



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 07:39 AM EDT

PDB ID : 5H2F  
Title : Crystal structure of the PsbM-deletion mutant of photosystem II  
Authors : Uto, S.; Kawakami, K.; Umena, Y.; Iwai, M.; Ikeuchi, M.; Shen, J.R.; Kamiya, N.  
Deposited on : unknown  
Resolution : 2.20 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-20029824  
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-20029824

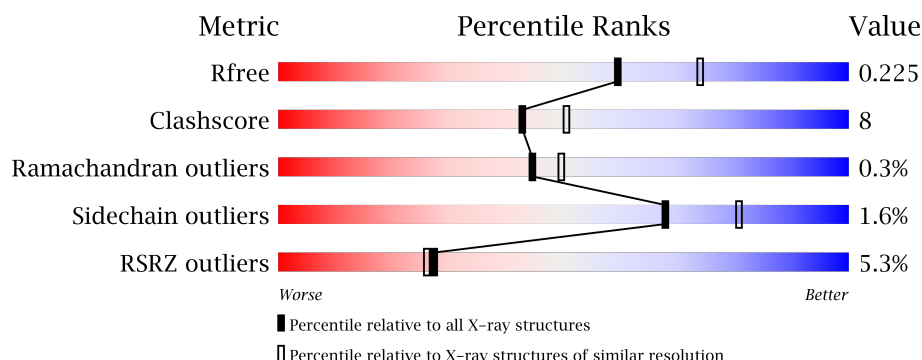
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



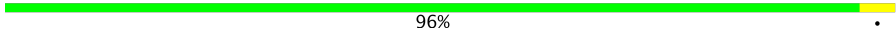

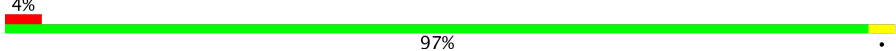


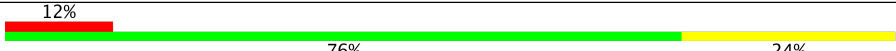
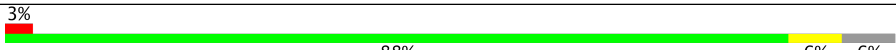

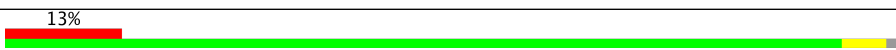
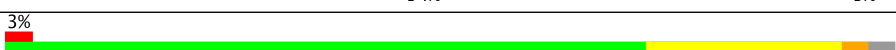
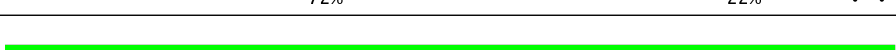
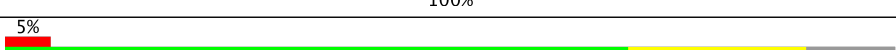

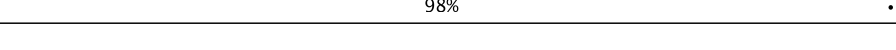
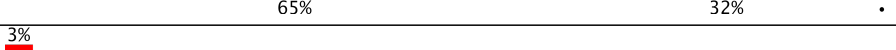
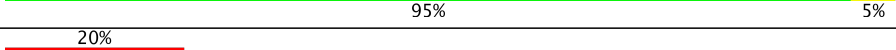

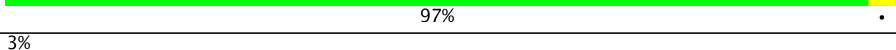

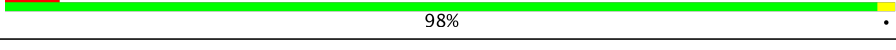

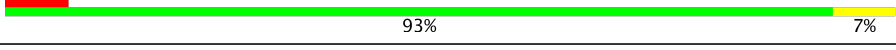
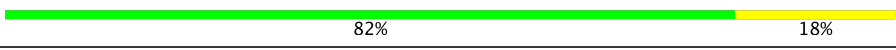
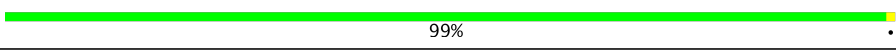

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	A	334	<div> <div>4%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	a	334	<div> <div>10%</div> <div>98%</div> <div>.</div> </div>
2	B	505	<div> <div>7%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
2	b	505	<div> <div>4%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
3	C	455	<div> <div>3%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	455	 96% .
4	D	342	 78% 21% .
4	d	342	 97% .
5	E	80	 13% 75% 23% ..
5	e	80	 15% 94% 5% .
6	F	33	 12% 76% 24%
6	f	33	 3% 88% 6% 6%
7	H	63	 2% 67% 32% .
7	h	63	 13% 94% 5% .
8	I	36	 3% 72% 22% . .
8	i	36	 100%
9	J	40	 5% 70% 20% 10%
9	j	40	 15% 98% .
10	K	37	 65% 32% .
10	k	37	 3% 95% 5%
11	L	35	 20% 86% 14%
11	l	35	 11% 97% .
12	O	243	 3% 78% 21%
12	o	243	 6% 98% .
13	T	30	 73% 27%
13	t	30	 7% 93% 7%
14	U	97	 82% 18%
14	u	97	 99% .
15	V	137	 84% 15% .
15	v	137	 2% 97% ..

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Mol	Chain	Length	Quality of chain
16	Y	29	
16	y	29	
17	X	37	
17	x	37	
18	Z	62	
18	z	62	

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
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	a	409	X	-	-	-
22	CLA	b	602	X	-	-	X
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	902	X	-	-	-
22	CLA	c	903	X	-	-	-
22	CLA	c	904	X	-	-	-
22	CLA	c	905	X	-	-	-
22	CLA	c	906	X	-	-	-
22	CLA	c	907	X	-	-	-
22	CLA	c	908	X	-	-	-
22	CLA	c	909	X	-	-	-
22	CLA	c	910	X	-	-	-
22	CLA	c	911	X	-	-	-
22	CLA	c	912	X	-	-	-
22	CLA	c	913	X	-	-	-
22	CLA	c	914	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	B	618	-	-	-	X
24	BCR	D	405	-	-	-	X
24	BCR	b	618	-	-	-	X
24	BCR	b	619	-	-	-	X
25	LMG	B	621	-	-	-	X
25	LMG	C	531	-	-	-	X
25	LMG	J	101	-	-	-	X
25	LMG	b	622	-	-	-	X
27	LHG	A	412	-	-	-	X
28	SQD	A	413	-	-	-	X
29	LMT	A	414	-	-	-	X
29	LMT	E	101	-	-	-	X
29	LMT	I	102	-	-	-	X
29	LMT	T	102	-	-	-	X
29	LMT	Z	101	-	-	-	X
29	LMT	a	419	-	-	-	X
29	LMT	c	921	-	-	-	X
29	LMT	c	931	-	-	-	X
29	LMT	f	102	-	-	-	X
29	LMT	t	101	-	-	-	X
30	UNL	A	415	-	-	-	X
30	UNL	B	624	-	-	-	X
30	UNL	D	413	-	-	-	X
30	UNL	I	104	-	-	-	X
30	UNL	J	103	-	-	-	X
30	UNL	T	101	-	-	-	X
30	UNL	U	201	-	-	-	X
30	UNL	a	417	-	-	-	X
30	UNL	a	420	-	-	-	X
30	UNL	i	104	-	-	-	X
30	UNL	j	103	-	-	-	X
30	UNL	t	102	-	-	-	X
30	UNL	u	201	-	-	-	X
31	DMS	B	628	-	-	-	X
31	DMS	B	631	-	-	-	X
31	DMS	B	638	-	-	X	-
31	DMS	B	640	-	-	-	X
31	DMS	C	528	-	-	-	X
31	DMS	C	530	-	-	-	X
31	DMS	C	535	-	-	-	X
31	DMS	C	536	-	-	-	X
31	DMS	C	540	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	DMS	D	417	-	-	-	X
31	DMS	F	101	-	-	-	X
31	DMS	L	102	-	-	-	X
31	DMS	O	304	-	-	X	X
31	DMS	O	307	-	-	-	X
31	DMS	O	310	-	-	X	X
31	DMS	O	312	-	-	-	X
31	DMS	O	313	-	-	-	X
31	DMS	U	203	-	-	-	X
31	DMS	V	204	-	-	-	X
31	DMS	V	209	-	-	-	X
31	DMS	V	211	-	-	-	X
31	DMS	V	212	-	-	X	-
31	DMS	a	424	-	-	-	X
31	DMS	a	425	-	-	-	X
31	DMS	b	629	-	-	-	X
31	DMS	b	630	-	-	-	X
31	DMS	b	638	-	-	-	X
31	DMS	c	924	-	-	-	X
31	DMS	c	925	-	-	-	X
31	DMS	c	926	-	-	-	X
31	DMS	c	927	-	-	-	X
31	DMS	c	929	-	-	-	X
31	DMS	c	934	-	-	-	X
31	DMS	c	935	-	-	-	X
31	DMS	c	939	-	-	-	X
31	DMS	f	103	-	-	-	X
31	DMS	i	106	-	-	-	X
31	DMS	o	302	-	-	-	X
31	DMS	o	303	-	-	-	X
31	DMS	o	305	-	-	-	X
31	DMS	o	307	-	-	-	X
31	DMS	u	205	-	-	-	X
31	DMS	v	210	-	-	-	X
31	DMS	v	211	-	-	-	X
34	HTG	B	626	-	-	-	X
34	HTG	D	414	-	-	-	X
34	HTG	D	415	-	-	-	X
34	HTG	V	203	-	-	-	X
34	HTG	b	632	-	-	-	X
35	DGD	C	519	-	-	-	X
35	DGD	D	407	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	DGD	d	406	-	-	-	X



## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 51892 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 Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2598	1706	428	449	15			
1	a	334	Total	C	N	O	S	0	1	0
			2555	1675	427	438	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	3	0
			3950	2596	661	680	13			
2	b	483	Total	C	N	O	S	0	1	0
			3780	2484	631	652	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3470	2274	580	603	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2732	1814	442	464	12			
4	d	341	Total	C	N	O	S	0	2	0
			2717	1805	441	459	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	79	Total	C	N	O	0	0	0
			635	417	101	117			
5	e	79	Total	C	N	O	0	0	0
			636	418	101	117			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	3	0
			522	347	87	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			288	196	45	46	1			
8	i	36	Total	C	N	O	S	0	0	0
			293	199	46	47	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			277	186	41	49	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	35	Total	C	N	O	0	0	0
			287	192	46	49			
11	l	35	Total	C	N	O	0	0	0
			287	192	46	49			

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	243	Total	C	N	O	S	0	1	0
			1853	1160	311	378	4			
12	o	243	Total	C	N	O	S	0	0	0
			1833	1149	305	375	4			

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	T	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			
13	t	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	97	Total	C	N	O	0	1	0
			782	496	132	154			
14	u	97	Total	C	N	O	0	0	0
			766	487	129	150			

- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	V	137	Total	C	N	O	S	0	1	0
			1066	677	177	208	4			
15	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
16	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

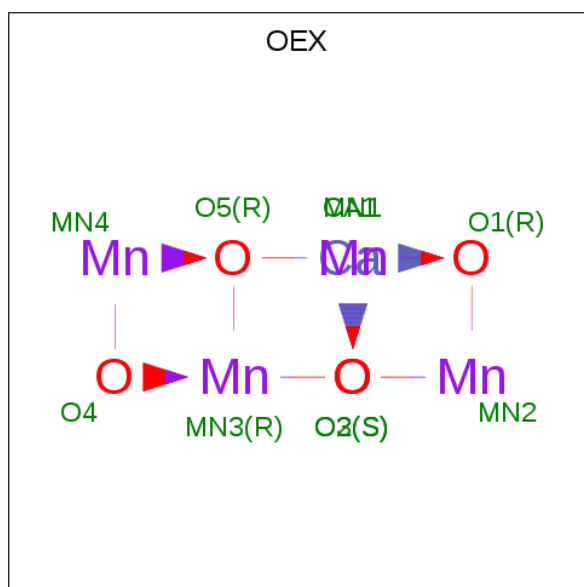
- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	37	Total	C	N	O	0	1	0
			269	183	40	46			
17	x	36	Total	C	N	O	0	0	0
			253	172	37	44			

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			453	311	68	72	2			
18	z	61	Total	C	N	O	S	0	0	0
			436	299	67	69	1			

- Molecule 19 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
19	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

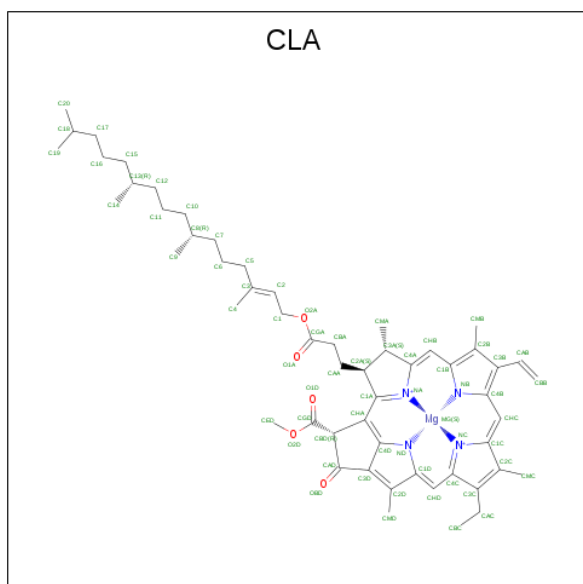
- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	0
			2	2		
21	a	2	Total	Cl	0	0
			2	2		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
22	b	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

