C1-O2A-CGA	2.27	122.23	116.77
9	m	103	BCL	CBC-CAC-C3C	2.28	118.67	113.51
9	A	102	BCL	C2A-C1A-CHA	2.28	127.96	123.92
9	5	102	BCL	CAC-C3C-C4C	2.28	117.64	112.58
11	x	304	UQ8	C35-C34-C36	2.28	119.25	115.29
9	z	102	BCL	CBB-CAB-C3B	2.29	127.05	120.39
9	7	101	BCL	CBB-CAB-C3B	2.29	127.05	120.39
10	x	302	BPH	C6-C5-C3	2.29	117.85	112.66
9	8	102	BCL	CBB-CAB-C3B	2.29	127.05	120.39
9	X	102	BCL	CHC-C1C-NC	2.29	127.68	124.51
9	X	102	BCL	OBD-CAD-C3D	2.29	132.25	128.03
9	AE	102	BCL	CBB-CAB-C3B	2.29	127.06	120.39
15	R	101	CRT	C34-C33-C35	2.30	121.76	118.10
9	u	101	BCL	OBD-CAD-C3D	2.30	132.26	128.03
9	G	102	BCL	C4A-NA-C1A	2.30	109.31	106.45
10	M	402	BPH	CHB-C1B-NB	2.30	129.15	124.64
9	p	104	BCL	CBB-CAB-C3B	2.30	127.09	120.39
9	i	102	BCL	C2A-C1A-CHA	2.31	128.01	123.92
9	j	101	BCL	C1-O2A-CGA	2.31	122.31	116.77
9	L	301	BCL	C4A-NA-C1A	2.31	109.32	106.45
15	U	102	CRT	C34-C33-C35	2.31	121.78	118.10
9	S	102	BCL	O2A-CGA-CBA	2.31	118.63	111.90
9	m	102	BCL	C2A-C1A-CHA	2.31	128.02	123.92
9	5	101	BCL	C3C-C2C-C1C	2.31	105.61	101.87
15	n	101	CRT	C24-C23-C25	2.31	121.78	118.10
15	n	101	CRT	C18-C17-C16	2.32	121.79	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	X	102	BCL	CAA-C2A-C3A	2.32	119.17	112.81
9	D	102	BCL	C1-O2A-CGA	2.32	122.35	116.77
9	AH	103	BCL	C1-C2-C3	2.33	130.24	125.96
9	F	101	BCL	CBB-CAB-C3B	2.33	127.17	120.39
9	I	101	BCL	C2A-C1A-CHA	2.33	128.05	123.92
9	x	303	BCL	O2A-CGA-CBA	2.33	118.69	111.90
9	4	102	BCL	CMD-C2D-C3D	2.34	129.23	124.89
9	x	301	BCL	CAC-C3C-C4C	2.34	117.77	112.58
7	C	501	HEM	CMB-C2B-C3B	2.34	129.24	124.89
9	N	102	BCL	CBB-CAB-C3B	2.34	127.20	120.39
15	U	102	CRT	C24-C23-C25	2.35	121.84	118.10
9	h	101	BCL	CMD-C2D-C3D	2.35	129.25	124.89
9	B	101	BCL	C2A-C1A-CHA	2.35	128.08	123.92
9	AE	102	BCL	C1-O2A-CGA	2.35	122.41	116.77
14	y	403	MQ8	C15-C16-C17	2.35	120.03	111.97
9	0	101	BCL	CBB-CAB-C3B	2.35	127.23	120.39
9	J	102	BCL	C1-O2A-CGA	2.36	122.42	116.77
9	r	101	BCL	C5-C3-C2	2.36	125.94	121.10
9	O	101	BCL	C1-O2A-CGA	2.36	122.44	116.77
9	u	101	BCL	C2A-C1A-CHA	2.36	128.11	123.92
9	9	103	BCL	C2A-C1A-CHA	2.37	128.11	123.92
9	AD	101	BCL	C1-O2A-CGA	2.37	122.46	116.77
11	L	304	UQ8	C20-C19-C21	2.37	119.40	115.29
15	U	102	CRT	C8-C7-C6	2.38	121.88	118.10
9	Y	101	BCL	C2A-C1A-CHA	2.38	128.14	123.92
9	5	101	BCL	CBB-CAB-C3B	2.38	127.32	120.39
9	AI	101	BCL	OBD-CAD-C3D	2.38	132.42	128.03
9	AD	101	BCL	C3C-C2C-C1C	2.39	105.73	101.87
15	f	102	CRT	O2-C38-C37	2.39	112.71	106.29
9	F	101	BCL	CHC-C1C-NC	2.40	127.83	124.51
9	L	305	BCL	CMD-C2D-C3D	2.40	129.34	124.89
11	x	304	UQ8	C32-C31-C29	2.41	121.08	112.93
9	N	102	BCL	CHC-C1C-NC	2.41	127.85	124.51
15	z	101	CRT	C29-C28-C30	2.41	121.95	118.10
9	r	101	BCL	O2A-CGA-CBA	2.42	118.93	111.90
9	h	101	BCL	CMB-C2B-C3B	2.42	129.39	124.89
15	AC	101	CRT	C29-C28-C30	2.42	121.96	118.10
9	U	101	BCL	CBB-CAB-C3B	2.43	127.45	120.39
15	P	102	CRT	C8-C7-C6	2.43	121.97	118.10
15	2	101	CRT	C34-C33-C35	2.43	121.97	118.10
9	y	401	BCL	CBB-CAB-C3B	2.43	127.46	120.39
9	D	101	BCL	C3C-C2C-C1C	2.44	105.81	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	101	BCL	O2A-CGA-CBA	2.44	119.00	111.90
9	B	101	BCL	C3C-C2C-C1C	2.44	105.81	101.87
9	V	101	BCL	OBD-CAD-C3D	2.45	132.54	128.03
9	x	305	BCL	OBD-CAD-C3D	2.45	132.54	128.03
15	6	101	CRT	C18-C17-C16	2.45	122.00	118.10
9	AL	102	BCL	CHC-C1C-NC	2.45	127.90	124.51
10	L	302	BPH	O2D-CGD-CBD	2.46	115.69	111.30
9	Q	101	BCL	C6-C5-C3	2.46	118.23	112.66
10	y	402	BPH	CHB-C1B-NB	2.46	129.46	124.64
15	y	404	CRT	C34-C33-C35	2.46	122.02	118.10
11	x	304	UQ8	O5-C5-C4	2.46	126.19	120.95
9	AH	103	BCL	C2A-C1A-CHA	2.46	128.28	123.92
9	v	102	BCL	C4A-NA-C1A	2.46	109.51	106.45
9	X	102	BCL	C2A-C1A-CHA	2.47	128.29	123.92
9	J	102	BCL	CBA-CAA-C2A	2.47	121.19	113.80
15	T	101	CRT	C18-C17-C16	2.47	122.04	118.10
9	AL	102	BCL	CBB-CAB-C3B	2.47	127.58	120.39
9	I	101	BCL	OBD-CAD-C3D	2.49	132.61	128.03
10	x	302	BPH	C1-O2A-CGA	2.49	122.74	116.77
9	P	101	BCL	CMD-C2D-C3D	2.49	129.51	124.89
9	m	103	BCL	CHC-C1C-NC	2.50	127.97	124.51
9	k	102	BCL	C1-O2A-CGA	2.50	122.77	116.77
9	AH	101	BCL	CBB-CAB-C3B	2.50	127.66	120.39
9	k	102	BCL	CHC-C1C-NC	2.50	127.97	124.51
9	5	102	BCL	CBC-CAC-C3C	2.50	119.19	113.51
9	U	101	BCL	OBD-CAD-C3D	2.51	132.64	128.03
10	x	302	BPH	O2A-CGA-CBA	2.51	119.20	111.90
15	A	103	CRT	C18-C17-C16	2.51	122.10	118.10
9	Q	101	BCL	CBC-CAC-C3C	2.51	119.21	113.51
9	AE	104	BCL	CHC-C1C-NC	2.51	127.99	124.51
12	t	301	PEF	C3-O3-C30	2.51	123.57	117.17
9	s	102	BCL	CBB-CAB-C3B	2.52	127.71	120.39
15	AJ	101	CRT	C9-C10-C11	2.52	130.95	123.23
9	AH	103	BCL	CBB-CAB-C3B	2.52	127.72	120.39
9	c	102	BCL	C2A-C1A-CHA	2.52	128.39	123.92
9	l	101	BCL	CBB-CAB-C3B	2.52	127.72	120.39
9	3	101	BCL	C1-O2A-CGA	2.52	122.82	116.77
9	X	102	BCL	C1-O2A-CGA	2.52	122.83	116.77
15	f	102	CRT	C18-C17-C16	2.53	122.12	118.10
9	y	401	BCL	C2A-C1A-CHA	2.53	128.40	123.92
9	V	101	BCL	CMD-C2D-C3D	2.53	129.59	124.89
9	m	102	BCL	OBD-CAD-C3D	2.53	132.69	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	5	101	BCL	CMD-C2D-C3D	2.54	129.60	124.89
9	X	102	BCL	CBB-CAB-C3B	2.54	127.77	120.39
10	L	302	BPH	C1-O2A-CGA	2.54	122.86	116.77
9	m	103	BCL	C2A-C1A-CHA	2.54	128.43	123.92
15	AD	102	CRT	C11-C12-C14	2.54	122.85	118.94
15	P	102	CRT	C13-C12-C11	2.55	122.15	118.10
15	AE	103	CRT	C29-C28-C30	2.55	122.16	118.10
15	y	404	CRT	C1-C4-C5	2.55	119.45	112.87
9	T	102	BCL	CMD-C2D-C3D	2.55	129.63	124.89
9	K	101	BCL	C2A-C1A-CHA	2.55	128.44	123.92
9	AL	102	BCL	C3C-C2C-C1C	2.56	106.00	101.87
15	AD	102	CRT	C14-C15-C16	2.56	131.07	123.23
9	p	102	BCL	CHC-C1C-NC	2.56	128.05	124.51
9	AH	103	BCL	OBD-CAD-C3D	2.56	132.74	128.03
15	p	103	CRT	C24-C23-C25	2.56	122.18	118.10
14	M	403	MQ8	C24-C23-C25	2.56	119.73	115.29
15	AD	102	CRT	C15-C16-C17	2.56	133.62	126.42
9	L	301	BCL	CMB-C2B-C3B	2.57	129.67	124.89
15	4	101	CRT	C29-C28-C30	2.58	122.20	118.10
9	AA	101	BCL	OBD-CAD-C3D	2.58	132.78	128.03
15	E	101	CRT	C8-C7-C6	2.58	122.21	118.10
15	U	102	CRT	C13-C12-C11	2.59	122.22	118.10
9	K	101	BCL	C3C-C2C-C1C	2.59	106.05	101.87
15	z	101	CRT	C18-C17-C16	2.59	122.22	118.10
15	2	101	CRT	C18-C17-C16	2.59	122.23	118.10
15	c	101	CRT	C24-C23-C25	2.59	122.23	118.10
15	AL	101	CRT	C24-C23-C25	2.60	122.24	118.10
9	I	101	BCL	CHC-C1C-NC	2.60	128.11	124.51
9	Y	101	BCL	OBD-CAD-C3D	2.60	132.82	128.03
15	f	102	CRT	C31-C30-C28	2.60	133.73	126.42
9	L	303	BCL	CBB-CAB-C3B	2.60	127.96	120.39
9	1	101	BCL	CMD-C2D-C3D	2.61	129.73	124.89
15	s	101	CRT	C36-C35-C33	2.61	129.83	125.89
9	R	102	BCL	C1-O2A-CGA	2.61	123.03	116.77
15	AJ	101	CRT	C20-C19-C17	2.61	131.04	127.31
7	o	503	HEM	C4A-C3A-C2A	2.61	108.81	107.00
9	k	102	BCL	OBD-CAD-C3D	2.61	132.84	128.03
9	L	303	BCL	CAA-CBA-CGA	2.61	121.22	113.35