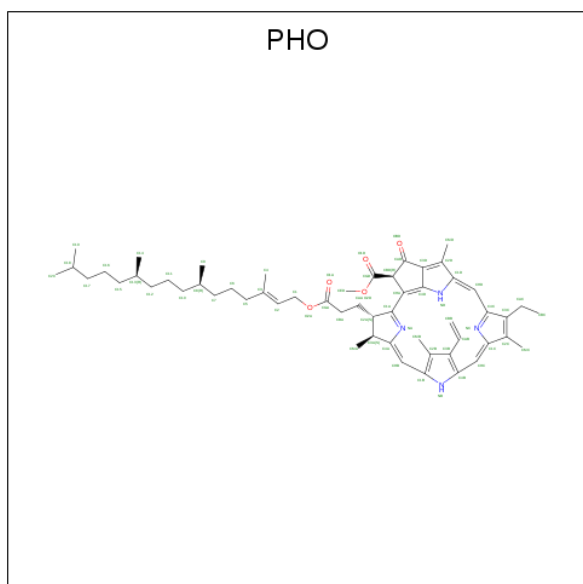
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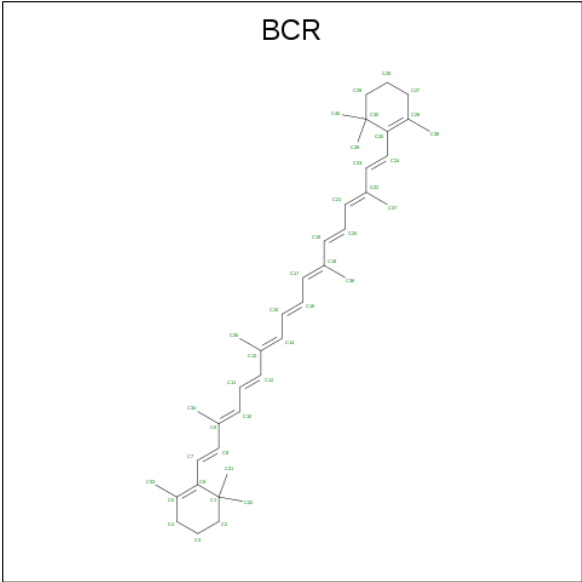
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	N	O		0	0
			64	55	4	5			
23	D	1	Total	C	N	O		0	0
			64	55	4	5			
23	a	1	Total	C	N	O		0	0
			64	55	4	5			
23	a	1	Total	C	N	O		0	0
			64	55	4	5			

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



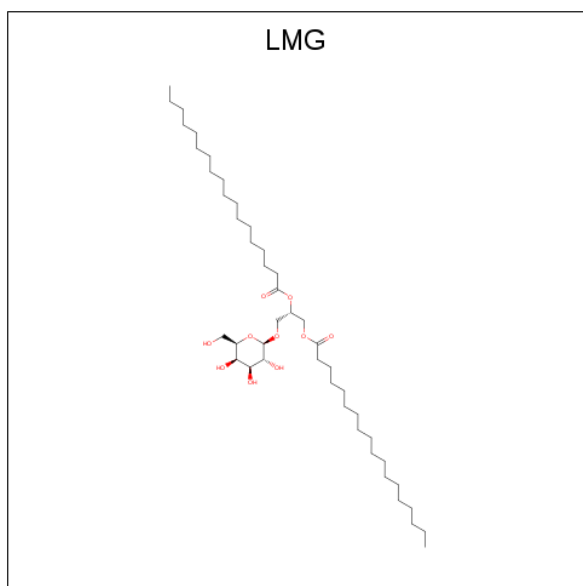
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 19 19	0	0
24	B	1	Total C 30 30	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	Y	1	Total C 39 39	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 20 20	0	0
24	b	1	Total C 31 31	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



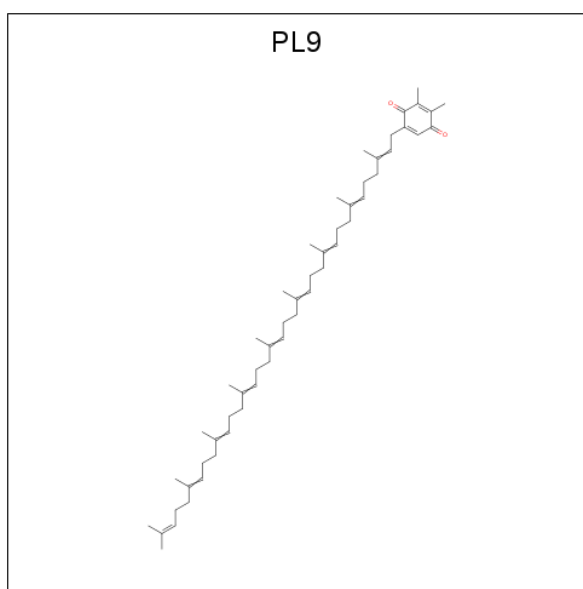
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 51 41 10	0	0
25	B	1	Total C O 40 30 10	0	0
25	C	1	Total C O 51 41 10	0	0
25	C	1	Total C O 40 30 10	0	0
25	D	1	Total C O 46 36 10	0	0
25	J	1	Total C O 45 35 10	0	0
25	b	1	Total C O 43 33 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	c	1	Total	C	O	0	0
			51	41	10		
25	c	1	Total	C	O	0	0
			49	39	10		
25	d	1	Total	C	O	0	0
			47	37	10		
25	i	1	Total	C	O	0	0
			51	41	10		
25	j	1	Total	C	O	0	0
			47	37	10		

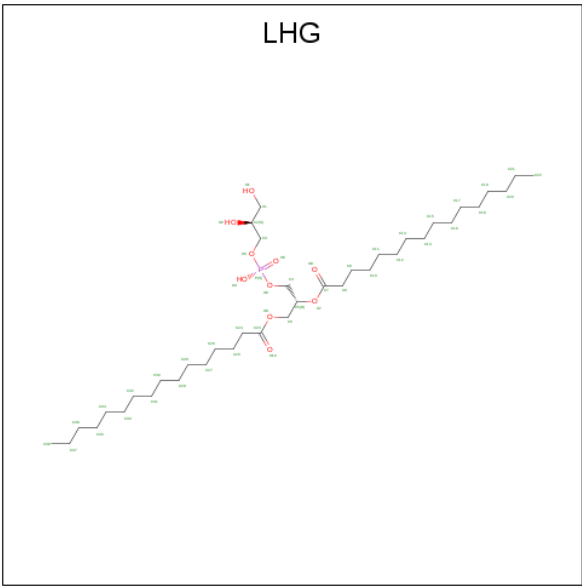
- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			55	53	2		
26	D	1	Total	C	O	0	0
			55	53	2		
26	a	1	Total	C	O	0	0
			55	53	2		
26	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

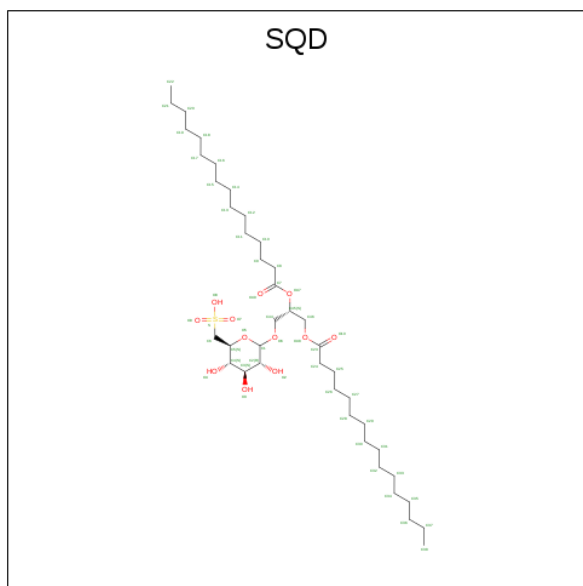
LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			31	22	8	1		
27	C	1	Total	C	O	P	0	0
			30	21	8	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			45	34	10	1		
27	L	1	Total	C	O	P	0	0
			40	29	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			45	34	10	1		
27	d	1	Total	C	O	P	0	0
			33	24	8	1		
27	d	1	Total	C	O	P	0	0
			49	38	10	1		
27	d	1	Total	C	O	P	0	0
			46	35	10	1		
27	l	1	Total	C	O	P	0	0
			49	38	10	1		

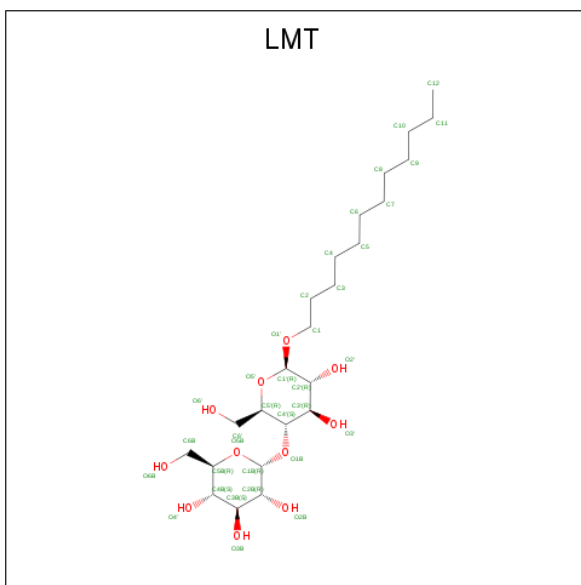
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			49	36	12	1		
28	C	1	Total	C	O	S	0	0
			54	41	12	1		
28	D	1	Total	C	O	S	0	0
			20	9	10	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			51	38	12	1		
28	b	1	Total	C	O	S	0	0
			38	26	11	1		
28	f	1	Total	C	O	S	0	0
			14	6	7	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total 35	C 24	O 11	0	0
29	B	1	Total 24	C 18	O 6	0	0
29	E	1	Total 24	C 18	O 6	0	0
29	I	1	Total 35	C 24	O 11	0	0
29	T	1	Total 24	C 18	O 6	0	0
29	Z	1	Total 35	C 24	O 11	0	0
29	a	1	Total 35	C 24	O 11	0	0
29	c	1	Total 35	C 24	O 11	0	0
29	c	1	Total 24	C 18	O 6	0	0
29	f	1	Total 25	C 19	O 6	0	0
29	t	1	Total 24	C 18	O 6	0	0

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	J	1	Total C 16 16	0	0

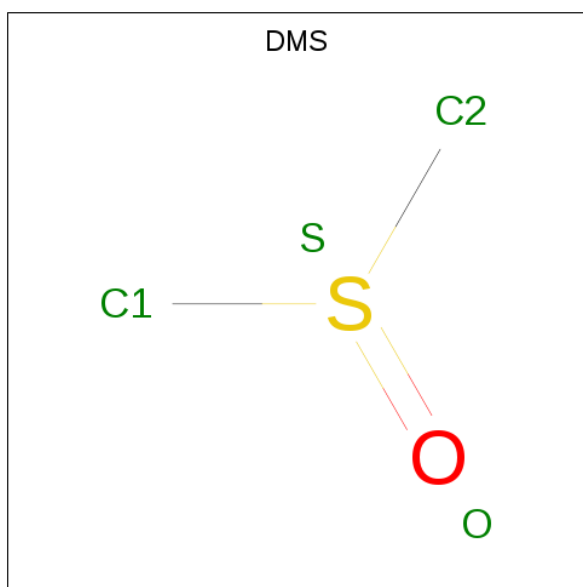
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	i	4	Total C 58 58	0	0
30	D	1	Total C 16 16	0	0
30	d	1	Total C 16 16	0	0
30	B	2	Total C 23 23	0	0
30	I	3	Total C 45 45	0	0
30	c	1	Total C 10 10	0	0
30	a	2	Total C 16 16	0	0
30	j	1	Total C 16 16	0	0
30	x	1	Total C 15 15	0	0
30	Z	1	Total C 9 9	0	0
30	A	1	Total C 5 5	0	0
30	T	1	Total C 13 13	0	0
30	U	1	Total C 14 14	0	0
30	X	1	Total C 16 16	0	0
30	O	1	Total C 16 16	0	0
30	t	1	Total C 16 16	0	0
30	u	1	Total C 11 11	0	0
30	b	2	Total C 27 27	0	0

- Molecule 31 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	A	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		
31	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	L	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0

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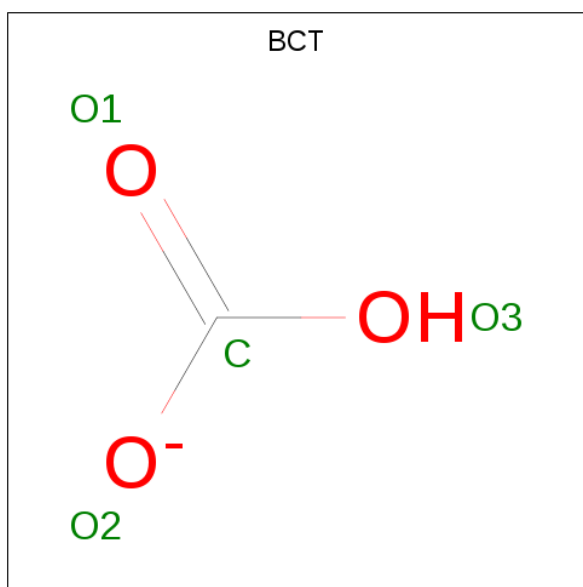
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	f	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



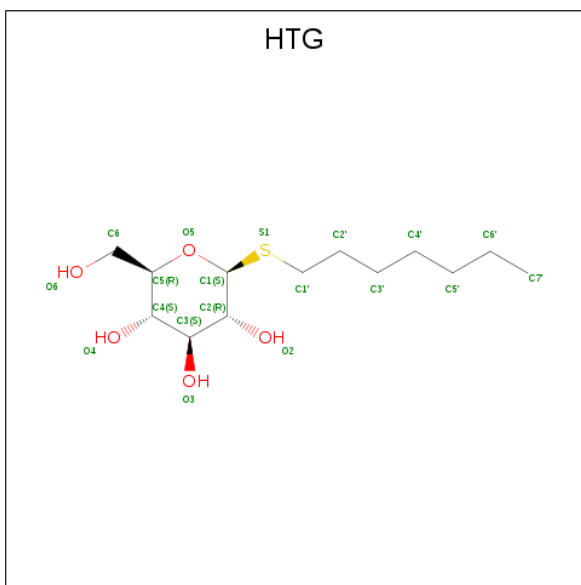
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			8	2	6		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	o	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	B	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		

- Molecule 34 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



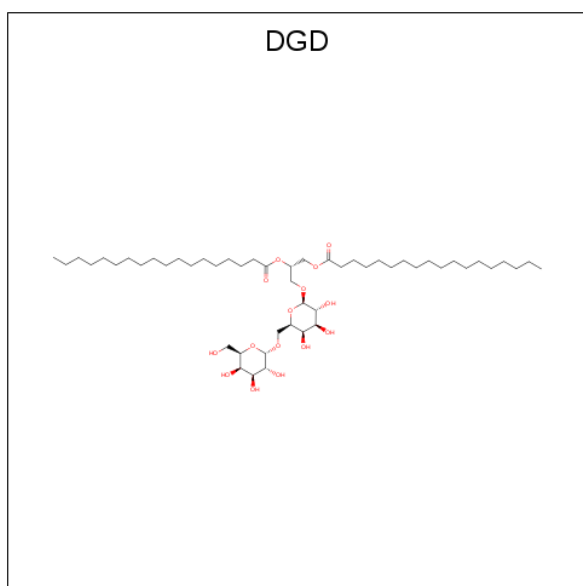
[illegible]

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			19	13	5	1		
34	l	1	Total	C	O	S	0	0
			19	13	5	1		
34	v	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