9	i	102	BCL	CHC-C1C-NC	2.61	128.13	124.51
9	F	101	BCL	CBC-CAC-C3C	2.61	119.44	113.51
9	L	301	BCL	C5-C3-C2	2.61	126.45	121.10
9	y	401	BCL	O2A-CGA-CBA	2.62	119.52	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	101	BCL	CMD-C2D-C3D	2.62	129.76	124.89
9	D	102	BCL	CHC-C1C-NC	2.63	128.15	124.51
9	x	301	BCL	OBD-CAD-C3D	2.63	132.88	128.03
9	p	104	BCL	C3C-C2C-C1C	2.63	106.12	101.87
9	1	101	BCL	CBB-CAB-C3B	2.64	128.07	120.39
9	P	101	BCL	CBC-CAC-C3C	2.65	119.51	113.51
9	3	101	BCL	C1-C2-C3	2.65	130.84	125.96
9	T	102	BCL	OBD-CAD-C3D	2.65	132.91	128.03
15	f	102	CRT	C1-C4-C5	2.65	119.72	112.87
9	w	101	BCL	C2A-C1A-CHA	2.65	128.62	123.92
9	i	102	BCL	C1-O2A-CGA	2.66	123.15	116.77
9	l	101	BCL	C2A-C1A-CHA	2.66	128.63	123.92
9	p	104	BCL	CHC-C1C-NC	2.66	128.19	124.51
9	AL	102	BCL	CBC-CAC-C3C	2.66	119.54	113.51
9	x	305	BCL	CBB-CAB-C3B	2.66	128.14	120.39
9	AD	101	BCL	CMD-C2D-C3D	2.67	129.84	124.89
9	AE	104	BCL	C1-O2A-CGA	2.67	123.19	116.77
9	AB	101	BCL	OBD-CAD-C3D	2.68	132.96	128.03
9	O	101	BCL	C3C-C2C-C1C	2.68	106.20	101.87
9	z	102	BCL	C3C-C2C-C1C	2.68	106.20	101.87
9	f	101	BCL	CMD-C2D-C3D	2.68	129.87	124.89
15	z	101	CRT	C24-C23-C25	2.69	122.38	118.10
15	T	101	CRT	C29-C28-C30	2.69	122.38	118.10
9	F	101	BCL	CMD-C2D-C3D	2.69	129.88	124.89
14	y	403	MQ8	C24-C23-C25	2.69	119.96	115.29
15	f	102	CRT	C6-C7-C9	2.69	123.07	118.94
9	d	101	BCL	CHC-C1C-NC	2.70	128.24	124.51
9	p	102	BCL	C1-O2A-CGA	2.70	123.24	116.77
15	AJ	101	CRT	C13-C12-C11	2.70	122.39	118.10
10	x	302	BPH	CHC-C4B-NB	2.70	130.14	124.97
15	AE	103	CRT	C13-C12-C11	2.70	122.41	118.10
9	R	102	BCL	CBB-CAB-C3B	2.70	128.25	120.39
9	K	101	BCL	CMD-C2D-C3D	2.71	129.91	124.89
15	AL	101	CRT	C34-C33-C35	2.71	122.41	118.10
15	N	101	CRT	C13-C12-C11	2.71	122.41	118.10
10	x	302	BPH	CHB-C1B-NB	2.71	129.96	124.64
9	AH	103	BCL	CMB-C2B-C3B	2.72	129.94	124.89
9	x	301	BCL	CBB-CAB-C3B	2.72	128.31	120.39
9	O	101	BCL	C2A-C1A-CHA	2.72	128.75	123.92
12	t	303	PEF	C3-O3-C30	2.73	124.12	117.17
9	x	303	BCL	CBC-CAC-C3C	2.76	119.77	113.51
15	9	102	CRT	C10-C9-C7	2.76	131.25	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	y	404	CRT	C13-C12-C11	2.77	122.51	118.10
7	o	501	HEM	CMC-C2C-C3C	2.77	130.03	124.89
9	L	301	BCL	CBC-CAC-C3C	2.77	119.80	113.51
11	x	304	UQ8	C36-C37-C38	2.78	121.50	111.97
15	AH	102	CRT	C24-C23-C25	2.78	122.53	118.10
9	f	101	BCL	C1-O2A-CGA	2.79	123.46	116.77
9	W	101	BCL	CMB-C2B-C3B	2.79	130.06	124.89
15	e	101	CRT	C8-C7-C6	2.79	122.54	118.10
15	i	101	CRT	C34-C33-C35	2.79	122.55	118.10
7	C	501	HEM	CMD-C2D-C3D	2.80	130.21	124.94
11	L	304	UQ8	C35-C34-C36	2.80	120.14	115.29
9	O	101	BCL	CMD-C2D-C3D	2.80	130.09	124.89
9	X	102	BCL	CMD-C2D-C3D	2.80	130.09	124.89
9	w	101	BCL	C1-O2A-CGA	2.80	123.50	116.77
15	Z	101	CRT	C34-C33-C35	2.80	122.57	118.10
15	Z	101	CRT	C13-C12-C11	2.81	122.57	118.10
10	L	302	BPH	CHC-C4B-NB	2.81	130.35	124.97
15	6	101	CRT	C8-C7-C6	2.81	122.57	118.10
16	t	302	PO4	O4-P-O2	2.81	118.22	107.90
10	y	402	BPH	O2A-CGA-CBA	2.81	120.08	111.90
11	x	304	UQ8	O3-C3-C2	2.82	125.36	116.60
15	f	102	CRT	C13-C12-C11	2.82	122.60	118.10
15	E	101	CRT	C34-C33-C35	2.83	122.61	118.10
10	M	402	BPH	CHC-C4B-NB	2.84	130.41	124.97
9	Q	101	BCL	CMD-C2D-C3D	2.84	130.16	124.89
10	M	402	BPH	CED-O2D-CGD	2.84	122.62	115.97
12	y	407	PEF	O3-C3-C2	2.84	115.79	108.66
15	9	102	CRT	C29-C28-C30	2.84	122.62	118.10
10	x	302	BPH	C4D-C3D-CAD	2.84	109.40	107.78
9	x	305	BCL	O2A-CGA-CBA	2.85	120.19	111.90
9	J	102	BCL	C2A-C1A-CHA	2.85	128.97	123.92
10	L	302	BPH	C4D-C3D-CAD	2.85	109.41	107.78
9	Z	102	BCL	CMB-C2B-C3B	2.86	130.19	124.89
9	m	103	BCL	CMD-C2D-C3D	2.86	130.20	124.89
9	e	102	BCL	CBB-CAB-C3B	2.86	128.72	120.39
15	J	101	CRT	C29-C28-C30	2.87	122.67	118.10
15	P	102	CRT	C34-C33-C35	2.87	122.67	118.10
9	G	102	BCL	OBD-CAD-C3D	2.87	133.32	128.03
9	AB	101	BCL	C1-O2A-CGA	2.89	123.70	116.77
11	x	304	UQ8	C6-C1-C2	2.89	123.31	120.29
9	d	101	BCL	C2A-C1A-CHA	2.89	129.04	123.92
9	L	305	BCL	CMB-C2B-C3B	2.90	130.28	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	101	CRT	C34-C33-C35	2.91	122.74	118.10
9	AE	102	BCL	C2A-C1A-CHA	2.93	129.11	123.92
9	B	101	BCL	CMD-C2D-C3D	2.93	130.33	124.89
9	4	102	BCL	C1-O2A-CGA	2.94	123.82	116.77
9	W	101	BCL	OBD-CAD-C3D	2.94	133.44	128.03
9	g	101	BCL	C2A-C1A-CHA	2.95	129.14	123.92
9	AE	102	BCL	C3C-C2C-C1C	2.95	106.63	101.87
17	S	101	PGW	O03-C01-C02	2.95	116.07	108.66
9	0	101	BCL	CMD-C2D-C3D	2.95	130.37	124.89
15	A	103	CRT	C1-C4-C5	2.96	120.51	112.87
15	c	101	CRT	C18-C17-C16	2.96	122.82	118.10
12	M	407	PEF	O2P-P-O1P	2.97	127.66	112.28
14	M	403	MQ8	C34-C33-C35	2.98	120.46	115.29
15	A	103	CRT	C34-C33-C35	2.98	122.85	118.10
9	Z	102	BCL	CBB-CAB-C3B	2.98	129.07	120.39
9	G	102	BCL	CMD-C2D-C3D	2.99	130.44	124.89
9	g	101	BCL	CMD-C2D-C3D	2.99	130.44	124.89
15	4	101	CRT	C35-C33-C32	2.99	123.54	118.94
15	n	101	CRT	C9-C10-C11	3.00	132.42	123.23
9	p	104	BCL	C2A-C1A-CHA	3.00	129.23	123.92
9	M	401	BCL	CBB-CAB-C3B	3.01	129.14	120.39
15	v	101	CRT	C13-C12-C11	3.01	122.90	118.10
9	0	101	BCL	C5-C3-C2	3.01	127.27	121.10
7	C	502	HEM	C1D-C2D-C3D	3.02	109.10	107.00
9	AE	102	BCL	OBD-CAD-C3D	3.02	133.59	128.03
15	y	404	CRT	C36-C35-C33	3.02	130.46	125.89
15	J	101	CRT	C8-C7-C6	3.02	122.91	118.10
12	m	101	PEF	O3-C3-C2	3.02	116.25	108.66
15	AD	102	CRT	C18-C17-C16	3.02	122.92	118.10
9	m	102	BCL	CMD-C2D-C3D	3.02	130.50	124.89
7	C	501	HEM	CMC-C2C-C3C	3.02	130.50	124.89
9	M	401	BCL	C2A-C1A-CHA	3.03	129.28	123.92
10	y	402	BPH	C4D-C3D-CAD	3.03	109.51	107.78
9	L	301	BCL	CBB-CAB-C3B	3.04	129.22	120.39
9	U	101	BCL	CMD-C2D-C3D	3.04	130.54	124.89
9	7	101	BCL	CMB-C2B-C3B	3.05	130.54	124.89
10	y	402	BPH	OBB-CAB-C3B	3.05	125.89	120.37
9	AH	101	BCL	CHC-C1C-NC	3.05	128.72	124.51
9	AI	101	BCL	C2A-C1A-CHA	3.05	129.32	123.92
15	s	101	CRT	C34-C33-C35	3.05	122.96	118.10
9	G	102	BCL	C2A-C1A-CHA	3.05	129.33	123.92
9	B	101	BCL	C1-O2A-CGA	3.05	124.10	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AH	101	BCL	OBD-CAD-C3D	3.06	133.66	128.03
9	AC	102	BCL	CMD-C2D-C3D	3.06	130.58	124.89
12	t	303	PEF	O3-C30-C31	3.07	126.24	112.44
15	4	101	CRT	C24-C23-C25	3.08	123.01	118.10
17	AE	101	PGW	C02-O01-C1	3.08	123.89	117.94
9	c	102	BCL	C1-O2A-CGA	3.09	124.18	116.77
9	AH	103	BCL	CMD-C2D-C3D	3.09	130.63	124.89
9	c	102	BCL	CMD-C2D-C3D	3.10	130.64	124.89
9	Q	101	BCL	CMB-C2B-C3B	3.10	130.64	124.89
9	S	102	BCL	CHC-C1C-NC	3.11	128.81	124.51
7	o	502	HEM	CMC-C2C-C3C	3.11	130.67	124.89
9	A	102	BCL	CMD-C2D-C3D	3.12	130.68	124.89
15	E	101	CRT	C18-C17-C16	3.12	123.07	118.10
7	C	504	HEM	C4C-C3C-C2C	3.13	109.08	106.90
9	AJ	102	BCL	CMD-C2D-C3D	3.14	130.71	124.89
9	i	102	BCL	CMD-C2D-C3D	3.14	130.72	124.89