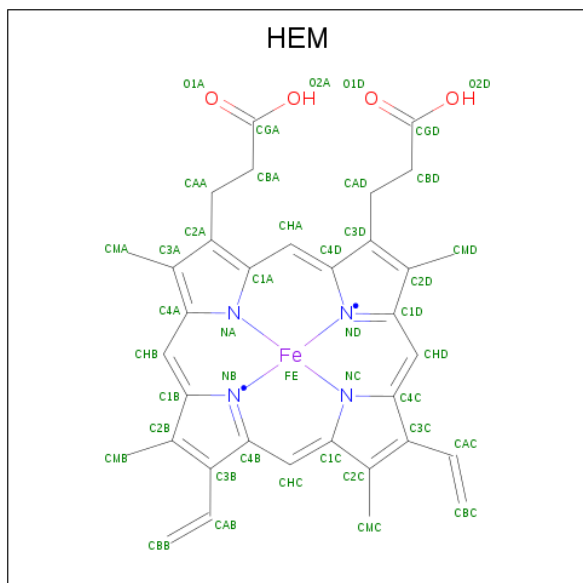
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	D	1	Total	C	O		0	0
			50	41	9			
35	H	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			

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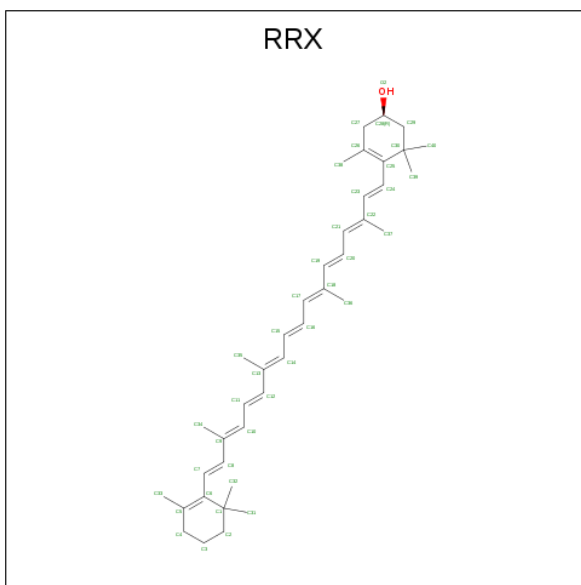
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total	C	O	0	0
			43	37	6		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
36	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	H	1	Total	C	O	0	0
			41	40	1		
37	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	J	1	Total	Mg	0	0
			1	1		
38	j	1	Total	Mg	0	0
			1	1		
38	K	1	Total	Mg	0	0
			1	1		
38	k	1	Total	Mg	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	132	Total	O	0	0
			132	132		
39	B	256	Total	O	0	6
			262	262		
39	C	174	Total	O	0	4
			178	178		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	D	130	Total 131	O 131	0	1
39	E	33	Total 35	O 35	0	2
39	F	4	Total 4	O 4	0	0
39	H	39	Total 39	O 39	0	0
39	I	5	Total 5	O 5	0	0
39	J	15	Total 16	O 16	0	1
39	K	7	Total 7	O 7	0	0
39	L	18	Total 19	O 19	0	1
39	O	161	Total 166	O 166	0	5
39	T	12	Total 12	O 12	0	0
39	U	72	Total 74	O 74	0	2
39	V	110	Total 113	O 113	0	3
39	Y	7	Total 8	O 8	0	1
39	X	15	Total 16	O 16	0	1
39	Z	5	Total 5	O 5	0	0
39	a	122	Total 123	O 123	0	1
39	b	251	Total 261	O 261	0	10
39	c	216	Total 220	O 220	0	4
39	d	115	Total 115	O 115	0	0
39	e	16	Total 17	O 17	0	1
39	f	4	Total 4	O 4	0	0

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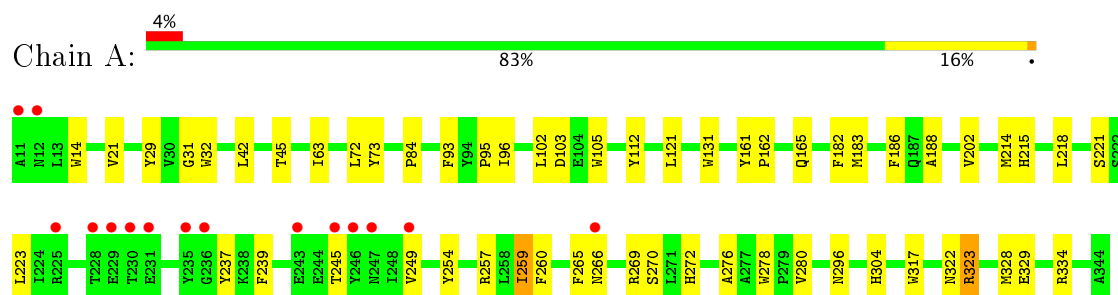
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	h	31	Total 31	O 31	0	0
39	i	5	Total 5	O 5	0	0
39	j	10	Total 10	O 10	0	0
39	k	9	Total 10	O 10	0	1
39	l	14	Total 15	O 15	0	1
39	o	153	Total 156	O 156	0	3
39	t	10	Total 10	O 10	0	0
39	u	75	Total 75	O 75	0	0
39	v	77	Total 82	O 82	0	5
39	y	1	Total 1	O 1	0	0
39	x	5	Total 5	O 5	0	0
39	z	8	Total 8	O 8	0	0

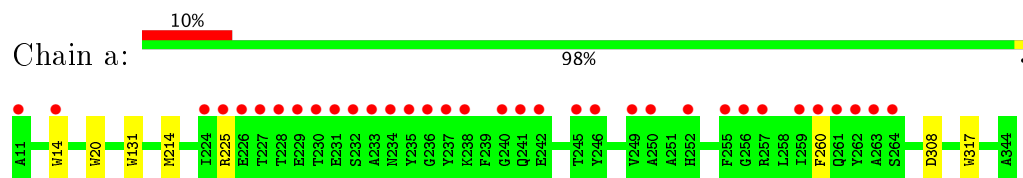
### 3 Residue-property plots

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.

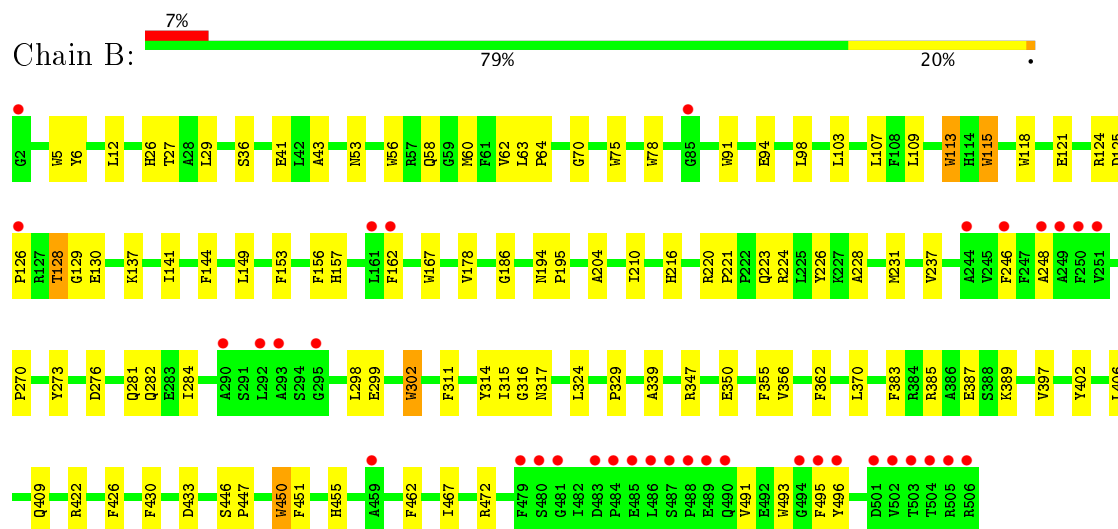
- Molecule 1: Photosystem II protein D1 1

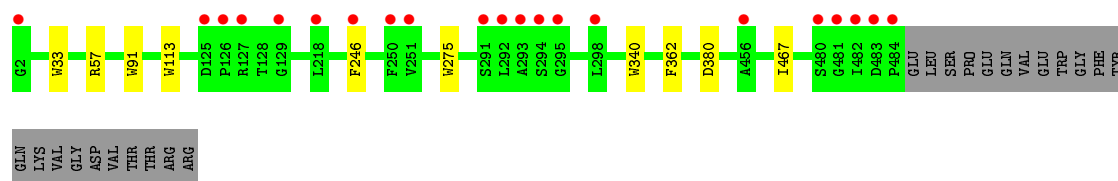


- Molecule 1: Photosystem II protein D1 1

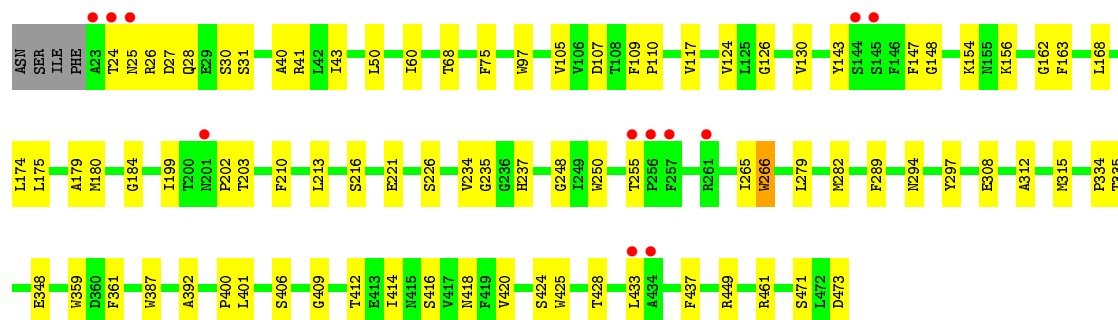
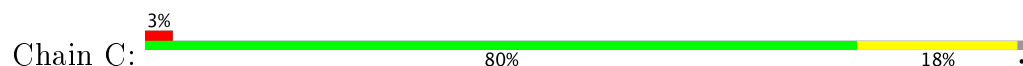


- Molecule 2: Photosystem II CP47 reaction center protein





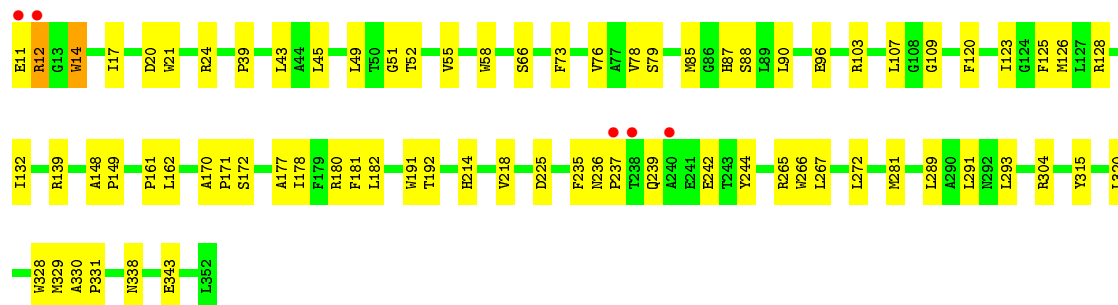
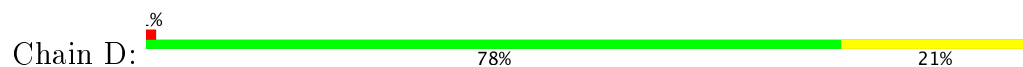
- Molecule 3: Photosystem II CP43 reaction center protein



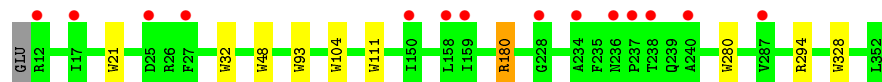
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein

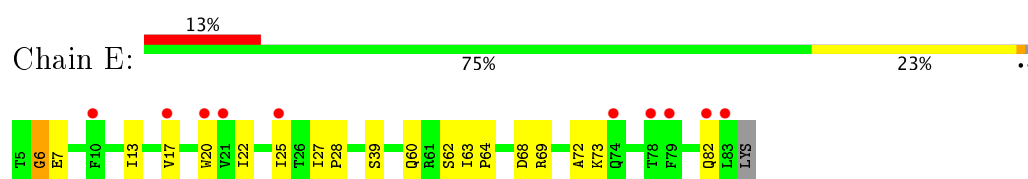


- Molecule 4: Photosystem II D2 protein

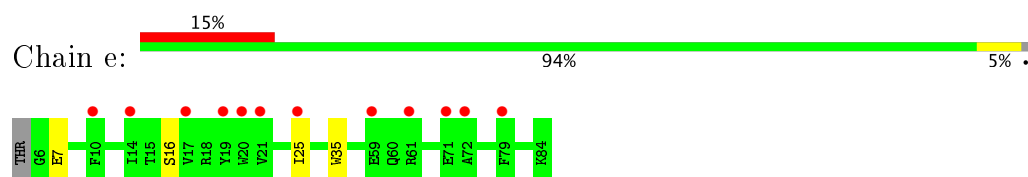


- Molecule 5: Cytochrome b559 subunit alpha

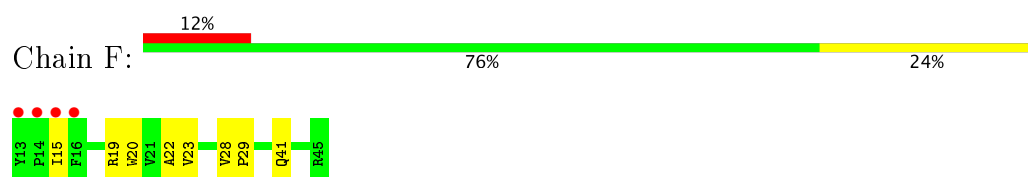




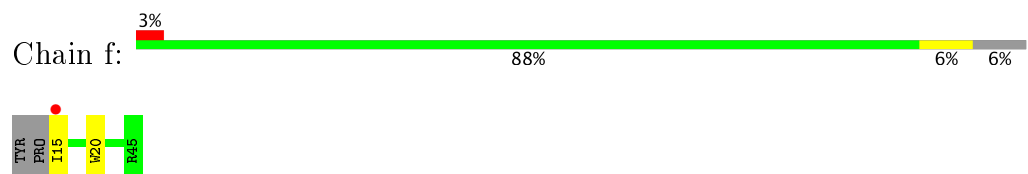
- Molecule 5: Cytochrome b559 subunit alpha



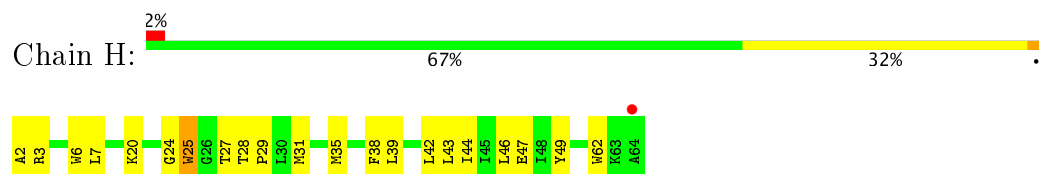
- Molecule 6: Cytochrome b559 subunit beta



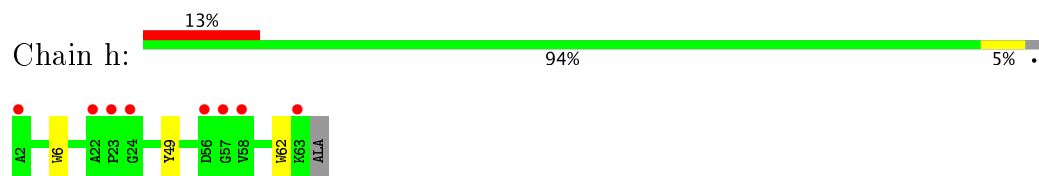
- Molecule 6: Cytochrome b559 subunit beta



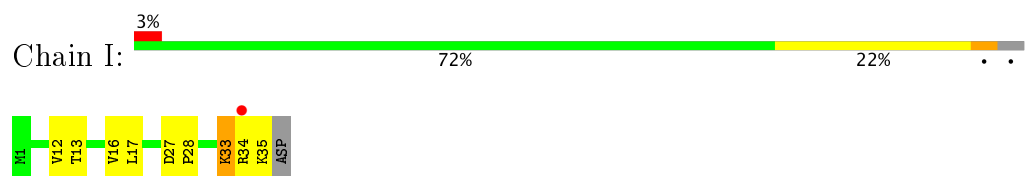
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  100%

There are no outlier residues recorded for this chain.

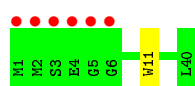
- Molecule 9: Photosystem II reaction center protein J

Chain J:  5% 70% 20% 10%



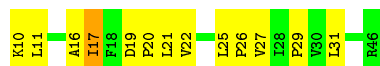
- Molecule 9: Photosystem II reaction center protein J

Chain j:  15% 98% .



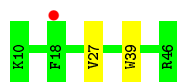
- Molecule 10: Photosystem II reaction center protein K

Chain K:  65% 32% .




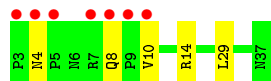
- Molecule 10: Photosystem II reaction center protein K

Chain k:  3% 95% 5%



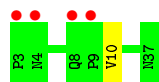
- Molecule 11: Photosystem II reaction center protein L

Chain L:  20% 86% 14%




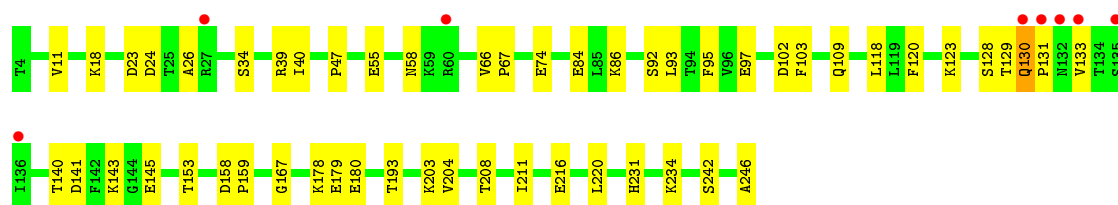
- Molecule 11: Photosystem II reaction center protein L

Chain l:  11% 97% .

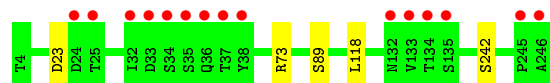


- Molecule 12: Photosystem II manganese-stabilizing polypeptide

Chain O:  3% 78% 21%



- Molecule 12: Photosystem II manganese-stabilizing polypeptide



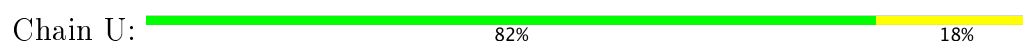
- Molecule 13: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein T



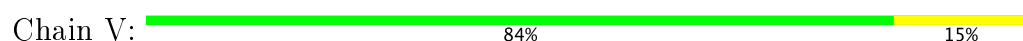
- Molecule 14: Photosystem II 12 kDa extrinsic protein



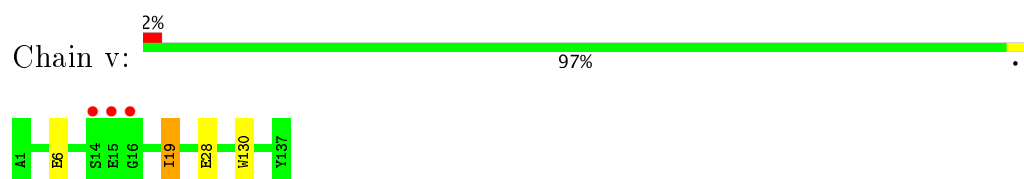
- Molecule 14: Photosystem II 12 kDa extrinsic protein



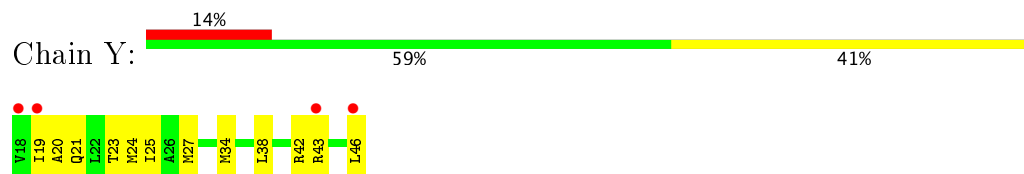
- Molecule 15: Cytochrome c-550



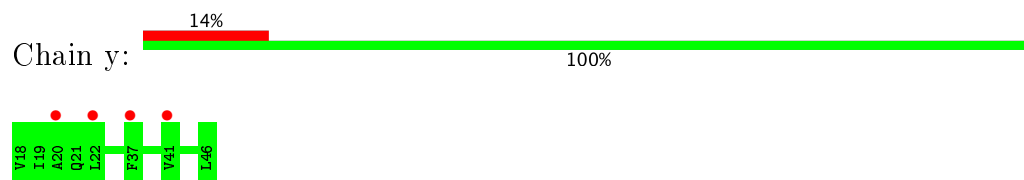
- Molecule 15: Cytochrome c-550



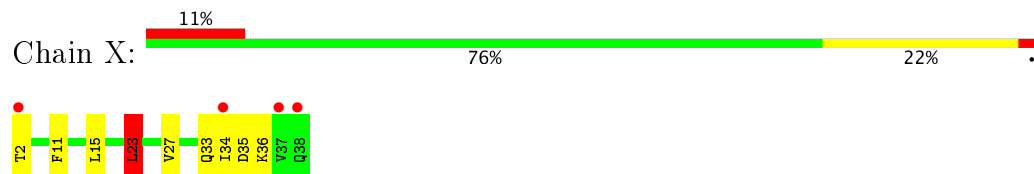
- Molecule 16: Photosystem II reaction center protein Ycf12



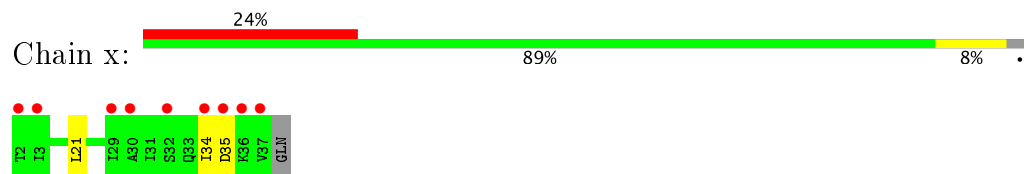
- Molecule 16: Photosystem II reaction center protein Ycf12



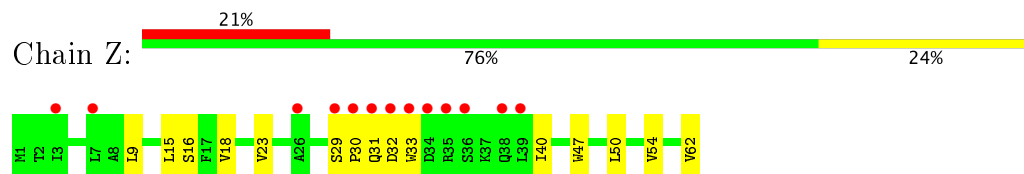
- Molecule 17: Photosystem II reaction center X protein



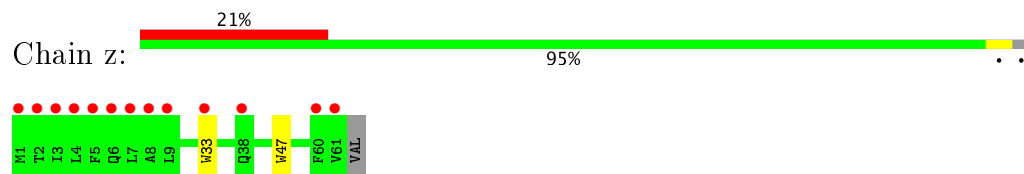
- Molecule 17: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center protein Z