9	Z	102	BCL	C2A-C1A-CHA	3.14	129.49	123.92
11	x	304	UQ8	O4-C4-C5	3.14	126.37	116.60
15	J	101	CRT	C4-C5-C6	3.15	129.10	124.57
9	AE	102	BCL	CMD-C2D-C3D	3.16	130.75	124.89
9	AD	101	BCL	CMB-C2B-C3B	3.16	130.75	124.89
9	U	101	BCL	CHC-C1C-NC	3.17	128.89	124.51
9	AE	104	BCL	CMD-C2D-C3D	3.17	130.77	124.89
9	D	101	BCL	CMD-C2D-C3D	3.18	130.79	124.89
15	T	101	CRT	C34-C33-C35	3.18	123.16	118.10
17	S	101	PGW	O01-C1-C2	3.18	117.07	111.10
15	AC	101	CRT	C18-C17-C16	3.18	123.17	118.10
15	AJ	101	CRT	C34-C33-C35	3.18	123.17	118.10
9	F	101	BCL	C1-O2A-CGA	3.19	124.43	116.77
9	AB	101	BCL	CMD-C2D-C3D	3.19	130.82	124.89
10	M	402	BPH	O2A-CGA-CBA	3.20	121.21	111.90
9	AK	101	BCL	CMD-C2D-C3D	3.20	130.83	124.89
9	L	303	BCL	OBD-CAD-C3D	3.21	133.93	128.03
9	AK	101	BCL	C2A-C1A-CHA	3.21	129.60	123.92
10	L	302	BPH	O2A-CGA-CBA	3.22	121.26	111.90
9	8	102	BCL	CMD-C2D-C3D	3.22	130.87	124.89
14	y	403	MQ8	C14-C13-C15	3.22	120.88	115.29
9	p	104	BCL	CMD-C2D-C3D	3.22	130.87	124.89
9	x	305	BCL	C3C-C2C-C1C	3.23	107.08	101.87
10	y	402	BPH	CHC-C4B-NB	3.23	131.16	124.97
9	x	305	BCL	C2A-C1A-CHA	3.23	129.65	123.92
9	p	104	BCL	OBD-CAD-C3D	3.23	133.98	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	101	BCL	CMD-C2D-C3D	3.24	130.90	124.89
9	D	102	BCL	C2A-C1A-CHA	3.24	129.66	123.92
15	AJ	101	CRT	C21-C20-C19	3.26	130.42	123.46
15	4	101	CRT	C18-C17-C16	3.27	123.31	118.10
9	m	103	BCL	C1-C2-C3	3.28	132.00	125.96
9	x	303	BCL	C2A-C1A-CHA	3.28	129.74	123.92
9	i	102	BCL	CMB-C2B-C3B	3.28	130.99	124.89
9	k	102	BCL	CMB-C2B-C3B	3.29	130.99	124.89
9	5	102	BCL	CMB-C2B-C3B	3.29	131.00	124.89
10	M	402	BPH	C4D-C3D-CAD	3.30	109.66	107.78
15	AJ	101	CRT	C36-C35-C33	3.32	130.92	125.89
12	H	304	PEF	O3-C3-C2	3.33	117.01	108.66
15	2	101	CRT	C13-C12-C11	3.33	123.40	118.10
9	Y	101	BCL	CMB-C2B-C3B	3.35	131.11	124.89
9	T	102	BCL	C1-O2A-CGA	3.35	124.81	116.77
9	L	303	BCL	CMB-C2B-C3B	3.36	131.12	124.89
15	T	101	CRT	C13-C12-C11	3.37	123.47	118.10
9	W	101	BCL	C1-O2A-CGA	3.38	124.88	116.77
9	7	101	BCL	C1-O2A-CGA	3.38	124.89	116.77
9	AA	101	BCL	CMD-C2D-C3D	3.39	131.18	124.89
9	U	101	BCL	CMB-C2B-C3B	3.39	131.19	124.89
9	1	102	BCL	CMB-C2B-C3B	3.40	131.20	124.89
15	Z	101	CRT	C24-C23-C25	3.40	123.52	118.10
11	L	304	UQ8	C15-C14-C16	3.41	121.20	115.29
9	X	102	BCL	CMB-C2B-C3B	3.43	131.26	124.89
9	K	101	BCL	CMB-C2B-C3B	3.44	131.28	124.89
9	AA	101	BCL	CMB-C2B-C3B	3.45	131.28	124.89
9	d	101	BCL	CMB-C2B-C3B	3.45	131.29	124.89
9	J	102	BCL	CMB-C2B-C3B	3.45	131.30	124.89
9	s	102	BCL	C2A-C1A-CHA	3.46	130.05	123.92
9	4	102	BCL	CMB-C2B-C3B	3.47	131.34	124.89
15	N	101	CRT	C1-C4-C5	3.48	121.84	112.87
15	X	101	CRT	C9-C10-C11	3.50	133.97	123.23
9	D	101	BCL	CMB-C2B-C3B	3.51	131.40	124.89
9	AE	102	BCL	CMB-C2B-C3B	3.51	131.40	124.89
9	e	102	BCL	CMD-C2D-C3D	3.51	131.40	124.89
9	9	103	BCL	CMB-C2B-C3B	3.52	131.42	124.89
15	8	101	CRT	C25-C23-C22	3.53	124.35	118.94
9	8	102	BCL	OBD-CAD-C3D	3.53	134.54	128.03
12	y	408	PEF	C3-C2-C1	3.55	119.86	111.86
15	e	101	CRT	C34-C33-C35	3.55	123.75	118.10
9	AI	101	BCL	O2A-CGA-CBA	3.55	122.23	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	o	503	HEM	CBA-CAA-C2A	3.55	119.27	112.48
15	Z	101	CRT	C18-C17-C16	3.56	123.77	118.10
9	9	103	BCL	C1-O2A-CGA	3.58	125.36	116.77
9	P	101	BCL	C2A-C1A-CHA	3.58	130.27	123.92
9	s	102	BCL	CMD-C2D-C3D	3.58	131.54	124.89
9	T	102	BCL	CMB-C2B-C3B	3.58	131.54	124.89
12	A	101	PEF	C3-O3-C30	3.59	126.29	117.17
9	AL	102	BCL	CMB-C2B-C3B	3.59	131.55	124.89
9	z	102	BCL	CMB-C2B-C3B	3.61	131.59	124.89
7	C	502	HEM	CMC-C2C-C3C	3.63	131.62	124.89
12	M	406	PEF	C3-O3-C30	3.63	126.40	117.17
11	L	304	UQ8	C10-C9-C11	3.63	121.59	115.29
9	y	401	BCL	C1-O2A-CGA	3.64	125.50	116.77
9	AI	101	BCL	CMB-C2B-C3B	3.65	131.66	124.89
7	o	502	HEM	C4A-C3A-C2A	3.65	109.53	107.00
7	o	504	HEM	C4A-C3A-C2A	3.66	109.54	107.00
9	Q	101	BCL	C1-O2A-CGA	3.66	125.56	116.77
9	g	101	BCL	CMB-C2B-C3B	3.66	131.69	124.89
9	x	305	BCL	C1-O2A-CGA	3.67	125.57	116.77
15	f	102	CRT	C32-C31-C30	3.67	134.49	123.23
9	W	101	BCL	CMD-C2D-C3D	3.67	131.71	124.89
15	N	101	CRT	C29-C28-C30	3.71	124.00	118.10
9	v	102	BCL	C2A-C1A-CHA	3.71	130.49	123.92
9	A	102	BCL	CMB-C2B-C3B	3.71	131.78	124.89
9	c	102	BCL	CMB-C2B-C3B	3.72	131.79	124.89
9	v	102	BCL	CMD-C2D-C3D	3.72	131.79	124.89
9	Z	102	BCL	CMD-C2D-C3D	3.74	131.83	124.89
9	r	101	BCL	CMB-C2B-C3B	3.78	131.90	124.89
12	L	306	PEF	O3P-C1-C2	3.78	119.83	108.61
9	u	101	BCL	CMB-C2B-C3B	3.80	131.93	124.89
14	M	403	MQ8	C14-C13-C15	3.81	121.89	115.29
9	U	101	BCL	O2D-CGD-CBD	3.81	118.11	111.30
9	m	102	BCL	CMB-C2B-C3B	3.82	131.98	124.89
9	p	102	BCL	CMB-C2B-C3B	3.82	131.98	124.89
9	AC	102	BCL	CMB-C2B-C3B	3.83	132.00	124.89
12	x	306	PEF	O2-C10-C11	3.83	118.30	111.10
15	6	101	CRT	C34-C33-C35	3.87	124.26	118.10
9	L	301	BCL	C2A-C1A-CHA	3.88	130.79	123.92
10	M	402	BPH	O2D-CGD-CBD	3.88	118.23	111.30
11	L	304	UQ8	C30-C29-C31	3.89	122.03	115.29
9	l	101	BCL	CMB-C2B-C3B	3.89	132.11	124.89
11	x	304	UQ8	C40-C39-C41	3.89	122.04	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	y	401	BCL	OBD-CAD-C3D	3.89	135.20	128.03
9	x	303	BCL	O2D-CGD-CBD	3.90	118.26	111.30
9	m	103	BCL	CMB-C2B-C3B	3.90	132.12	124.89
9	1	102	BCL	C2A-C1A-CHA	3.90	130.84	123.92
9	Y	101	BCL	CBC-CAC-C3C	3.91	122.37	113.51
9	L	301	BCL	O2A-CGA-CBA	3.91	123.28	111.90
9	L	301	BCL	O2D-CGD-CBD	3.92	118.31	111.30
9	8	102	BCL	CMB-C2B-C3B	3.92	132.17	124.89
9	S	102	BCL	CMB-C2B-C3B	3.93	132.18	124.89
17	AE	101	PGW	O01-C1-C2	3.93	118.48	111.10
9	k	102	BCL	C2A-C1A-CHA	3.95	130.92	123.92
12	H	303	PEF	O2-C10-C11	3.95	118.52	111.10
9	5	102	BCL	C2A-C1A-CHA	3.96	130.94	123.92
12	y	408	PEF	O2-C10-C11	3.96	118.54	111.10
9	1	102	BCL	CMD-C2D-C3D	3.99	132.30	124.89
9	Y	101	BCL	CAC-C3C-C4C	4.01	121.48	112.58
9	I	101	BCL	CMB-C2B-C3B	4.03	132.37	124.89
9	R	102	BCL	CMB-C2B-C3B	4.03	132.37	124.89
15	v	101	CRT	C29-C28-C30	4.04	124.53	118.10
9	AK	101	BCL	CMB-C2B-C3B	4.05	132.40	124.89
9	x	303	BCL	CAC-C3C-C4C	4.06	121.59	112.58
9	v	102	BCL	CMB-C2B-C3B	4.07	132.44	124.89
9	w	101	BCL	CMB-C2B-C3B	4.07	132.45	124.89
9	w	101	BCL	O2D-CGD-CBD	4.08	118.59	111.30
15	v	101	CRT	C4-C5-C6	4.09	130.45	124.57
9	s	102	BCL	CMB-C2B-C3B	4.09	132.48	124.89
9	V	101	BCL	CMB-C2B-C3B	4.09	132.48	124.89
9	F	101	BCL	CMB-C2B-C3B	4.12	132.54	124.89
9	m	103	BCL	OBD-CAD-C3D	4.13	135.64	128.03
9	x	301	BCL	C4A-NA-C1A	4.13	111.58	106.45
9	L	303	BCL	C6-C5-C3	4.13	122.03	112.66
9	Q	101	BCL	O2D-CGD-CBD	4.15	118.71	111.30
11	L	304	UQ8	C40-C39-C41	4.17	122.52	115.29
9	x	305	BCL	CMD-C2D-C3D	4.19	132.67	124.89
12	A	101	PEF	O2-C10-C11	4.21	119.01	111.10
15	R	101	CRT	C18-C17-C16	4.23	124.84	118.10
7	C	502	HEM	C4A-C3A-C2A	4.24	109.95	107.00