- Molecule 18: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.95Å 226.99Å 285.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 46.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.3 (46.79-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.174 , 0.226 0.174 , 0.225	Depositor DCC
$R_{free}$ test set	19307 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	51892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: LHG, HTG, MG, OEX, PHO, DGD, CL, CA, SQD, LMT, CLA, PL9, DMS, FE2, RRX, BCT, HEM, FME, UNL, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.86	3/2686 (0.1%)	0.76	2/3666 (0.1%)
1	a	0.87	4/2640 (0.2%)	0.77	1/3604 (0.0%)
2	B	0.87	10/4099 (0.2%)	0.77	5/5591 (0.1%)
2	b	0.85	5/3917 (0.1%)	0.78	3/5342 (0.1%)
3	C	0.85	6/3583 (0.2%)	0.76	1/4880 (0.0%)
3	c	0.83	9/3638 (0.2%)	0.76	1/4953 (0.0%)
4	D	0.91	5/2836 (0.2%)	0.77	0/3866
4	d	0.88	8/2818 (0.3%)	0.75	2/3842 (0.1%)
5	E	0.73	0/654	0.73	0/895
5	e	0.71	1/655 (0.2%)	0.72	0/896
6	F	0.83	1/278 (0.4%)	0.62	0/379
6	f	0.78	1/257 (0.4%)	0.66	0/349
7	H	0.83	3/541 (0.6%)	0.74	0/737
7	h	0.80	2/517 (0.4%)	0.68	0/704
8	I	0.67	0/285	0.67	0/385
8	i	0.63	0/290	0.64	0/392
9	J	0.80	1/257 (0.4%)	0.72	0/349
9	j	0.79	1/283 (0.4%)	0.67	0/384
10	K	0.71	0/303	0.73	0/416
10	k	0.74	1/296 (0.3%)	0.70	0/408
11	L	0.74	0/294	0.73	0/399
11	l	0.72	0/294	0.71	0/399
12	O	0.69	0/1887	0.80	0/2561
12	o	0.63	0/1864	0.78	1/2535 (0.0%)
13	T	0.79	0/252	0.72	0/342
13	t	0.74	0/252	0.69	0/342
14	U	0.76	0/796	0.82	0/1078
14	u	0.71	0/777	0.79	0/1054
15	V	0.78	0/1090	0.78	0/1480
15	v	0.69	1/1082 (0.1%)	0.75	0/1472
16	Y	0.54	0/216	0.72	0/289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	y	0.48	0/208	0.67	0/278
17	X	0.55	0/275	0.68	1/373 (0.3%)
17	x	0.56	0/256	0.65	0/349
18	Z	0.69	1/463 (0.2%)	0.67	0/636
18	z	0.65	2/447 (0.4%)	0.62	0/614
All	All	0.81	65/41286 (0.2%)	0.76	17/56239 (0.0%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	387	TRP	CD2-CE2	7.25	1.50	1.41
2	B	78	TRP	CD2-CE2	6.94	1.49	1.41
1	A	317	TRP	CD2-CE2	6.86	1.49	1.41
3	c	365	TRP	CD2-CE2	6.65	1.49	1.41
1	A	278	TRP	CD2-CE2	6.57	1.49	1.41
2	b	33	TRP	CD2-CE2	6.42	1.49	1.41
2	b	275	TRP	CD2-CE2	6.39	1.49	1.41
2	B	56	TRP	CD2-CE2	6.37	1.49	1.41
4	d	48	TRP	CD2-CE2	6.21	1.48	1.41
4	D	58	TRP	CD2-CE2	6.12	1.48	1.41
4	d	93	TRP	CD2-CE2	6.10	1.48	1.41
2	B	5	TRP	CD2-CE2	6.04	1.48	1.41
2	B	167	TRP	CD2-CE2	6.00	1.48	1.41
3	c	250	TRP	CD2-CE2	5.98	1.48	1.41
3	c	387	TRP	CD2-CE2	5.95	1.48	1.41
15	v	130	TRP	CD2-CE2	5.90	1.48	1.41
3	c	443	TRP	CD2-CE2	5.86	1.48	1.41
2	B	450	TRP	CD2-CE2	5.84	1.48	1.41
4	d	104	TRP	CD2-CE2	5.80	1.48	1.41
7	H	62	TRP	CD2-CE2	5.74	1.48	1.41
3	C	266	TRP	CD2-CE2	5.69	1.48	1.41
1	A	14	TRP	CD2-CE2	5.68	1.48	1.41
2	B	302	TRP	CD2-CE2	5.62	1.48	1.41
10	k	39	TRP	CD2-CE2	5.62	1.48	1.41
3	C	425	TRP	CD2-CE2	5.58	1.48	1.41
7	H	25	TRP	CD2-CE2	5.57	1.48	1.41
4	d	21	TRP	CD2-CE2	5.56	1.48	1.41
6	f	20	TRP	CD2-CE2	5.56	1.48	1.41
18	z	33	TRP	CD2-CE2	5.55	1.48	1.41
2	B	115	TRP	CD2-CE2	5.52	1.48	1.41
1	a	131	TRP	CD2-CE2	5.46	1.48	1.41
3	C	250	TRP	CD2-CE2	5.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	11	TRP	CD2-CE2	5.44	1.47	1.41
4	d	32	TRP	CD2-CE2	5.39	1.47	1.41
1	a	14	TRP	CD2-CE2	5.38	1.47	1.41
3	c	359	TRP	CD2-CE2	5.37	1.47	1.41
2	b	91	TRP	CD2-CE2	5.37	1.47	1.41
2	B	91	TRP	CD2-CE2	5.37	1.47	1.41
6	F	20	TRP	CD2-CE2	5.35	1.47	1.41
3	C	359	TRP	CD2-CE2	5.34	1.47	1.41
3	c	35	TRP	CD2-CE2	5.32	1.47	1.41
2	b	340	TRP	CD2-CE2	5.32	1.47	1.41
2	B	493	TRP	CD2-CE2	5.29	1.47	1.41
1	a	20	TRP	CD2-CE2	5.27	1.47	1.41
4	D	21	TRP	CD2-CE2	5.25	1.47	1.41
1	a	317	TRP	CD2-CE2	5.25	1.47	1.41
4	D	87	HIS	CG-CD2	5.25	1.44	1.35
4	d	328	TRP	CD2-CE2	5.23	1.47	1.41
2	b	113	TRP	CD2-CE2	5.22	1.47	1.41
4	D	14	TRP	CD2-CE2	5.19	1.47	1.41
3	c	259	TRP	CD2-CE2	5.19	1.47	1.41
18	z	47	TRP	CD2-CE2	5.18	1.47	1.41
18	Z	33	TRP	CD2-CE2	5.16	1.47	1.41
7	h	6	TRP	CD2-CE2	5.16	1.47	1.41
2	B	113	TRP	CD2-CE2	5.13	1.47	1.41
4	d	280	TRP	CD2-CE2	5.12	1.47	1.41
4	D	328	TRP	CD2-CE2	5.08	1.47	1.41
3	c	36	TRP	CD2-CE2	5.05	1.47	1.41
9	j	11	TRP	CD2-CE2	5.04	1.47	1.41
3	C	97	TRP	CD2-CE2	5.04	1.47	1.41
4	d	111	TRP	CD2-CE2	5.04	1.47	1.41
3	c	97	TRP	CD2-CE2	5.04	1.47	1.41
5	e	35	TRP	CD2-CE2	5.04	1.47	1.41
7	H	6	TRP	CD2-CE2	5.03	1.47	1.41
7	h	62	TRP	CD2-CE2	5.02	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	57	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	b	57	ARG	NE-CZ-NH1	6.84	123.72	120.30
3	C	473	ASP	CB-CG-OD1	6.78	124.40	118.30
4	d	180	ARG	NE-CZ-NH1	-5.99	117.31	120.30
2	B	433	ASP	CB-CG-OD1	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	385	ARG	NE-CZ-NH2	-5.71	117.44	120.30
12	o	73	ARG	NE-CZ-NH1	-5.58	117.51	120.30
4	d	294	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	298	LEU	CA-CB-CG	5.32	127.54	115.30
2	B	422	ARG	NE-CZ-NH2	-5.28	117.66	120.30
17	X	23	LEU	CA-CB-CG	5.28	127.43	115.30
1	A	131	TRP	CA-CB-CG	-5.24	103.75	113.70
2	b	380	ASP	CB-CG-OD2	-5.18	113.63	118.30
2	B	433	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	323	ARG	NE-CZ-NH1	5.10	122.85	120.30
3	c	357	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	a	308	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2484	59	0
1	a	2555	0	2420	0	0
2	B	3950	0	3776	99	0
2	b	3780	0	3636	0	0
3	C	3470	0	3380	56	0
3	c	3521	0	3439	0	0
4	D	2732	0	2640	74	0
4	d	2717	0	2628	0	0
5	E	635	0	613	14	0
5	e	636	0	609	0	0
6	F	269	0	277	7	0
6	f	250	0	261	0	0
7	H	522	0	547	20	0
7	h	501	0	526	0	0
8	I	288	0	307	5	0
8	i	293	0	309	0	0
9	J	251	0	257	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	277	0	0
10	K	293	0	305	15	0
10	k	286	0	285	0	0
11	L	287	0	299	5	0
11	l	287	0	299	0	0
12	O	1853	0	1819	48	0
12	o	1833	0	1783	0	0
13	T	253	0	247	5	0
13	t	253	0	247	0	0
14	U	782	0	786	12	0
14	u	766	0	765	0	0
15	V	1066	0	1075	26	0
15	v	1058	0	1053	0	0
16	Y	215	0	246	12	0
16	y	207	0	221	0	0
17	X	269	0	297	6	0
17	x	253	0	274	0	0
18	Z	453	0	471	8	0
18	z	436	0	431	0	0
19	A	10	0	0	0	0
19	a	10	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	185	0	193	15	0
22	B	1014	0	1091	73	0
22	C	836	0	915	39	0
22	D	195	0	216	7	0
22	a	256	0	277	0	0
22	b	1016	0	1096	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
23	A	64	0	74	1	0
23	D	64	0	74	5	0
23	a	128	0	148	0	0
24	A	40	0	56	0	0
24	B	89	0	121	8	0
24	C	80	0	112	5	0
24	D	40	0	56	1	0
24	K	40	0	56	2	0
24	Y	39	0	53	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	0	0
24	b	91	0	123	0	0
24	c	80	0	112	0	0
24	d	40	0	56	0	0
24	k	40	0	56	0	0
24	y	40	0	56	0	0
25	A	51	0	72	2	0
25	B	40	0	50	3	0
25	C	91	0	122	3	0
25	D	46	0	62	5	0
25	J	45	0	60	2	0
25	b	43	0	56	0	0
25	c	100	0	140	0	0
25	d	47	0	64	0	0
25	i	51	0	72	0	0
25	j	47	0	64	0	0
26	A	55	0	80	11	0
26	D	55	0	80	5	0
26	a	55	0	80	0	0
26	d	55	0	80	0	0
27	A	31	0	36	1	0
27	C	30	0	33	1	0
27	D	143	0	211	18	0
27	L	40	0	53	7	0
27	a	94	0	137	0	0
27	d	128	0	178	0	0
27	l	49	0	74	0	0
28	A	49	0	64	2	0
28	C	54	0	78	6	0
28	D	20	0	16	0	0
28	a	105	0	147	0	0
28	b	38	0	47	0	0
28	f	14	0	8	0	0
28	l	54	0	78	0	0
29	A	35	0	46	6	0
29	B	24	0	35	3	0
29	E	24	0	35	1	0
29	I	35	0	46	0	0
29	T	24	0	35	1	0
29	Z	35	0	46	1	0
29	a	35	0	46	0	0
29	c	59	0	81	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	f	25	0	35	0	0
29	t	24	0	35	0	0
30	A	5	0	0	0	0
30	B	23	0	0	0	0
30	D	16	0	0	0	0
30	I	45	0	0	1	0
30	J	16	0	0	1	0
30	O	16	0	0	0	0
30	T	13	0	0	0	0
30	U	14	0	0	1	0
30	X	16	0	0	1	0
30	Z	9	0	0	0	0
30	a	16	0	0	0	0
30	b	27	0	0	0	0
30	c	10	0	0	0	0
30	d	16	0	0	0	0
30	i	58	0	0	0	0
30	j	16	0	0	0	0
30	t	16	0	0	0	0
30	u	11	0	0	0	0
30	x	15	0	0	0	0
31	A	20	0	30	2	0
31	B	60	0	90	15	0
31	C	60	0	90	3	0
31	D	12	0	18	0	0
31	F	4	0	6	0	0
31	H	4	0	6	0	0
31	I	8	0	12	0	0
31	L	4	0	6	0	0
31	O	48	0	72	24	0
31	U	8	0	12	1	0
31	V	40	0	60	19	0
31	a	20	0	30	0	0
31	b	36	0	54	0	0
31	c	76	0	114	0	0
31	d	20	0	30	0	0
31	f	4	0	6	0	0
31	i	4	0	6	0	0
31	l	12	0	18	0	0
31	o	28	0	42	0	0
31	t	12	0	18	0	0
31	u	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	v	36	0	54	0	0
32	A	8	0	0	1	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	57	0	78	4	0
34	C	47	0	67	2	0
34	D	38	0	52	10	0
34	V	14	0	13	0	0
34	b	95	0	130	0	0
34	c	19	0	26	0	0
34	l	19	0	26	0	0
34	v	16	0	17	0	0
35	C	186	0	246	3	0
35	D	50	0	69	0	0
35	H	62	0	82	4	0
35	c	186	0	246	0	0
35	d	43	0	62	0	0
35	h	62	0	82	0	0
36	E	43	0	30	1	0
36	V	43	0	30	1	0
36	e	43	0	30	0	0
36	v	43	0	30	0	0
37	H	41	0	56	12	0
37	h	41	0	56	0	0
38	J	1	0	0	0	0
38	K	1	0	0	0	0
38	j	1	0	0	0	0
38	k	1	0	0	0	0
39	A	132	0	0	1	0
39	B	262	0	0	13	0
39	C	178	0	0	3	0
39	D	131	0	0	5	0
39	E	35	0	0	1	0
39	F	4	0	0	0	0
39	H	39	0	0	1	0
39	I	5	0	0	0	0
39	J	16	0	0	0	0
39	K	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	L	19	0	0	0	0
39	O	166	0	0	13	0
39	T	12	0	0	0	0
39	U	74	0	0	3	0
39	V	113	0	0	5	0
39	X	16	0	0	0	0
39	Y	8	0	0	0	0
39	Z	5	0	0	1	0
39	a	123	0	0	0	0
39	b	261	0	0	0	0
39	c	220	0	0	0	0
39	d	115	0	0	0	0
39	e	17	0	0	0	0
39	f	4	0	0	0	0
39	h	31	0	0	0	0
39	i	5	0	0	0	0
39	j	10	0	0	0	0
39	k	10	0	0	0	0
39	l	15	0	0	0	0
39	o	156	0	0	0	0
39	t	10	0	0	0	0
39	u	75	0	0	0	0
39	v	82	0	0	0	0
39	x	5	0	0	0	0
39	y	1	0	0	0	0
39	z	8	0	0	0	0
All	All	51892	0	50274	587	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 8.

All (587) 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)
22:B:608:CLA:H52	22:B:608:CLA:H92	2.73	1.10
22:B:608:CLA:H52	22:B:608:CLA:C9	3.21	1.05
2:B:125:ASP:HB3	2:B:128:THR:CG2	4.42	1.05
12:O:66:VAL:HG13	12:O:67:PRO:HD2	1.37	1.05
26:D:406:PL9:C33	27:L:101:LHG:H223	1.87	1.04
1:A:214:MET:HG2	26:A:411:PL9:H102	1.37	1.02
2:B:356:VAL:H	31:B:638:DMS:H21	18.54	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:HD12	10:K:17:ILE:H	1.27	0.96
22:B:608:CLA:H92	22:B:608:CLA:C5	3.22	0.96
2:B:125:ASP:HB3	2:B:128:THR:HG22	5.00	0.92
31:O:310:DMS:H12	39:O:501:HOH:O	1.69	0.91
27:D:411:LHG:H161	27:D:411:LHG:H322	1.52	0.91
1:A:304:HIS:HE1	31:V:212:DMS:H13	1.35	0.90
12:O:133:VAL:HG22	31:O:304:DMS:C2	2.02	0.90
2:B:347[A]:ARG:NH2	39:B:701:HOH:O	2.09	0.86
12:O:66:VAL:CG1	12:O:67:PRO:HD2	2.04	0.86
10:K:17:ILE:H	10:K:17:ILE:CD1	1.88	0.85
24:B:620:BCR:H331	24:B:620:BCR:HC8	2.39	0.84
31:B:628:DMS:H13	39:B:711:HOH:O	1.75	0.84
22:A:405:CLA:HMB1	22:A:405:CLA:HBB1	1.57	0.84
4:D:338:ASN:HB3	39:D:614:HOH:O	1.77	0.83
10:K:17:ILE:HD12	10:K:17:ILE:N	1.93	0.83
27:A:412:LHG:H352	30:I:105:UNL:C3	2.09	0.82
10:K:21:LEU:HD13	16:Y:24:MET:HE3	2.14	0.82
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.61	0.81
1:A:214:MET:HG2	26:A:411:PL9:C10	2.10	0.81
28:C:501:SQD:H381	9:J:22:ILE:HD11	1.63	0.81
1:A:304:HIS:HE1	31:V:212:DMS:C1	1.95	0.80
22:B:614:CLA:HMB1	22:B:614:CLA:HBB1	1.80	0.80
3:C:148:GLY:O	3:C:156:LYS:NZ	2.50	0.79
31:B:642:DMS:H13	39:B:853:HOH:O	1.83	0.78
13:T:2:GLU:HG2	13:T:6:TYR:CE2	2.43	0.78
22:D:401:CLA:HMB1	22:D:401:CLA:HBB1	1.66	0.78
24:B:620:BCR:H331	24:B:620:BCR:C8	2.48	0.78
4:D:242:GLU:HG3	4:D:244:TYR:O	3.24	0.77
12:O:133:VAL:HG22	31:O:304:DMS:H21	1.64	0.77
12:O:208:THR:O	31:O:305:DMS:C1	9.83	0.77
10:K:19:ASP:HB3	10:K:20:PRO:HD3	1.67	0.76
3:C:40:ALA:O	3:C:43:ILE:HG13	1.86	0.76
15:V:129[B]:LYS:HB3	31:V:210:DMS:S	26.59	0.76
14:U:9:LEU:HA	39:U:332:HOH:O	38.51	0.75
1:A:304:HIS:CE1	31:V:212:DMS:H13	2.21	0.75
27:D:411:LHG:H142	27:D:411:LHG:H331	1.68	0.74
4:D:343[B]:GLU:OE2	34:D:415:HTG:H2	1.87	0.74
29:A:414:LMT:H2B	4:D:304:ARG:HH22	1.53	0.74
4:D:85:MET:HE2	4:D:90[A]:LEU:HD21	1.83	0.74
27:D:409:LHG:O9	27:L:101:LHG:HC81	1.88	0.73
2:B:125:ASP:CB	2:B:128:THR:HG22	5.94	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.92	0.73
2:B:125:ASP:HB3	2:B:128:THR:HG23	4.94	0.72
12:O:208:THR:O	31:O:305:DMS:H12	9.78	0.72
15:V:126:LEU:O	15:V:129[A]:LYS:HD2	1.89	0.72
22:B:608:CLA:H203	27:D:409:LHG:H122	1.71	0.72
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.25	0.71
15:V:27:LEU:HD21	31:V:206:DMS:C1	2.20	0.71
2:B:125:ASP:OD2	2:B:128:THR:HG22	6.31	0.71
2:B:299:GLU:HG3	39:B:879:HOH:O	5.52	0.71
22:C:507:CLA:HBB1	22:C:507:CLA:HMB1	1.70	0.71
31:O:312:DMS:H21	39:O:467:HOH:O	1.89	0.71
12:O:179:GLU:HG3	31:O:312:DMS:H11	1.73	0.70
2:B:282:GLN:NE2	39:B:701:HOH:O	19.94	0.70
2:B:467:ILE:HG13	4:D:126:MET:HE2	2.74	0.70
2:B:383:PHE:CZ	12:O:167:GLY:HA2	2.62	0.70
3:C:461:ARG:HG3	39:D:534:HOH:O	1.91	0.70
1:A:183:MET:HA	22:A:405:CLA:HMD2	1.75	0.69
4:D:14:TRP:CD1	34:D:414:HTG:H61	2.28	0.69
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.75	0.68
2:B:446:SER:HB2	2:B:447:PRO:CD	2.22	0.68
1:A:304:HIS:CE1	31:V:212:DMS:C1	2.76	0.68
1:A:121[A]:LEU:HD23	25:A:410:LMG:H202	1.74	0.68
2:B:36:SER:OG	24:B:619:BCR:H362	2.38	0.68
4:D:343[A]:GLU:OE2	39:D:501:HOH:O	2.11	0.68
15:V:27:LEU:HD21	31:V:206:DMS:H13	1.76	0.68
3:C:279:LEU:HD22	22:C:510:CLA:HED2	1.76	0.67
12:O:133:VAL:HG22	31:O:304:DMS:H23	1.74	0.67
10:K:16:ALA:O	10:K:19:ASP:HB2	1.94	0.67
7:H:2:ALA:N	39:H:201:HOH:O	2.28	0.67
2:B:467:ILE:HG13	4:D:126:MET:CE	2.92	0.66
12:O:178:LYS:HG2	31:O:304:DMS:C2	61.65	0.66
15:V:124:LYS:HE2	39:V:356:HOH:O	20.05	0.66
5:E:68:ASP:O	5:E:72:ALA:HB2	1.96	0.66
27:D:409:LHG:HC12	27:L:101:LHG:O5	1.96	0.65
2:B:356:VAL:N	31:B:638:DMS:H21	17.71	0.65
25:B:621:LMG:H112	25:B:621:LMG:H312	1.79	0.65
2:B:26:HIS:HB2	22:B:613:CLA:HMB2	1.79	0.65
27:D:411:LHG:H331	27:D:411:LHG:C14	2.25	0.65
22:B:605:CLA:H43	22:B:606:CLA:H2	1.80	0.64
3:C:279:LEU:HD12	3:C:282:MET:CE	2.27	0.64
18:Z:50:LEU:O	18:Z:54:VAL:HG23	2.57	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:408:CLA:HBB1	22:A:408:CLA:HMB1	2.01	0.64
22:D:403:CLA:HMB1	22:D:403:CLA:HBB1	2.15	0.64
2:B:462:PHE:CE1	22:B:614:CLA:HMB3	2.45	0.63
22:C:510:CLA:HBB1	22:C:510:CLA:HMB1	1.81	0.63
37:H:101:RRX:H46	37:H:101:RRX:H55	1.95	0.63
4:D:85:MET:CE	4:D:96:GLU:HG2	2.28	0.63
14:U:9:LEU:HA	39:U:301:HOH:O	1.98	0.63
3:C:179:ALA:O	3:C:184:GLY:HA2	2.21	0.62
2:B:350:GLU:HG3	31:B:631:DMS:C1	2.30	0.62
22:D:404:CLA:HBB1	22:D:404:CLA:HMB1	1.81	0.62
12:O:74[A]:GLU:OE2	39:O:401:HOH:O	2.16	0.62
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.82	0.61
26:A:411:PL9:H403	6:F:22:ALA:HB2	1.82	0.61
5:E:22:ILE:O	5:E:25:ILE:HG22	4.25	0.61
12:O:102:ASP:OD1	12:O:123:LYS:NZ	2.85	0.61
1:A:265:PHE:HE2	26:A:411:PL9:H122	1.64	0.61
1:A:215:HIS:HA	26:A:411:PL9:O1	2.01	0.60
6:F:15:ILE:O	6:F:15:ILE:HG23	3.17	0.60
5:E:20:TRP:CD1	9:J:8:ILE:HD13	2.35	0.60
34:D:415:HTG:H3	15:V:55:ARG:HH12	1.66	0.60
22:C:507:CLA:HMC2	22:C:508:CLA:H102	1.83	0.60
37:H:101:RRX:H46	37:H:101:RRX:C33	2.62	0.60
22:C:512:CLA:HMB1	22:C:512:CLA:HBB1	1.83	0.60
12:O:18:LYS:HE3	39:O:490:HOH:O	52.84	0.60
4:D:85:MET:CE	4:D:90[A]:LEU:HD21	2.38	0.60
22:C:511:CLA:HMB1	22:C:511:CLA:HBB1	1.83	0.59
2:B:350:GLU:HG3	31:B:631:DMS:H12	1.84	0.59
25:D:412:LMG:H352	34:D:414:HTG:H6'2	1.84	0.59
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.99	0.59
1:A:223:LEU:HD22	4:D:265:ARG:HG2	1.84	0.59
17:X:34:ILE:C	17:X:36:LYS:H	3.45	0.58
22:B:606:CLA:C14	22:B:611:CLA:HED2	2.33	0.58
26:D:406:PL9:C32	27:L:101:LHG:H223	2.32	0.58
22:B:615:CLA:HED3	11:L:8:GLN:O	2.44	0.58
12:O:47:PRO:HG3	12:O:120:PHE:CE1	2.38	0.58
7:H:3[A]:ARG:HB2	7:H:3[A]:ARG:HH11	4.79	0.58
7:H:3[A]:ARG:HB2	7:H:3[A]:ARG:NH1	5.31	0.58
4:D:49:LEU:HD21	25:J:101:LMG:H341	1.84	0.58
4:D:85:MET:HE3	4:D:96:GLU:HG2	1.96	0.58
1:A:265:PHE:O	26:A:411:PL9:H531	2.04	0.58
2:B:137:LYS:O	2:B:141:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:606:CLA:HBB1	22:B:606:CLA:HHC	2.81	0.57
2:B:223:GLN:NE2	39:B:703:HOH:O	2.37	0.57
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.86	0.57
37:H:101:RRX:C23	37:H:101:RRX:H17	2.69	0.57
15:V:78:ASN:OD1	15:V:96:ARG:NH1	2.77	0.57
24:B:620:BCR:HC8	24:B:620:BCR:C33	2.93	0.57
27:D:409:LHG:HC92	27:L:101:LHG:HC92	1.86	0.57
29:A:414:LMT:H2B	4:D:304:ARG:NH2	2.18	0.57
22:C:502:CLA:HMD2	22:C:503:CLA:H101	1.87	0.57
2:B:356:VAL:HG23	31:B:638:DMS:H22	18.56	0.57
22:B:615:CLA:HBB1	22:B:615:CLA:HMB1	1.86	0.57
31:O:310:DMS:C1	39:O:427:HOH:O	2.52	0.56
12:O:39:ARG:HD3	39:O:413:HOH:O	2.04	0.56
2:B:29:LEU:HD11	24:B:618:BCR:H19C	2.65	0.56
26:A:411:PL9:H221	23:D:402:PHO:HMA2	1.87	0.56
10:K:21:LEU:HB2	16:Y:24:MET:HE3	3.90	0.56
1:A:322:ASN:OD1	3:C:412:THR:HA	2.23	0.56
1:A:329:GLU:HG3	39:A:617:HOH:O	23.17	0.56
1:A:96:ILE:HD12	22:A:408:CLA:HMD1	1.86	0.56
2:B:248:ALA:HB2	22:B:604:CLA:H51	1.87	0.56
4:D:90[B]:LEU:HG	4:D:109:GLY:HA2	2.06	0.56
34:D:415:HTG:C3	15:V:55:ARG:HH12	2.19	0.56
23:A:407:PHO:HBB1	23:A:407:PHO:HMB1	1.87	0.56
12:O:39:ARG:NH1	39:O:404:HOH:O	2.39	0.56
2:B:103:LEU:HD21	22:B:606:CLA:HMC3	1.96	0.56
22:B:609:CLA:H203	22:B:610:CLA:H191	2.63	0.56
3:C:437:PHE:CE1	22:C:511:CLA:HMB3	2.41	0.56
22:D:401:CLA:HMC1	22:D:401:CLA:HBC2	1.88	0.56
29:B:622:LMT:H11	25:D:412:LMG:HC92	1.88	0.55
9:J:18:GLY:HA3	24:Y:101:BCR:H371	2.11	0.55
2:B:339:ALA:HB2	12:O:58:ASN:HB3	45.08	0.55
2:B:125:ASP:CB	2:B:128:THR:CG2	5.31	0.55
24:C:515:BCR:H331	24:C:515:BCR:C8	2.36	0.55
16:Y:20:ALA:O	16:Y:24:MET:HG2	2.07	0.55
22:B:611:CLA:HBB1	22:B:611:CLA:HHC	1.87	0.55
2:B:281:GLN:NE2	39:B:702:HOH:O	48.71	0.55
12:O:208:THR:O	31:O:305:DMS:H13	8.97	0.55
3:C:126:GLY:O	3:C:130:VAL:HG23	2.54	0.55
8:I:13:THR:O	8:I:17:LEU:HG	2.07	0.55
15:V:129[B]:LYS:HB3	31:V:212:DMS:S	2.47	0.55
2:B:63:LEU:N	2:B:64:PRO:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:20:PRO:HB3	16:Y:21:GLN:HG3	1.88	0.55
2:B:389:LYS:NZ	34:D:415:HTG:H2'2	2.22	0.54
27:D:411:LHG:H161	27:D:411:LHG:C32	2.32	0.54
1:A:265:PHE:CE2	26:A:411:PL9:H122	2.42	0.54
2:B:324:LEU:HA	4:D:293[B]:LEU:HG	5.32	0.54
2:B:128:THR:HG23	2:B:130:GLU:H	4.46	0.54
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.90	0.54
15:V:27:LEU:HD21	31:V:206:DMS:H11	1.88	0.54
28:A:413:SQD:H272	2:B:109:LEU:HD13	60.26	0.54
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.88	0.54
22:B:611:CLA:OBD	22:B:611:CLA:H152	2.18	0.54
12:O:216:GLU:CD	12:O:234:LYS:HD2	2.28	0.54
28:C:501:SQD:H302	22:C:509:CLA:H71	1.90	0.54
12:O:66:VAL:CG1	12:O:67:PRO:CD	2.83	0.54
22:B:608:CLA:H191	26:D:406:PL9:H303	1.89	0.54
9:J:18:GLY:O	9:J:22:ILE:HD12	2.08	0.54
12:O:55:GLU:OE2	12:O:231:HIS:CD2	4.77	0.54
4:D:11:GLU:O	4:D:12:ARG:CB	2.56	0.53
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.09	0.53
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.53
2:B:314:TYR:CE1	2:B:316:GLY:HA3	2.43	0.53
24:C:516:BCR:H331	24:C:516:BCR:C8	2.39	0.53
22:C:505:CLA:H112	35:C:519:DGD:HBF1	1.89	0.53
15:V:129[A]:LYS:HB3	31:V:210:DMS:S	27.15	0.53
29:B:622:LMT:H11	25:D:412:LMG:C9	2.39	0.53
16:Y:23:THR:HG22	16:Y:27:MET:CE	3.21	0.53
22:C:509:CLA:HBB1	22:C:509:CLA:HMB1	1.90	0.53
14:U:58:VAL:HG12	14:U:79:LEU:HD22	2.27	0.53
17:X:23:LEU:O	17:X:27:VAL:HG23	2.08	0.53
1:A:221:SER:HB2	4:D:139:ARG:O	2.09	0.53
18:Z:9:LEU:HD13	18:Z:54:VAL:HG11	2.54	0.53
22:A:406:CLA:HMD3	4:D:182:LEU:HD11	1.89	0.53
27:D:410:LHG:H171	27:L:101:LHG:H201	1.91	0.53
15:V:126:LEU:O	15:V:129[A]:LYS:CD	2.56	0.53
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.64	0.53
2:B:355:PHE:O	2:B:370:LEU:HA	2.32	0.53
22:B:603:CLA:H201	35:H:102:DGD:HBT1	3.13	0.53
30:U:201:UNL:C4	39:U:346:HOH:O	2.57	0.53
22:B:616:CLA:H161	7:H:7:LEU:HD21	2.30	0.52
14:U:38:TYR:HB2	14:U:41:LEU:HD12	1.91	0.52