9	AJ	102	BCL	CMB-C2B-C3B	4.25	132.78	124.89
9	G	102	BCL	CMB-C2B-C3B	4.27	132.82	124.89
9	e	102	BCL	CMB-C2B-C3B	4.27	132.82	124.89
9	5	101	BCL	CMB-C2B-C3B	4.28	132.83	124.89
9	X	102	BCL	O2D-CGD-CBD	4.29	118.96	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AD	101	BCL	O2D-CGD-CBD	4.31	119.00	111.30
9	D	102	BCL	CMD-C2D-C3D	4.33	132.92	124.89
9	0	101	BCL	CMB-C2B-C3B	4.33	132.93	124.89
11	x	304	UQ8	C25-C24-C26	4.34	122.81	115.29
7	C	501	HEM	CAD-CBD-CGD	4.35	120.10	112.66
9	N	102	BCL	CMB-C2B-C3B	4.35	132.97	124.89
9	AH	101	BCL	O2D-CGD-CBD	4.36	119.09	111.30
15	X	101	CRT	C21-C20-C19	4.36	132.78	123.46
9	y	401	BCL	CMB-C2B-C3B	4.38	133.02	124.89
9	L	303	BCL	O2D-CGD-CBD	4.41	119.18	111.30
12	m	101	PEF	O2-C10-C11	4.42	119.39	111.10
9	AE	104	BCL	CMB-C2B-C3B	4.48	133.20	124.89
9	5	102	BCL	CMD-C2D-C3D	4.48	133.20	124.89
9	v	102	BCL	O2D-CGD-CBD	4.49	119.33	111.30
9	AH	101	BCL	CMB-C2B-C3B	4.50	133.24	124.89
9	M	401	BCL	OBD-CAD-C3D	4.51	136.33	128.03
15	U	102	CRT	C3-C1-C2	4.52	119.24	110.31
9	d	101	BCL	C1-O2A-CGA	4.52	127.61	116.77
11	x	304	UQ8	C30-C29-C31	4.52	123.13	115.29
9	K	101	BCL	O2D-CGD-CBD	4.52	119.38	111.30
15	J	101	CRT	C5-C6-C7	4.52	132.72	125.89
15	k	101	CRT	C25-C23-C22	4.53	125.89	118.94
9	B	101	BCL	CMB-C2B-C3B	4.53	133.30	124.89
12	M	408	PEF	O2-C10-C11	4.53	119.61	111.10
15	c	101	CRT	C3-C1-C2	4.55	119.30	110.31
10	x	302	BPH	O2D-CGD-CBD	4.55	119.42	111.30
9	k	102	BCL	O2D-CGD-CBD	4.57	119.47	111.30
9	AE	102	BCL	O2D-CGD-CBD	4.58	119.49	111.30
9	3	101	BCL	CMB-C2B-C3B	4.59	133.41	124.89
9	I	101	BCL	O2D-CGD-CBD	4.60	119.53	111.30
9	x	303	BCL	CMB-C2B-C3B	4.61	133.45	124.89
9	p	104	BCL	CMB-C2B-C3B	4.62	133.46	124.89
9	f	101	BCL	CMB-C2B-C3B	4.62	133.47	124.89
15	s	101	CRT	C3-C1-C2	4.63	119.48	110.31
9	G	102	BCL	O2D-CGD-CBD	4.66	119.63	111.30
11	x	304	UQ8	C15-C14-C16	4.66	123.38	115.29
9	O	101	BCL	O2D-CGD-CBD	4.66	119.63	111.30
15	i	101	CRT	C3-C1-C2	4.66	119.53	110.31
15	9	102	CRT	C3-C1-C2	4.69	119.59	110.31
9	AB	101	BCL	O2D-CGD-CBD	4.74	119.76	111.30
15	n	101	CRT	C10-C9-C7	4.76	134.10	127.31
9	j	101	BCL	CMB-C2B-C3B	4.79	133.79	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AB	101	BCL	CMB-C2B-C3B	4.82	133.83	124.89
9	AI	101	BCL	O2D-CGD-CBD	4.83	119.94	111.30
9	AI	101	BCL	CMD-C2D-C3D	4.83	133.86	124.89
9	0	101	BCL	O2D-CGD-CBD	4.84	119.94	111.30
9	T	102	BCL	O2D-CGD-CBD	4.84	119.95	111.30
9	D	102	BCL	CMB-C2B-C3B	4.85	133.89	124.89
9	R	102	BCL	O2D-CGD-CBD	4.86	119.99	111.30
9	M	401	BCL	CMB-C2B-C3B	4.86	133.91	124.89
9	m	102	BCL	O2D-CGD-CBD	4.87	120.01	111.30
9	AC	102	BCL	O2D-CGD-CBD	4.88	120.03	111.30
9	AA	101	BCL	O2D-CGD-CBD	4.89	120.03	111.30
9	P	101	BCL	CMB-C2B-C3B	4.89	133.97	124.89
15	v	101	CRT	C8-C7-C6	4.91	125.92	118.10
9	p	104	BCL	O2D-CGD-CBD	4.91	120.08	111.30
15	R	101	CRT	C3-C1-C2	4.92	120.05	110.31
9	1	101	BCL	CMB-C2B-C3B	4.93	134.04	124.89
9	p	102	BCL	O2D-CGD-CBD	4.94	120.12	111.30
9	AK	101	BCL	O2D-CGD-CBD	4.94	120.13	111.30
9	u	101	BCL	O2D-CGD-CBD	4.95	120.14	111.30
12	y	407	PEF	O2-C10-C11	4.97	120.44	111.10
15	AE	103	CRT	C3-C1-C2	4.99	120.17	110.31
9	r	101	BCL	O2D-CGD-CBD	4.99	120.22	111.30
9	B	101	BCL	O2D-CGD-CBD	4.99	120.22	111.30
9	AH	103	BCL	O2D-CGD-CBD	5.05	120.32	111.30
9	N	102	BCL	O2D-CGD-CBD	5.06	120.34	111.30
15	E	101	CRT	C3-C1-C2	5.07	120.34	110.31
15	6	101	CRT	C3-C1-C2	5.09	120.38	110.31
15	G	101	CRT	C3-C1-C2	5.12	120.43	110.31
9	W	101	BCL	O2D-CGD-CBD	5.13	120.46	111.30
9	3	101	BCL	O2D-CGD-CBD	5.14	120.48	111.30
9	7	101	BCL	O2D-CGD-CBD	5.14	120.48	111.30
10	x	302	BPH	C1C-NC-C4C	5.14	115.16	110.54
15	z	101	CRT	C3-C1-C2	5.14	120.48	110.31
9	F	101	BCL	O2D-CGD-CBD	5.15	120.50	111.30
9	O	101	BCL	CMB-C2B-C3B	5.16	134.47	124.89
9	D	101	BCL	O2D-CGD-CBD	5.20	120.59	111.30
9	j	101	BCL	O2D-CGD-CBD	5.20	120.60	111.30
15	M	404	CRT	C3-C1-C2	5.20	120.60	110.31
9	e	102	BCL	O2D-CGD-CBD	5.21	120.61	111.30
9	P	101	BCL	O2D-CGD-CBD	5.23	120.65	111.30
12	H	301	PEF	O2-C10-C11	5.24	120.94	111.10
9	c	102	BCL	O2D-CGD-CBD	5.24	120.67	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	101	BCL	O2D-CGD-CBD	5.26	120.70	111.30
9	m	103	BCL	O2D-CGD-CBD	5.27	120.71	111.30
9	5	101	BCL	O2D-CGD-CBD	5.31	120.79	111.30
15	k	101	CRT	C3-C1-C2	5.33	120.85	110.31
9	V	101	BCL	O2D-CGD-CBD	5.34	120.84	111.30
12	y	408	PEF	C3-O3-C30	5.36	130.82	117.17
9	y	401	BCL	O2D-CGD-CBD	5.39	120.94	111.30
15	y	404	CRT	C3-C1-C2	5.44	121.07	110.31
12	H	304	PEF	O2-C10-C11	5.44	121.32	111.10
12	t	303	PEF	O2-C10-C11	5.46	121.35	111.10
15	8	101	CRT	C3-C1-C2	5.48	121.15	110.31
9	1	102	BCL	O2D-CGD-CBD	5.55	121.22	111.30
9	8	102	BCL	O2D-CGD-CBD	5.56	121.23	111.30
12	y	406	PEF	O2-C10-C11	5.57	121.56	111.10
15	n	101	CRT	C3-C1-C2	5.59	121.36	110.31
9	Y	101	BCL	O2D-CGD-CBD	5.60	121.31	111.30
9	J	102	BCL	O2D-CGD-CBD	5.60	121.31	111.30
9	i	102	BCL	O2D-CGD-CBD	5.61	121.33	111.30
9	h	101	BCL	O2D-CGD-CBD	5.63	121.36	111.30
9	S	102	BCL	O2D-CGD-CBD	5.64	121.37	111.30
15	A	103	CRT	C3-C1-C2	5.64	121.46	110.31
9	A	102	BCL	O2D-CGD-CBD	5.64	121.37	111.30
9	d	101	BCL	O2D-CGD-CBD	5.65	121.40	111.30
9	9	103	BCL	O2D-CGD-CBD	5.67	121.43	111.30
15	4	101	CRT	C3-C1-C2	5.69	121.56	110.31
15	p	103	CRT	C3-C1-C2	5.69	121.57	110.31
10	L	302	BPH	C1C-NC-C4C	5.69	115.66	110.54
9	z	102	BCL	O2D-CGD-CBD	5.72	121.52	111.30
9	L	305	BCL	O2D-CGD-CBD	5.72	121.52	111.30
9	D	102	BCL	O2D-CGD-CBD	5.73	121.55	111.30
9	Z	102	BCL	O2D-CGD-CBD	5.76	121.59	111.30
9	AE	104	BCL	O2D-CGD-CBD	5.78	121.62	111.30
15	f	102	CRT	C3-C1-C2	5.79	121.76	110.31
10	M	402	BPH	C1C-NC-C4C	5.82	115.77	110.54
9	1	101	BCL	O2D-CGD-CBD	5.85	121.75	111.30
9	x	305	BCL	O2D-CGD-CBD	5.88	121.81	111.30
9	AL	102	BCL	O2D-CGD-CBD	5.89	121.82	111.30
9	g	101	BCL	O2D-CGD-CBD	5.97	121.96	111.30
9	f	101	BCL	O2D-CGD-CBD	5.97	121.97	111.30
15	AD	102	CRT	C3-C1-C2	5.98	122.14	110.31
9	x	301	BCL	O2D-CGD-CBD	5.99	122.00	111.30
15	v	101	CRT	C3-C1-C2	6.00	122.18	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AH	102	CRT	C3-C1-C2	6.01	122.20	110.31
15	J	101	CRT	C3-C1-C2	6.05	122.27	110.31
15	N	101	CRT	C3-C1-C2	6.07	122.31	110.31
12	M	406	PEF	O2-C10-C11	6.07	122.50	111.10
10	y	402	BPH	C1C-NC-C4C	6.11	116.04	110.54
9	M	401	BCL	O2D-CGD-CBD	6.12	122.23	111.30
15	v	101	CRT	C5-C6-C7	6.26	135.36	125.89
9	s	102	BCL	O2D-CGD-CBD	6.34	122.63	111.30
9	AJ	102	BCL	O2D-CGD-CBD	6.47	122.87	111.30
9	4	102	BCL	O2D-CGD-CBD	6.49	122.91	111.30
9	L	303	BCL	C1-O2A-CGA	6.64	132.70	116.77
10	L	302	BPH	C4A-NA-C1A	7.02	113.84	108.16
10	x	302	BPH	C4A-NA-C1A	7.18	113.96	108.16
9	5	102	BCL	O2D-CGD-CBD	7.26	124.27	111.30
15	T	101	CRT	C3-C1-C2	7.32	124.78	110.31
10	M	402	BPH	C4A-NA-C1A	7.86	114.51	108.16
10	y	402	BPH	C4A-NA-C1A	8.46	115.00	108.16