2:B:41:GLU:HB3	2:B:60:MET:SD	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:33:LYS:O	8:I:35:LYS:HG3	2.33	0.52
3:C:28:GLN:NE2	28:C:501:SQD:O7	2.36	0.52
22:C:505:CLA:H42	35:C:518:DGD:HB42	1.91	0.52
1:A:266:ASN:HD22	4:D:237:PRO:HG3	4.70	0.52
10:K:21:LEU:HD13	16:Y:24:MET:CE	2.54	0.52
12:O:158:ASP:HB2	12:O:159:PRO:CD	2.39	0.52
5:E:7:GLU:HG2	6:F:19:ARG:CZ	4.04	0.52
25:D:412:LMG:O9	25:D:412:LMG:O2	2.19	0.52
4:D:123:ILE:HD11	35:H:102:DGD:HAW1	4.10	0.52
34:D:415:HTG:H7'3	14:U:37:GLN:HE22	1.74	0.52
22:C:514:CLA:C4B	24:C:515:BCR:H383	2.40	0.52
12:O:40:ILE:HD12	12:O:95:PHE:CD2	2.73	0.52
3:C:437:PHE:CZ	22:C:511:CLA:HMB3	2.46	0.51
22:B:605:CLA:HMD2	22:B:613:CLA:H203	1.91	0.51
12:O:39:ARG:HG3	12:O:246:ALA:HB2	4.01	0.51
2:B:125:ASP:CG	2:B:128:THR:HG22	6.43	0.51
22:B:608:CLA:H193	4:D:281:MET:SD	2.50	0.51
22:B:614:CLA:HMB1	22:B:614:CLA:CBB	2.65	0.51
1:A:63:ILE:HB	3:C:335:THR:HG21	1.92	0.51
8:I:12:VAL:O	8:I:16:VAL:HG23	2.11	0.51
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.93	0.51
22:B:602:CLA:C9	37:H:101:RRX:H25	3.02	0.51
12:O:133:VAL:HG13	31:O:304:DMS:H23	1.93	0.51
31:C:530:DMS:H11	39:C:737:HOH:O	2.09	0.51
34:D:415:HTG:H62	39:V:301:HOH:O	2.11	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.54	0.51
2:B:128:THR:HB	2:B:130:GLU:H	1.75	0.51
2:B:355:PHE:HA	31:B:638:DMS:C2	17.76	0.51
3:C:143:TYR:HE2	34:C:532:HTG:H61	1.76	0.51
24:K:101:BCR:H331	24:K:101:BCR:C8	2.65	0.51
3:C:147:PHE:CD2	22:C:514:CLA:H3A	2.46	0.51
14:U:45:LEU:HD21	14:U:71:GLN:HB3	2.42	0.50
2:B:121:GLU:HA	7:H:2:ALA:HB1	1.93	0.50
2:B:299:GLU:HG2	2:B:402:TYR:HD1	2.04	0.50
3:C:334:PRO:HA	12:O:153:THR:OG1	2.11	0.50
31:O:310:DMS:H11	39:O:427:HOH:O	2.10	0.50
2:B:115:TRP:CD2	24:B:618:BCR:H292	2.47	0.50
29:A:414:LMT:H12	34:B:623:HTG:H5	48.98	0.50
3:C:279:LEU:HD12	3:C:282:MET:HE1	1.92	0.50
3:C:60:ILE:HG22	22:C:504:CLA:HHH	1.94	0.50
12:O:178:LYS:HG2	31:O:304:DMS:H23	62.04	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:CD2	4:D:265:ARG:HG2	2.42	0.50
10:K:25:LEU:N	10:K:26:PRO:CD	2.98	0.50
12:O:103:PHE:HA	12:O:120:PHE:O	2.21	0.50
29:A:414:LMT:H32	2:B:43:ALA:HA	42.43	0.49
22:B:609:CLA:H111	4:D:120:PHE:CE1	3.14	0.49
23:D:402:PHO:HMB1	23:D:402:PHO:HBB1	1.93	0.49
22:B:606:CLA:HHC	22:B:606:CLA:CBB	2.82	0.49
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.47	0.49
2:B:221:PRO:HA	22:B:610:CLA:HED3	2.14	0.49
3:C:180:MET:HG2	3:C:199:ILE:O	2.12	0.49
16:Y:38:LEU:O	16:Y:42:ARG:HG2	4.41	0.49
1:A:103:ASP:OD1	31:A:419:DMS:H21	2.13	0.49
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.49
35:C:519:DGD:HBN1	27:D:411:LHG:H222	1.95	0.49
2:B:462:PHE:CZ	22:B:614:CLA:HMB3	2.75	0.49
22:B:606:CLA:HBB1	22:B:607:CLA:C5	2.43	0.49
2:B:62:VAL:HB	22:B:606:CLA:HED3	2.11	0.49
3:C:308:GLU:HB2	3:C:361:PHE:CE2	2.47	0.49
12:O:129:THR:HA	12:O:141:ASP:O	2.13	0.49
1:A:237:TYR:CB	4:D:265:ARG:HD2	2.43	0.49
4:D:272:LEU:HD23	4:D:272:LEU:C	2.34	0.48
22:B:615:CLA:OBD	11:L:10:VAL:CG2	4.65	0.48
26:A:411:PL9:H251	26:A:411:PL9:H272	1.66	0.48
31:B:638:DMS:H13	39:B:778:HOH:O	2.13	0.48
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.29	0.48
3:C:31:SER:CB	3:C:41:ARG:HG2	2.53	0.48
1:A:121[B]:LEU:HD11	22:C:506:CLA:H152	1.94	0.48
26:D:406:PL9:H401	11:L:29:LEU:HD23	1.94	0.48
26:A:411:PL9:H301	4:D:45:LEU:HD22	1.96	0.48
2:B:12:LEU:HB2	22:B:613:CLA:HMC2	2.24	0.48
1:A:249:VAL:HG12	2:B:491:VAL:HG23	1.95	0.48
3:C:117:VAL:HG12	25:C:531:LMG:H222	1.95	0.48
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.14	0.48
12:O:193:THR:HG21	12:O:220:LEU:HD12	2.15	0.48
12:O:145:GLU:CB	31:O:303:DMS:H23	2.43	0.48
15:V:72:LEU:HD12	15:V:120:LEU:HD11	2.93	0.48
1:A:304:HIS:CE1	31:V:212:DMS:H12	2.47	0.48
2:B:355:PHE:HA	31:B:638:DMS:H21	18.51	0.48
22:C:502:CLA:H42	22:C:503:CLA:HMD1	1.95	0.48
3:C:174:LEU:HB3	22:C:503:CLA:H161	1.95	0.48
27:D:410:LHG:H192	13:T:17:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:V:207:DMS:H22	39:V:380:HOH:O	2.14	0.48
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.48
4:D:73:PHE:CZ	25:J:101:LMG:H182	5.49	0.48
18:Z:23:VAL:HG22	18:Z:40:ILE:HG12	2.61	0.48
2:B:162:PHE:O	22:B:607:CLA:HHD	2.17	0.47
3:C:461:ARG:HD2	4:D:225:ASP:OD1	2.14	0.47
22:B:610:CLA:H42	25:D:412:LMG:H171	1.95	0.47
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.47
16:Y:42:ARG:HD2	18:Z:29:SER:OG	4.07	0.47
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.49	0.47
4:D:236:ASN:O	4:D:239:GLN:HG2	2.19	0.47
7:H:38:PHE:HB2	37:H:101:RRX:C10	2.59	0.47
12:O:55:GLU:OE2	12:O:231:HIS:HD2	5.61	0.47
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.47
22:B:604:CLA:H18	22:B:610:CLA:H91	2.67	0.47
22:B:609:CLA:HMB1	22:B:609:CLA:HBB1	1.95	0.47
3:C:202:PRO:HB3	3:C:234:VAL:HG12	2.44	0.47
22:B:609:CLA:H142	7:H:39:LEU:HD21	2.54	0.47
14:U:27:LEU:HD22	14:U:49:ILE:HG21	2.06	0.47
3:C:414:ILE:HD13	31:V:212:DMS:C1	2.44	0.47
17:X:34:ILE:O	17:X:36:LYS:N	3.96	0.47
2:B:228:ALA:HB2	29:B:622:LMT:H21	1.96	0.47
7:H:28:THR:HB	7:H:29:PRO:HD3	2.26	0.47
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.79	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.96	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.57	0.47
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.96	0.47
22:D:401:CLA:CMC	22:D:401:CLA:HBC2	2.45	0.47
39:B:829:HOH:O	31:O:304:DMS:H11	83.40	0.47
3:C:75:PHE:HZ	3:C:105:VAL:HG21	2.10	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
24:Y:101:BCR:H312	18:Z:16:SER:HB3	1.96	0.47
31:B:638:DMS:C1	39:B:778:HOH:O	2.63	0.47
12:O:145:GLU:HB2	31:O:303:DMS:H23	1.96	0.47
18:Z:47:TRP:CD2	29:Z:101:LMT:H111	2.50	0.47
1:A:270:SER:HB2	28:C:501:SQD:O49	2.16	0.47
2:B:451:PHE:CD1	2:B:451:PHE:C	2.99	0.47
1:A:257:ARG:O	4:D:128:ARG:NH2	3.15	0.47
24:K:101:BCR:H371	24:K:101:BCR:H24C	1.91	0.47
31:O:303:DMS:H11	39:O:550:HOH:O	2.14	0.47
1:A:237:TYR:HD2	1:A:245:THR:HB	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:CD1	29:A:414:LMT:H3B	2.50	0.46
4:D:52:THR:HB	4:D:76:VAL:CG2	2.45	0.46
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.97	0.46
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.20	0.46
31:O:310:DMS:H13	39:O:427:HOH:O	2.13	0.46
1:A:29:TYR:CE1	1:A:31:GLY:HA3	2.66	0.46
4:D:343[B]:GLU:HG3	39:V:301:HOH:O	2.14	0.46
27:D:411:LHG:H111	27:D:411:LHG:H162	1.96	0.46
4:D:343[B]:GLU:CD	34:D:415:HTG:H2	2.36	0.46
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.98	0.46
4:D:178:ILE:O	4:D:181:PHE:HB3	2.15	0.46
22:C:511:CLA:H192	22:C:511:CLA:HBC3	1.98	0.46
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.45	0.46
2:B:450:TRP:CZ3	4:D:293[B]:LEU:HD21	4.66	0.46
22:C:505:CLA:H201	27:D:411:LHG:C34	2.46	0.46
22:C:509:CLA:C2B	22:C:511:CLA:HBA1	2.45	0.46
2:B:216:HIS:HE1	22:B:610:CLA:C1A	2.40	0.46
22:C:513:CLA:C11	22:C:514:CLA:H141	2.46	0.46
15:V:79:PRO:HD3	15:V:94:SER:HB3	1.97	0.46
22:C:503:CLA:H61	22:C:513:CLA:H42	1.98	0.46
22:C:513:CLA:H92	22:C:514:CLA:H203	1.97	0.46
17:X:11:PHE:O	17:X:15[A]:LEU:HG	2.16	0.46
2:B:276:ASP:OD1	31:B:641:DMS:H22	2.15	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	2.22	0.46
4:D:162:LEU:HD21	35:H:102:DGD:HA21	1.97	0.46
22:C:505:CLA:H191	27:D:411:LHG:C34	2.46	0.46
4:D:55:VAL:O	4:D:66:SER:HB3	2.15	0.46
37:H:101:RRX:H48	37:H:101:RRX:H47	2.05	0.46
1:A:269:ARG:HD2	4:D:235:PHE:HB2	2.58	0.46
2:B:350:GLU:HG3	31:B:631:DMS:S	2.56	0.46
2:B:406:LEU:O	2:B:409:GLN:HG3	2.88	0.45
2:B:186:GLY:HA3	39:B:839:HOH:O	57.46	0.45
22:B:602:CLA:H203	22:B:602:CLA:H151	5.79	0.45
4:D:39:PRO:O	4:D:43:LEU:HG	2.17	0.45
22:B:602:CLA:HMC1	7:H:44:ILE:HG21	2.30	0.45
3:C:154:LYS:HG2	3:C:266:TRP:CE3	3.14	0.45
22:B:610:CLA:HMC2	37:H:101:RRX:H44	1.99	0.45
22:B:607:CLA:H102	22:B:607:CLA:H61	1.61	0.45
22:B:608:CLA:HBB1	22:B:608:CLA:HMB1	1.97	0.45
22:B:602:CLA:H161	37:H:101:RRX:C16	5.62	0.45
12:O:93:LEU:O	12:O:128:SER:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:129[B]:LYS:HE3	15:V:136:TYR:O	3.74	0.45
22:B:605:CLA:C3B	22:B:614:CLA:HMC3	2.65	0.45
22:C:514:CLA:NB	24:C:515:BCR:H383	2.31	0.45
15:V:30:LYS:HG3	15:V:118:HIS:CE1	2.52	0.45
22:B:605:CLA:HBB1	22:B:605:CLA:HMB1	1.99	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.46	0.45
9:J:26:GLY:HA2	30:J:103:UNL:C10	3.43	0.45
12:O:92:SER:HB3	12:O:131:PRO:HA	1.99	0.45
3:C:294:ASN:HA	3:C:297:TYR:O	2.17	0.45
3:C:400:PRO:C	3:C:401:LEU:HD12	2.64	0.45
4:D:79:SER:HA	4:D:172:SER:HB3	1.97	0.45
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.82	0.45
26:D:406:PL9:H322	27:L:101:LHG:H223	1.98	0.45
16:Y:23:THR:HG22	16:Y:27:MET:HE1	3.26	0.45
22:B:606:CLA:HBB1	22:B:607:CLA:H51	1.99	0.45
22:B:609:CLA:C14	7:H:39:LEU:HD21	2.79	0.45
4:D:52:THR:HB	4:D:76:VAL:HG21	1.97	0.45
12:O:86:LYS:HE3	39:O:549:HOH:O	2.15	0.45
14:U:53:ALA:HB1	14:U:54:PRO:HA	2.12	0.45
18:Z:62:VAL:C	39:Z:203:HOH:O	2.55	0.45
4:D:266:TRP:CG	27:D:410:LHG:HC2	2.51	0.45
2:B:495:PHE:C	2:B:496:TYR:HD1	2.21	0.44
22:B:611:CLA:CBB	22:B:611:CLA:HHC	2.46	0.44
22:B:616:CLA:HMB1	22:B:616:CLA:HBB1	2.29	0.44
15:V:41:HIS:HA	15:V:45:ILE:O	2.17	0.44
22:A:408:CLA:HBA1	22:A:408:CLA:C4A	2.69	0.44
22:B:612:CLA:H72	22:B:612:CLA:H112	1.68	0.44
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.44
2:B:118:TRP:CZ2	11:L:4:ASN:HA	2.52	0.44
15:V:118:HIS:CE1	15:V:122:GLU:HG2	2.53	0.44
3:C:68:THR:OG1	22:C:504:CLA:HED1	2.17	0.44
3:C:266:TRP:CZ3	22:C:508:CLA:HAC2	2.52	0.44
25:C:531:LMG:HC8	25:C:531:LMG:HC1	1.77	0.44
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.44
5:E:39:SER:HB3	29:E:101:LMT:H6E	1.99	0.44
25:C:520:LMG:H241	9:J:22:ILE:HG12	1.99	0.44
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.84	0.44
4:D:24:ARG:NH2	17:X:35:ASP:OD2	2.51	0.44
5:E:60:GLN:NE2	5:E:62:SER:O	2.49	0.44
12:O:97:GLU:OE2	12:O:102:ASP:OD2	2.36	0.44
1:A:121[B]:LEU:CD2	22:A:408:CLA:HMB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:602:CLA:H91	37:H:101:RRX:H25	2.10	0.44
2:B:237:VAL:HG11	22:B:611:CLA:H201	3.16	0.44
2:B:226:TYR:HA	2:B:231:MET:HG3	1.99	0.44