There are no chirality outliers.

All (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
9	g	101	BCL	CED-O2D-CGD-CBD
9	O	101	BCL	CED-O2D-CGD-CBD
9	X	102	BCL	CED-O2D-CGD-CBD
9	AE	104	BCL	CED-O2D-CGD-CBD
9	z	102	BCL	CED-O2D-CGD-CBD
9	AB	101	BCL	CED-O2D-CGD-CBD
9	N	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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
9	D	102	BCL	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
9	X	102	BCL	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

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

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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

All (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
5	A	53	VAL	15.0
5	Y	3	THR	14.4
5	A	52	PRO	13.3
5	O	52	PRO	13.2
5	AE	54	SER	13.0
5	7	3	THR	12.2
5	u	13	LEU	12.1
5	K	57	ALA	11.8
5	A	59	GLY	11.8

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Mol	Chain	Res	Type	RSRZ
5	p	54	SER	11.6
5	Y	61	LYS	11.3
6	v	45	TRP	11.3
5	S	58	LEU	11.2
4	t	3	ALA	11.1
5	p	46	TRP	11.0
5	m	55	TYR	10.7
5	Q	54	SER	10.5
5	7	13	LEU	10.1
5	K	56	GLN	9.9
5	AA	60	LYS	9.9
6	AF	11	ASP	9.8
5	K	58	LEU	9.7
5	D	13	LEU	9.6
6	s	45	TRP	9.6
5	r	13	LEU	9.5
5	O	53	VAL	9.4
6	N	45	TRP	9.3
5	m	54	SER	9.3
5	l	54	SER	9.3
5	3	61	LYS	9.3
5	I	58	LEU	9.2
5	9	54	SER	9.1
5	I	59	GLY	9.1
5	Y	52	PRO	9.0
5	AK	13	LEU	9.0
5	K	52	PRO	9.0
5	AC	50	ASN	9.0
5	3	52	PRO	8.9
5	Y	2	PHE	8.8
5	w	52	PRO	8.8
6	e	45	TRP	8.7
5	O	56	GLN	8.6
5	d	13	LEU	8.6
5	F	53	VAL	8.5
5	A	13	LEU	8.4
5	p	47	LEU	8.3
5	S	55	TYR	8.3
5	h	12	TRP	8.2
5	3	59	GLY	8.2
6	AL	45	TRP	8.2
5	Y	51	ILE	8.2

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Mol	Chain	Res	Type	RSRZ
6	AH	45	TRP	8.1
6	z	9	LEU	8.1
6	q	45	TRP	8.1
5	F	8	LEU	8.0
5	j	3	THR	7.9
5	AA	8	LEU	7.9
5	AA	53	VAL	7.9
5	h	57	ALA	7.9
6	AD	45	TRP	7.9
5	AE	42	THR	7.9
5	9	2	PHE	7.8
5	K	60	LYS	7.8
5	S	57	ALA	7.8
5	AC	53	VAL	7.7
5	K	59	GLY	7.7
5	A	54	SER	7.6
5	d	6	ALA	7.6
5	3	46	TRP	7.5
5	W	57	ALA	7.5
5	9	50	ASN	7.5
5	9	55	TYR	7.5
5	f	54	SER	7.4
5	h	5	ASN	7.3
5	9	3	THR	7.3
5	F	7	ASN	7.3
5	u	46	TRP	7.2
4	H	55	VAL	7.2
5	A	58	LEU	7.2
5	O	55	TYR	7.1
5	O	57	ALA	7.1
5	D	57	ALA	7.0
5	l	61	LYS	7.0
5	Y	4	MET	7.0
5	K	8	LEU	7.0
6	n	17	PHE	7.0
5	D	6	ALA	6.9
6	AH	46	LEU	6.9
6	z	45	TRP	6.9
5	AI	8	LEU	6.8
6	P	45	TRP	6.8
5	F	2	PHE	6.8
5	U	51	ILE	6.8

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Mol	Chain	Res	Type	RSRZ
6	g	45	TRP	6.8
5	Y	53	VAL	6.8
5	r	51	ILE	6.8
5	3	44	LEU	6.8
5	u	14	ILE	6.7
5	AA	59	GLY	6.7
6	c	17	PHE	6.7
5	9	53	VAL	6.7
5	AE	41[A]	SER	6.7
5	AK	12	TRP	6.7
5	AG	55	TYR	6.6
6	R	45	TRP	6.6
5	AC	51	ILE	6.6
4	H	56	VAL	6.6
5	D	7	ASN	6.6
5	m	10	LYS	6.6
4	t	7	HIS	6.5
5	O	54	SER	6.5
5	AC	52	PRO	6.4
5	AK	54	SER	6.4
5	AI	46	TRP	6.4
6	AL	9	LEU	6.4
5	F	4	MET	6.4
4	t	2	SER	6.3
5	l	10	LYS	6.3
5	9	58	LEU	6.3
5	l	53	VAL	6.3
5	Q	57	ALA	6.3
5	f	53	VAL	6.3
6	Z	45	TRP	6.2
5	D	5	ASN	6.2
5	S	52	PRO	6.2
1	o	121	ILE	6.2
5	AG	52	PRO	6.2
5	f	58	LEU	6.2
5	U	13	LEU	6.1
5	r	54	SER	6.0
5	F	50	ASN	6.0
6	N	8	GLY	6.0
5	d	46	TRP	6.0
2	L	14	GLY	5.9
5	5	3	THR	5.9

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Mol	Chain	Res	Type	RSRZ
5	A	60	LYS	5.9
5	A	39	VAL	5.9
5	AG	53	VAL	5.9
6	z	46	LEU	5.9
5	K	61	LYS	5.8
5	Y	13	LEU	5.8
5	K	2	PHE	5.8
6	AL	46	LEU	5.7
5	W	13	LEU	5.7
5	j	8	LEU	5.7
1	o	154	THR	5.7
3	y	198	TYR	5.7
4	t	56	VAL	5.7
5	A	51	ILE	5.7
5	f	59	GLY	5.7
5	S	51	ILE	5.7
5	S	53	VAL	5.6
5	p	5	ASN	5.6
5	w	46	TRP	5.6
4	t	55	VAL	5.6
5	F	59	GLY	5.6
5	I	57	ALA	5.6
5	l	52	PRO	5.6
6	s	9	LEU	5.6
5	h	46	TRP	5.6
1	o	82	LEU	5.6
6	8	42	TYR	5.6
5	7	61	LYS	5.6
5	d	58	LEU	5.5
5	AA	3	THR	5.5
5	l	55	TYR	5.5
5	3	53	VAL	5.5
6	n	42	TYR	5.5
5	f	52	PRO	5.5
5	AG	54	SER	5.5
6	n	21	PHE	5.5
2	x	120	LEU	5.5
5	U	52	PRO	5.5
1	o	150	VAL	5.5
4	t	4	GLY	5.5
5	I	7	ASN	5.5
5	m	13	LEU	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	k	45	TRP	5.4
6	i	46	LEU	5.4
4	H	2	SER	5.4
5	5	57	ALA	5.4
5	AI	53	VAL	5.4
5	AI	58	LEU	5.3
6	0	17	PHE	5.3
4	t	182	LEU	5.3
6	J	9	LEU	5.3
5	h	51	ILE	5.3
5	AE	58	LEU	5.3
5	7	57	ALA	5.3
5	D	10	LYS	5.3
5	K	46	TRP	5.3
5	d	54	SER	5.3
5	p	10	LYS	5.3
5	m	6	ALA	5.2
5	AK	53	VAL	5.2
5	7	54	SER	5.2
5	w	37	MET	5.2
6	0	41	LEU	5.2
5	U	58	LEU	5.2
5	j	2	PHE	5.1
5	D	55	TYR	5.1
5	9	57	ALA	5.1
2	x	14	GLY	5.1
5	u	6	ALA	5.1
5	1	46	TRP	5.1
5	l	7	ASN	5.1
5	I	11	ILE	5.1
5	d	8	LEU	5.1
5	I	14	ILE	5.1
5	AK	46	TRP	5.1
5	O	42	THR	5.1
6	J	45	TRP	5.1
5	AI	42	THR	5.1
1	C	82	LEU	5.0
1	C	210	ILE	5.0
5	AK	11	ILE	5.0
4	H	202	PHE	5.0
5	S	54	SER	5.0
2	L	2	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
5	1	52	PRO	5.0
6	z	44	PRO	5.0
5	m	57	ALA	5.0
5	U	53	VAL	4.9
5	K	54	SER	4.9
5	Q	58	LEU	4.9
5	d	7	ASN	4.9
5	j	57	ALA	4.9
5	1	54	SER	4.9
6	J	28	TRP	4.8
5	d	52	PRO	4.8
1	o	204	LEU	4.8
5	F	3	THR	4.8
5	AA	13	LEU	4.8
5	AK	10	LYS	4.8
3	y	195	ASN	4.8
4	H	41	LEU	4.8
5	AI	52	PRO	4.8
4	H	3	ALA	4.8
5	K	53	VAL	4.8
5	7	6	ALA	4.8
5	h	13	LEU	4.8
6	8	17	PHE	4.8
5	p	13	LEU	4.8
6	c	46	LEU	4.8
5	Y	46	TRP	4.8
5	u	47	LEU	4.8
6	B	9	LEU	4.8
5	m	58	LEU	4.7
6	2	13	GLU	4.7
6	6	45	TRP	4.7
5	AC	3	THR	4.7
5	W	54	SER	4.7
5	Q	55	TYR	4.7
5	5	46	TRP	4.7
5	7	58	LEU	4.7
6	AD	46	LEU	4.7
5	h	54	SER	4.7
5	O	60	LYS	4.7
6	i	10	THR	4.6
5	f	10	LYS	4.6
5	r	52	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
4	t	176	GLU	4.6
5	l	60	LYS	4.6
5	u	60	LYS	4.6
6	i	45	TRP	4.6
2	x	155	PHE	4.6
6	n	43	ARG	4.6
5	9	51	ILE	4.6
5	3	60	LYS	4.6
6	2	9	LEU	4.6
5	O	13	LEU	4.5
1	o	210	ILE	4.5
5	p	55	TYR	4.5
5	l	59	GLY	4.5
5	AC	4	MET	4.5
5	AC	2	PHE	4.5
5	r	47	LEU	4.5
6	AL	21	PHE	4.5
1	C	303	LEU	4.5
5	I	53	VAL	4.5
5	Y	54	SER	4.5
5	m	8	LEU	4.5
5	w	8	LEU	4.5
6	B	11	ASP	4.5
6	8	45	TRP	4.5
1	C	332	LYS	4.5
1	o	321	ALA	4.4
5	O	2	PHE	4.4
1	C	329	GLY	4.4
5	9	52	PRO	4.4
6	0	46	LEU	4.4
5	F	51	ILE	4.4
5	7	53	VAL	4.4
5	r	53	VAL	4.4
6	R	46	LEU	4.4
1	C	121	ILE	4.3
5	I	48	ASP	4.3
2	x	58	PRO	4.3
5	AC	14	ILE	4.3
5	h	8	LEU	4.3
6	e	10	THR	4.3
5	S	12	TRP	4.3
5	m	44	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
4	H	39	TYR	4.3
6	G	12	ASP	4.3
5	D	8	LEU	4.3
5	I	46	TRP	4.3
5	W	12	TRP	4.3
5	A	50	ASN	4.3
6	T	45	TRP	4.3
6	R	44	PRO	4.3
6	P	14	ALA	4.3
6	c	9	LEU	4.3
1	C	330	LEU	4.2
1	o	323	MET	4.2
4	t	214	ILE	4.2
6	P	9	LEU	4.2
5	u	57	ALA	4.2
5	r	55	TYR	4.2
5	AI	47	LEU	4.2
5	AC	55	TYR	4.2
1	o	177	GLY	4.2
5	AA	2	PHE	4.2
5	f	2	PHE	4.2
5	j	51	ILE	4.2
1	o	176	SER	4.2
5	AE	43	ASP	4.2
6	B	43	ARG	4.2
5	W	4	MET	4.2
5	AE	14	ILE	4.2
6	P	7	THR	4.2
1	o	324	ALA	4.2
1	o	72	ALA	4.1
6	8	16	GLU	4.1
5	Q	3	THR	4.1
5	9	13	LEU	4.1
5	r	48	ASP	4.1
5	A	10	LYS	4.1
5	D	61	LYS	4.1
5	Q	2	PHE	4.1
5	l	3	THR	4.1
5	U	54	SER	4.1
5	r	14	ILE	4.1
5	9	49	ASP	4.1
4	H	149	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
5	D	52	PRO	4.1
5	u	12	TRP	4.0
6	E	45	TRP	4.0
5	r	46	TRP	4.0
4	t	242	TYR	4.0
5	l	57	ALA	4.0
5	W	52	PRO	4.0
5	A	14	ILE	4.0
5	p	8	LEU	4.0
5	AG	44	LEU	4.0
6	0	42	TYR	4.0
5	1	44	LEU	4.0
5	AG	14	ILE	4.0
5	5	52	PRO	4.0
5	AE	7	ASN	4.0
5	AI	57	ALA	4.0
5	w	53	VAL	4.0
5	AE	59	GLY	4.0
5	D	59	GLY	4.0
5	l	58	LEU	4.0
6	q	46	LEU	3.9
5	w	41	SER	3.9
6	V	45	TRP	3.9
6	0	9	LEU	3.9
1	o	233	PHE	3.9
5	AG	57	ALA	3.9
5	1	13	LEU	3.9
5	d	59	GLY	3.9
6	2	10	THR	3.9
6	6	14	ALA	3.9
1	C	68	THR	3.9
6	AJ	7	THR	3.9
6	T	13	GLU	3.9
6	AJ	9	LEU	3.9
6	B	10	THR	3.9
5	l	13	LEU	3.9
6	N	46	LEU	3.9
5	S	44	LEU	3.9
5	D	11	ILE	3.9
2	L	13	ARG	3.8
5	AG	46	TRP	3.8
6	AF	10	THR	3.8

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Mol	Chain	Res	Type	RSRZ
6	k	14	ALA	3.8
5	m	50	ASN	3.8
5	9	8	LEU	3.8
5	AI	54	SER	3.8
5	1	4	MET	3.8
5	AC	58	LEU	3.8
5	AK	3	THR	3.8
6	v	46	LEU	3.7
5	K	11	ILE	3.7
6	AH	7	THR	3.7
5	U	50	ASN	3.7
5	D	41	SER	3.7
5	S	13	LEU	3.7
6	k	46	LEU	3.7
6	N	43	ARG	3.7
5	AI	61	LYS	3.7
5	1	55	TYR	3.7
6	c	45	TRP	3.7
6	R	43	ARG	3.7
1	C	114	GLY	3.7
4	H	214	ILE	3.7
5	u	55	TYR	3.7
5	I	13	LEU	3.7
6	G	9	LEU	3.7
6	R	39	ALA	3.7
1	C	122	TYR	3.7
5	D	14	ILE	3.7
5	j	13	LEU	3.7
5	Q	53	VAL	3.7
5	l	50	ASN	3.7
6	P	13	GLU	3.7
5	D	54	SER	3.6
5	d	57	ALA	3.6
5	AE	57	ALA	3.6
5	AE	44	LEU	3.6
6	N	9	LEU	3.6
5	D	58	LEU	3.6
5	AE	13	LEU	3.6
5	u	49	ASP	3.6
2	x	246	ALA	3.6
5	AC	57	ALA	3.6
1	o	197	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
5	AG	42	THR	3.6
6	J	41	LEU	3.6
6	c	42	TYR	3.6
6	N	44	PRO	3.6
5	I	12	TRP	3.6
1	o	97	VAL	3.5
4	H	5	ILE	3.5
5	5	2	PHE	3.5
5	AA	7	ASN	3.5
5	S	3	THR	3.5
5	p	2	PHE	3.5
5	A	12	TRP	3.5
5	AA	51	ILE	3.5
6	n	14	ALA	3.5
5	A	44	LEU	3.5
6	g	11	ASP	3.5
5	AI	60	LYS	3.5
5	m	47	LEU	3.5
3	M	294	TRP	3.5
5	r	7	ASN	3.5
1	C	284	ILE	3.5
5	p	7	ASN	3.5
5	u	58	LEU	3.5
6	P	8	GLY	3.5
5	W	46	TRP	3.5
5	5	58	LEU	3.5
6	g	46	LEU	3.5
5	AA	61	LYS	3.5
6	AF	45	TRP	3.5
1	C	290	VAL	3.4
5	m	53	VAL	3.4
1	C	77	GLN	3.4
5	m	12	TRP	3.4
5	l	47	LEU	3.4
5	l	14	ILE	3.4
1	C	150	VAL	3.4
4	H	182	LEU	3.4
3	y	189	PHE	3.4
6	AH	43	ARG	3.4
6	c	8	GLY	3.4
5	I	47	LEU	3.4
3	M	36	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
5	S	61	LYS	3.4
5	p	58	LEU	3.4
6	8	39	ALA	3.4
5	O	10	LYS	3.4
5	AI	59	GLY	3.4
5	w	30	VAL	3.4
5	w	44	LEU	3.4
6	AB	41	LEU	3.4
6	z	15	LYS	3.4
5	I	52	PRO	3.4
6	AF	12	ASP	3.4
5	l	41	SER	3.4
1	C	72	ALA	3.3
5	l	51	ILE	3.3
6	G	45	TRP	3.3
5	F	6	ALA	3.3
6	B	13	GLU	3.3
5	D	53	VAL	3.3
5	AE	60	LYS	3.3
5	j	52	PRO	3.3
5	AE	53	VAL	3.3
6	2	39	ALA	3.3
5	D	60	LYS	3.3
5	AA	54	SER	3.3
5	AK	47	LEU	3.3
5	F	52	PRO	3.3
5	p	44	LEU	3.3
1	C	261	GLN	3.3
6	n	45	TRP	3.2
2	L	176	PHE	3.2
2	L	215	VAL	3.2
5	AA	23	SER	3.2
5	1	61	LYS	3.2
1	C	135	ARG	3.2
2	x	78	PRO	3.2
6	N	17	PHE	3.2
6	AB	11	ASP	3.2
6	z	8	GLY	3.2
6	c	43	ARG	3.2
3	M	198	TYR	3.2
6	0	45	TRP	3.2
6	q	9	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
5	F	9	TYR	3.2
1	o	143	ALA	3.2
5	d	60	LYS	3.2
5	j	56	GLN	3.2
5	7	21	LEU	3.2
6	AB	45	TRP	3.2
5	AG	58	LEU	3.1
5	AC	7	ASN	3.1
5	u	15	LEU	3.1
6	AH	41	LEU	3.1
6	g	41	LEU	3.1
4	H	201	ARG	3.1
1	C	76	TYR	3.1
6	B	15	LYS	3.1
5	AC	46	TRP	3.1
4	t	134	VAL	3.1
5	AE	15	LEU	3.1
6	AF	44	PRO	3.1
5	Q	61	LYS	3.1
5	j	10	LYS	3.1
6	8	15	LYS	3.1
6	T	14	ALA	3.1
5	A	55	TYR	3.1
5	I	55	TYR	3.1
6	B	42	TYR	3.1
1	C	70	PRO	3.1
1	o	116	TRP	3.1
6	E	39	ALA	3.1
4	t	43	SER	3.1
5	AE	23	SER	3.1
5	AA	55	TYR	3.1
6	k	9	LEU	3.1
5	m	4	MET	3.1
4	H	215	LYS	3.1
6	B	41	LEU	3.1
1	o	112	VAL	3.1
5	K	7	ASN	3.1
5	D	12	TRP	3.1
1	o	162	PRO	3.1
4	t	200	SER	3.1
5	AA	43	ASP	3.1
5	AA	58	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	x	80	LEU	3.1
6	N	36	HIS	3.1
5	F	54	SER	3.1
6	v	17	PHE	3.1
1	C	302	PRO	3.0
6	s	10	THR	3.0
3	M	142	MET	3.0
5	F	46	TRP	3.0
5	AI	44	LEU	3.0
4	t	209	VAL	3.0
6	2	12	ASP	3.0
5	Y	47	LEU	3.0
3	y	307	TYR	3.0
5	3	4	MET	3.0
5	h	11	ILE	3.0
4	H	151	PRO	3.0
5	AC	13	LEU	3.0
5	m	5	ASN	3.0
5	AA	26	ALA	3.0
5	p	39	VAL	3.0
6	v	23	GLN	3.0
6	z	16	GLU	3.0
1	C	252	ASN	3.0
1	o	85	LEU	3.0
5	Y	55	TYR	3.0
3	y	125	SER	3.0
5	W	7	ASN	3.0
5	w	28	GLN	3.0
6	k	42	TYR	3.0
1	o	332	LYS	3.0
5	A	26	ALA	2.9
6	i	21	PHE	2.9
5	p	53	VAL	2.9
5	f	44	LEU	2.9
6	AH	39	ALA	2.9
6	AJ	19	ALA	2.9
6	k	43	ARG	2.9
1	o	93	THR	2.9
5	7	14	ILE	2.9
5	AA	29	ILE	2.9
5	I	8	LEU	2.9
5	l	6	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
5	5	4	MET	2.9
5	9	23	SER	2.9
5	w	23	SER	2.9
4	t	84	PRO	2.9
6	AH	40	TRP	2.9
1	C	287	LEU	2.9
2	x	101	CYS	2.9
6	E	46	LEU	2.9
5	Y	6	ALA	2.9
6	T	39	ALA	2.9
5	D	40	LEU	2.9
6	0	16	GLU	2.9
5	AC	15	LEU	2.9
3	M	287	SER	2.9
1	o	125	VAL	2.9
5	j	14	ILE	2.9
3	y	317	TYR	2.9
6	AF	39	ALA	2.8
6	8	43	ARG	2.8
6	q	39	ALA	2.8
5	U	7	ASN	2.8
1	C	256	PHE	2.8
5	Q	14	ILE	2.8
6	n	46	LEU	2.8
5	AE	52	PRO	2.8
1	C	271	TYR	2.8
5	AE	26	ALA	2.8
5	Y	59	GLY	2.8
4	H	42	ASP	2.8
5	F	12	TRP	2.8
6	8	46	LEU	2.8
5	r	2	PHE	2.8
4	t	5	ILE	2.8
5	Y	14	ILE	2.8
5	Y	39	VAL	2.8
6	AD	17	PHE	2.8
5	AI	7	ASN	2.8
5	W	58	LEU	2.8
5	AC	8	LEU	2.8
4	H	204	LYS	2.8
5	p	3	THR	2.8
6	z	28	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
4	H	194	LEU	2.8
6	e	9	LEU	2.8
6	8	14	ALA	2.8
2	L	238	ILE	2.7
5	AA	9	TYR	2.7
4	t	175	SER	2.7
5	AA	30	VAL	2.7
6	8	26	TYR	2.7
6	P	36	HIS	2.7
5	AC	23	SER	2.7
6	0	43	ARG	2.7
4	t	162	GLU	2.7
4	H	4	GLY	2.7
1	o	152	CYS	2.7
1	o	70	PRO	2.7
5	3	47	LEU	2.7
5	m	40	LEU	2.7
6	k	24	SER	2.7
4	t	6	THR	2.7
5	AE	10	LYS	2.7
6	AD	14	ALA	2.7
6	AL	17	PHE	2.7
5	AE	4	MET	2.7
5	3	5	ASN	2.7
5	AA	6	ALA	2.7
6	n	13	GLU	2.7
6	k	10	THR	2.7
5	h	4	MET	2.7
6	AJ	21	PHE	2.7
5	A	61	LYS	2.7
6	v	9	LEU	2.7
6	AF	40	TRP	2.6
2	x	15	GLY	2.6
1	o	89	GLU	2.6
1	o	43	TYR	2.6
4	H	100	LEU	2.6
1	o	38	VAL	2.6
6	n	15	LYS	2.6
5	w	34	LEU	2.6
5	U	12	TRP	2.6
5	w	54	SER	2.6
2	L	43	THR	2.6

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Mol	Chain	Res	Type	RSRZ
6	J	14	ALA	2.6
5	7	23	SER	2.6
4	t	54	LYS	2.6
5	r	12	TRP	2.6
2	x	202	LEU	2.6
5	AI	13	LEU	2.6
6	AF	46	LEU	2.6
5	O	3	THR	2.6
1	o	282	ASN	2.6
5	AE	3	THR	2.6
5	D	30	VAL	2.6
5	K	10	LYS	2.6
5	AA	46	TRP	2.6
5	S	11	ILE	2.6
5	S	15	LEU	2.6
5	3	12	TRP	2.6
5	h	44	LEU	2.6
5	m	9	TYR	2.6
4	H	54	LYS	2.6
5	A	8	LEU	2.6
5	U	46	TRP	2.5
5	A	40	LEU	2.5
5	Y	44	LEU	2.5
1	o	90	PHE	2.5
5	h	3	THR	2.5
1	o	76	TYR	2.5
5	7	12	TRP	2.5
6	z	14	ALA	2.5
5	O	59	GLY	2.5
5	F	11	ILE	2.5
5	f	19	ARG	2.5
6	0	44	PRO	2.5
5	f	50	ASN	2.5
5	f	57	ALA	2.5
2	L	224	PHE	2.5
5	u	2	PHE	2.5
5	W	56	GLN	2.5
5	AK	57	ALA	2.5
1	o	37	GLY	2.5
1	o	114	GLY	2.5
5	F	5	ASN	2.5
1	C	131	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
4	H	18	ALA	2.5
1	C	333	THR	2.5
1	o	151	THR	2.5
6	AJ	10	THR	2.5
6	4	9	LEU	2.5
6	k	23	GLN	2.5
5	F	10	LYS	2.5
2	x	154	GLY	2.5
3	M	314	VAL	2.5
6	6	17	PHE	2.5
5	7	55	TYR	2.5
5	w	39	VAL	2.5
6	n	41	LEU	2.5
1	o	128	ARG	2.5
5	D	39	VAL	2.5
5	7	7	ASN	2.5
2	L	105	ALA	2.5
4	t	86	ALA	2.5
5	A	57	ALA	2.5
5	AC	9	TYR	2.5
3	y	106	ILE	2.5
2	x	119	LYS	2.4
5	S	8	LEU	2.4
5	AG	13	LEU	2.4
5	A	46	TRP	2.4
5	l	40	LEU	2.4
2	L	41	CYS	2.4
5	h	47	LEU	2.4
1	C	78	ASN	2.4
5	K	21	LEU	2.4
6	6	46	LEU	2.4
5	9	59	GLY	2.4
6	i	18	HIS	2.4
1	o	271	TYR	2.4
5	D	47	LEU	2.4
6	R	41	LEU	2.4
4	t	133	ILE	2.4
1	C	204	LEU	2.4
5	F	44	LEU	2.4
5	I	60	LYS	2.4
5	u	59	GLY	2.4
2	L	24	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
5	7	26	ALA	2.4
5	7	11	ILE	2.4
5	p	48	ASP	2.4
5	w	60	LYS	2.4
1	C	237	MET	2.4
5	D	26	ALA	2.4
3	y	68	ILE	2.4
5	w	14	ILE	2.4
6	AJ	45	TRP	2.4
5	j	46	TRP	2.4
5	l	46	TRP	2.4
5	7	30	VAL	2.4
5	D	56	GLN	2.4
1	C	327	TYR	2.4
6	v	26	TYR	2.4
1	o	131	PHE	2.3
2	L	15	GLY	2.3
5	f	6	ALA	2.3
6	k	20	ILE	2.3
5	S	39	VAL	2.3
6	V	7	THR	2.3
5	I	56	GLN	2.3
5	r	10	LYS	2.3
6	k	12	ASP	2.3
1	o	73	SER	2.3
5	D	23	SER	2.3
2	x	223	THR	2.3
5	u	7	ASN	2.3
6	g	21	PHE	2.3
6	i	43	ARG	2.3
1	C	134	VAL	2.3
5	Y	60	LYS	2.3
6	J	17	PHE	2.3
1	o	280	ASN	2.3
5	p	40	LEU	2.3
5	9	27	PHE	2.3
6	s	21	PHE	2.3
5	F	56	GLN	2.3
2	L	101	CYS	2.3
2	x	41	CYS	2.3
3	M	23	LEU	2.3
5	1	47	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	5	47	LEU	2.3
6	V	39	ALA	2.3
5	3	54	SER	2.3
1	C	124	LYS	2.3
4	t	171	TRP	2.3
5	7	60	LYS	2.3
5	p	14	ILE	2.3
3	M	74	ASN	2.3
3	M	160	LEU	2.3
5	w	13	LEU	2.3
5	AI	14	ILE	2.3
5	f	21	LEU	2.3
6	J	20	ILE	2.3
6	AJ	20	ILE	2.3
6	B	12	ASP	2.3
1	o	172	PRO	2.3
5	Q	11	ILE	2.3
1	C	138	ASN	2.3
5	I	6	ALA	2.3
5	m	30	VAL	2.3
5	p	50	ASN	2.3
5	w	57	ALA	2.3
5	AG	8	LEU	2.3
5	h	26	ALA	2.3
6	J	19	ALA	2.3
6	v	21	PHE	2.3
6	i	42	TYR	2.3
6	G	8	GLY	2.3
6	AB	46	LEU	2.3
5	7	51	ILE	2.3
6	6	18	HIS	2.3
5	AA	5	ASN	2.3
6	AL	25	MET	2.3
4	H	118	ASP	2.2
3	y	196	LEU	2.2
6	AJ	16	GLU	2.2
5	K	12	TRP	2.2
6	G	41	LEU	2.2
6	T	9	LEU	2.2
3	y	60	SER	2.2
5	w	21	LEU	2.2
1	C	75	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	t	85	VAL	2.2
5	3	8	LEU	2.2
6	Z	46	LEU	2.2
6	8	37	LEU	2.2
3	M	30	ARG	2.2
5	9	41	SER	2.2
2	x	171	TYR	2.2
5	3	6	ALA	2.2
6	2	11	ASP	2.2
3	M	140	LEU	2.2
5	f	46	TRP	2.2
5	D	42	THR	2.2
4	H	183	GLU	2.2
4	H	200	SER	2.2
5	A	6	ALA	2.2
5	h	55	TYR	2.2
3	y	255	THR	2.2
4	t	210	LYS	2.2
5	K	55	TYR	2.2
5	j	4	MET	2.2
5	m	59	GLY	2.2
6	J	32	VAL	2.2
2	L	268	TRP	2.1
5	W	44	LEU	2.1
5	AE	6	ALA	2.1
4	t	151	PRO	2.1
4	t	174	ARG	2.1
6	c	37	LEU	2.1
4	t	83	ALA	2.1
1	C	112	VAL	2.1
5	d	14	ILE	2.1
4	t	100	LEU	2.1
6	4	10	THR	2.1
5	W	53	VAL	2.1
1	C	288	ASN	2.1
5	Q	7	ASN	2.1
2	L	100	ILE	2.1
3	y	305	PRO	2.1
5	S	4	MET	2.1
3	M	217	ALA	2.1
5	j	61	LYS	2.1
6	P	43	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	o	81	VAL	2.1
5	W	42	THR	2.1
5	u	50	ASN	2.1
5	9	56	GLN	2.1
5	Q	52	PRO	2.1
5	5	44	LEU	2.1
5	f	17	PRO	2.1
5	w	27	PHE	2.1
6	AL	14	ALA	2.1
5	Q	59	GLY	2.1
5	AI	37	MET	2.1
5	AK	4	MET	2.1
3	y	36	PHE	2.1
6	8	21	PHE	2.1
5	u	11	ILE	2.1
5	w	59	GLY	2.1
5	f	7	ASN	2.1
5	f	60	LYS	2.1
5	O	23	SER	2.1
5	d	48	ASP	2.1
6	s	12	ASP	2.1
5	w	33	LEU	2.1
6	AL	44	PRO	2.1
4	t	132	LYS	2.1
6	AB	15	LYS	2.1
1	o	284	ILE	2.1
5	AG	56	GLN	2.1
5	l	12	TRP	2.1
5	w	26	ALA	2.1
6	c	16	GLU	2.1
2	L	47	VAL	2.1
2	L	59	THR	2.1
5	m	39	VAL	2.1
5	d	53	VAL	2.1
5	l	37	MET	2.1
1	C	324	ALA	2.0
3	y	319	THR	2.0
4	H	40	PRO	2.0
5	AC	10	LYS	2.0
6	i	17	PHE	2.0
4	H	124	ASP	2.0
6	X	45	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
4	H	181	TYR	2.0
6	B	14	ALA	2.0
1	o	199	PRO	2.0
5	I	33	LEU	2.0
5	9	17	PRO	2.0
2	x	153	HIS	2.0
2	x	228	ILE	2.0
6	E	41	LEU	2.0
4	H	148	ASP	2.0
4	t	118	ASP	2.0
1	o	243	LEU	2.0
5	F	57	ALA	2.0
2	L	104	GLY	2.0
2	x	112	ARG	2.0
5	d	5	ASN	2.0
1	o	283	TYR	2.0
1	o	235	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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

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

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

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

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

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