22:B:606:CLA:H141	22:B:611:CLA:HED2	1.98	0.44
22:A:408:CLA:H203	22:C:507:CLA:H101	2.00	0.44
3:C:50:LEU:HD12	22:C:513:CLA:HMD3	1.98	0.44
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.48	0.44
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.00	0.44
22:B:606:CLA:H122	22:B:611:CLA:HMA2	2.00	0.44
3:C:348:GLU:OE2	12:O:11:VAL:HA	2.17	0.44
22:C:504:CLA:HBB1	22:C:504:CLA:HMB1	1.99	0.44
28:C:501:SQD:H111	27:C:522:LHG:H261	2.00	0.44
37:H:101:RRX:H47	37:H:101:RRX:H43	1.77	0.44
7:H:43:LEU:O	7:H:47:GLU:HG3	2.37	0.44
22:B:603:CLA:H41	7:H:46:LEU:HA	1.98	0.44
15:V:2:GLU:OE2	31:V:207:DMS:C1	2.66	0.44
7:H:3[A]:ARG:CB	7:H:3[A]:ARG:HH11	4.72	0.43
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.99	0.43
22:A:408:CLA:H162	22:A:408:CLA:H203	4.19	0.43
28:C:501:SQD:H132	28:C:501:SQD:H162	1.40	0.43
4:D:90[A]:LEU:HA	4:D:90[A]:LEU:HD23	1.41	0.43
22:B:610:CLA:HMD1	7:H:27:THR:HB	2.25	0.43
39:D:630:HOH:O	30:X:101:UNL:C1	2.66	0.43
1:A:202:VAL:HG11	22:A:406:CLA:C3D	2.47	0.43
22:B:614:CLA:H121	25:B:621:LMG:H232	1.99	0.43
22:B:617:CLA:HBB1	22:B:617:CLA:HMB1	1.99	0.43
4:D:267:LEU:HD23	4:D:267:LEU:C	2.53	0.43
5:E:17:VAL:HG23	9:J:7:ARG:CB	2.49	0.43
16:Y:23:THR:HG22	16:Y:27:MET:HE2	4.13	0.43
22:B:608:CLA:H112	22:B:608:CLA:H91	1.76	0.43
22:B:615:CLA:H51	24:B:618:BCR:H372	2.00	0.43
22:C:503:CLA:H193	34:C:521:HTG:H2'1	2.00	0.43
9:J:18:GLY:O	9:J:22:ILE:CD1	2.67	0.43
2:B:224:ARG:HG3	7:H:25:TRP:CD2	2.53	0.43
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.09	0.43
23:D:402:PHO:HBC2	23:D:402:PHO:HHD	2.01	0.43
15:V:41:HIS:CD2	36:V:202:HEM:NB	3.02	0.43
32:A:421[B]:BCT:O3	4:D:214:HIS:CE1	2.71	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.18	0.43
12:O:178:LYS:HG2	31:O:304:DMS:H21	60.99	0.43
1:A:102:LEU:HD23	1:A:102:LEU:HA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:PHE:O	2:B:157:HIS:HB3	2.19	0.43
12:O:204:VAL:HG13	12:O:211:ILE:HG22	2.53	0.43
1:A:161:TYR:CZ	1:A:165:GLN:HG3	2.60	0.43
4:D:170:ALA:HB1	4:D:171:PRO:HD2	2.01	0.43
31:B:628:DMS:C1	39:D:502:HOH:O	2.66	0.43
5:E:13:ILE:HG21	36:E:102:HEM:HAD2	2.00	0.43
18:Z:15:LEU:O	18:Z:18:VAL:HG22	2.19	0.43
1:A:103:ASP:OD1	31:A:419:DMS:C2	2.66	0.43
22:B:615:CLA:OBD	11:L:10:VAL:HG22	5.40	0.43
3:C:414:ILE:HD13	31:V:212:DMS:H11	2.01	0.43
3:C:163:PHE:CD2	22:C:513:CLA:HAB	2.54	0.43
5:E:6:GLY:HA2	39:E:216:HOH:O	51.11	0.43
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.70	0.42
22:B:602:CLA:H72	22:B:602:CLA:H2	4.71	0.42
1:A:239:PHE:O	13:T:29:ILE:HA	3.23	0.42
2:B:284:ILE:CG2	2:B:302:TRP:CZ3	3.34	0.42
25:A:410:LMG:H291	3:C:216:SER:HA	2.01	0.42
3:C:312:ALA:HB1	3:C:392:ALA:O	2.19	0.42
3:C:424:SER:O	3:C:428:THR:HG23	2.38	0.42
27:D:409:LHG:H361	27:D:409:LHG:HC82	2.00	0.42
3:C:124:VAL:HB	24:C:515:BCR:H362	2.00	0.42
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.55	0.42
14:U:87:VAL:HG22	31:U:203:DMS:H13	2.01	0.42
3:C:210:PHE:HA	3:C:213:LEU:HD12	3.05	0.42
4:D:291:LEU:HD21	35:H:102:DGD:CGB	2.50	0.42
15:V:31:ARG:HG2	15:V:31:ARG:HH11	2.69	0.42
22:B:616:CLA:H112	22:B:616:CLA:H152	4.01	0.42
31:C:540:DMS:H11	39:C:638:HOH:O	2.19	0.42
10:K:11:LEU:HD11	10:K:22:VAL:HG21	2.07	0.42
2:B:144:PHE:CE2	2:B:210:ILE:HG23	2.67	0.42
27:D:409:LHG:H332	27:D:409:LHG:H121	2.00	0.42
12:O:140:THR:HG23	31:O:304:DMS:H22	2.00	0.42
1:A:218:LEU:HD12	26:A:411:PL9:C3	2.49	0.42
2:B:94:GLU:HG2	34:B:623:HTG:H2'1	4.71	0.42
10:K:19:ASP:HB3	10:K:20:PRO:CD	2.45	0.42
14:U:36:ILE:HG13	14:U:42:TYR:CG	2.55	0.42
15:V:26:TYR:CE2	15:V:118:HIS:HD2	6.87	0.42
1:A:73:TYR:HD1	29:A:414:LMT:H3B	1.83	0.42
2:B:113:TRP:CD1	22:B:617:CLA:HBA2	3.16	0.42
2:B:98:LEU:HB2	34:B:623:HTG:H7'3	2.02	0.42
22:D:401:CLA:H162	22:D:401:CLA:H203	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:33:LYS:HB3	8:I:34:ARG:H	1.56	0.42
12:O:23:ASP:O	12:O:203:LYS:HE3	4.65	0.42
1:A:45:THR:HG23	22:A:408:CLA:H201	26.36	0.42
22:B:606:CLA:H143	22:B:611:CLA:HED2	2.18	0.42
3:C:409:GLY:HA2	31:V:201:DMS:S	2.59	0.42
22:A:408:CLA:C20	22:C:507:CLA:H101	2.49	0.42
2:B:387:GLU:HG2	34:D:415:HTG:H5'1	2.02	0.42
7:H:42:LEU:HD23	7:H:42:LEU:HA	1.93	0.42
37:H:101:RRX:H3	17:X:2:THR:N	2.18	0.42
6:F:19:ARG:O	6:F:23:VAL:HG23	2.51	0.42
1:A:323:ARG:HB3	4:D:329:MET:HA	2.02	0.41
22:B:610:CLA:HMB2	22:B:611:CLA:C2B	2.54	0.41
12:O:180:GLU:H	12:O:180:GLU:CD	2.24	0.41
3:C:26:ARG:NH2	16:Y:46:LEU:OXT	2.82	0.41
22:A:406:CLA:HAB	22:A:406:CLA:HHC	1.80	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.84	0.41
3:C:25:ASN:HA	3:C:30:SER:CB	2.50	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.41
31:B:629:DMS:H11	39:B:734:HOH:O	59.94	0.41
8:I:27:ASP:N	8:I:28:PRO:CD	3.09	0.41
24:Y:101:BCR:HC8	24:Y:101:BCR:H311	2.61	0.41
1:A:259:ILE:HG22	1:A:260:PHE:N	2.87	0.41
1:A:21:VAL:HG11	1:A:32:TRP:CE3	2.88	0.41
13:T:28:ARG:HA	13:T:28:ARG:HD3	1.87	0.41
22:A:405:CLA:H193	22:A:405:CLA:H161	1.70	0.41
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.55	0.41
2:B:75:TRP:CH2	34:B:626:HTG:H2'1	2.80	0.41
37:H:101:RRX:H28	37:H:101:RRX:H32	1.89	0.41
2:B:124:ARG:HD2	2:B:129:GLY:O	2.20	0.41
2:B:467:ILE:HG13	4:D:126:MET:HE1	2.29	0.41
2:B:6:TYR:OH	27:D:409:LHG:HC11	2.21	0.41
3:C:433:LEU:HD13	22:C:503:CLA:CHC	2.50	0.41
22:C:507:CLA:HBB1	22:C:507:CLA:CMB	2.47	0.41
3:C:168:LEU:HD21	22:C:510:CLA:H62	2.02	0.41
15:V:118:HIS:CE1	15:V:122:GLU:CG	3.04	0.41
2:B:156:PHE:HB3	2:B:162:PHE:HB3	2.08	0.41
22:B:608:CLA:H2	25:B:621:LMG:H161	2.01	0.41
2:B:270:PRO:HG2	2:B:317:ASN:O	2.70	0.41
2:B:446:SER:CB	2:B:447:PRO:CD	2.91	0.41
22:C:508:CLA:HMB1	22:C:508:CLA:HBB1	2.02	0.41
23:D:402:PHO:ND	23:D:402:PHO:NC	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:405:BCR:C8	24:D:405:BCR:H331	2.50	0.41
7:H:31:MET:O	7:H:35:MET:HG3	2.54	0.41
10:K:31:LEU:HD23	10:K:31:LEU:HA	2.25	0.41
15:V:5:PRO:HD3	31:V:205:DMS:C1	2.50	0.41
1:A:182:PHE:O	1:A:186:PHE:HB2	2.28	0.41
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.50	0.41
14:U:45:LEU:O	14:U:49:ILE:HG13	2.20	0.41
1:A:21:VAL:HG11	1:A:32:TRP:CZ3	3.12	0.41
12:O:143:LYS:HE3	31:O:306:DMS:C2	2.51	0.41
2:B:137:LYS:NZ	39:B:709:HOH:O	59.82	0.41
10:K:21:LEU:O	10:K:25:LEU:HG	2.53	0.41
31:O:312:DMS:C2	39:O:467:HOH:O	2.59	0.41
1:A:42:LEU:HD23	28:A:413:SQD:H192	2.02	0.40
2:B:224:ARG:HG2	7:H:24:GLY:O	2.22	0.40
2:B:273:TYR:HA	2:B:276:ASP:HB2	2.03	0.40
3:C:109:PHE:N	3:C:110:PRO:CD	2.97	0.40
2:B:121:GLU:CA	7:H:2:ALA:HB1	2.50	0.40
2:B:339:ALA:CB	12:O:58:ASN:HB3	45.19	0.40
2:B:115:TRP:CZ3	24:B:618:BCR:H401	2.57	0.40
22:B:609:CLA:HMB3	4:D:126:MET:HG2	2.51	0.40
22:B:613:CLA:HHC	22:B:613:CLA:HAB	1.91	0.40
31:C:536:DMS:H22	39:C:750:HOH:O	2.21	0.40
4:D:103:ARG:O	4:D:107:LEU:HG	2.34	0.40
12:O:130:GLN:NE2	12:O:141:ASP:H	2.20	0.40
12:O:179:GLU:HA	31:O:307:DMS:H12	35.72	0.40
1:A:72:LEU:HD21	29:T:102:LMT:H41	2.03	0.40
2:B:194:ASN:HA	2:B:195:PRO:HD2	1.90	0.40
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.09	0.40
13:T:20:ALA:O	13:T:24:ARG:HB3	2.21	0.40
15:V:124:LYS:CE	39:V:356:HOH:O	19.87	0.40
15:V:129[A]:LYS:HB3	31:V:212:DMS:S	2.61	0.40
1:A:276:ALA:O	1:A:280:VAL:HG23	2.41	0.40
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.21	0.40
12:O:130:GLN:HG2	39:O:480:HOH:O	26.57	0.40
14:U:83:THR:OG1	14:U:84:VAL:N	2.74	0.40
16:Y:34:MET:HE2	16:Y:34:MET:HA	2.29	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.03	0.40
22:A:408:CLA:H41	22:A:408:CLA:H61	1.70	0.40
2:B:149:LEU:HB2	22:B:605:CLA:H171	2.22	0.40
2:B:204:ALA:CB	22:B:603:CLA:HAB	2.61	0.40
3:C:107:ASP:O	3:C:110:PRO:HD2	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:GLU:O	3:C:226:SER:HB3	2.27	0.40
4:D:125:PHE:CE1	23:D:402:PHO:HBD	2.57	0.40
4:D:17:ILE:O	4:D:20:ASP:HB2	2.22	0.40
6:F:15:ILE:O	6:F:15:ILE:CG2	3.28	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	44	49
1	a	333/334 (100%)	321 (96%)	11 (3%)	1 (0%)	44	49
2	B	506/505 (100%)	495 (98%)	11 (2%)	0	100	100
2	b	482/505 (95%)	465 (96%)	17 (4%)	0	100	100
3	C	449/455 (99%)	434 (97%)	13 (3%)	2 (0%)	38	41
3	c	454/455 (100%)	435 (96%)	18 (4%)	1 (0%)	51	58
4	D	343/342 (100%)	336 (98%)	6 (2%)	1 (0%)	44	49
4	d	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
5	E	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	14	11
5	e	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
6	F	31/33 (94%)	31 (100%)	0	0	100	100
6	f	29/33 (88%)	29 (100%)	0	0	100	100
7	H	64/63 (102%)	60 (94%)	4 (6%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	5	2
9	j	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	0	100	100
11	l	33/35 (94%)	33 (100%)	0	0	100	100
12	O	242/243 (100%)	228 (94%)	12 (5%)	2 (1%)	22	21
12	o	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
13	T	28/30 (93%)	28 (100%)	0	0	100	100
13	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	U	96/97 (99%)	92 (96%)	4 (4%)	0	100	100
14	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
15	v	136/137 (99%)	126 (93%)	9 (7%)	1 (1%)	25	24
16	Y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
16	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
17	X	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
17	x	34/37 (92%)	31 (91%)	1 (3%)	2 (6%)	2	0
18	Z	60/62 (97%)	56 (93%)	1 (2%)	3 (5%)	2	1
18	z	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
All	All	5100/5190 (98%)	4921 (96%)	163 (3%)	16 (0%)	44	49

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
3	C	24	THR
3	C	416	SER
5	E	6	GLY
18	Z	31	GLN
18	Z	32	ASP
3	c	416	SER
15	v	19	ILE
17	x	35	ASP
9	J	6	GLY

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Mol	Chain	Res	Type
12	O	34	SER
18	Z	30	PRO
1	a	225	ARG
12	O	26	ALA
1	A	259	ILE
17	x	34	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/270 (97%)	263 (100%)	0	100	100
1	a	252/270 (93%)	250 (99%)	2 (1%)	85	92
2	B	391/403 (97%)	386 (99%)	5 (1%)	73	85
2	b	378/403 (94%)	375 (99%)	3 (1%)	85	92
3	C	347/356 (98%)	341 (98%)	6 (2%)	66	79
3	c	356/356 (100%)	350 (98%)	6 (2%)	66	79
4	D	278/277 (100%)	276 (99%)	2 (1%)	87	93
4	d	276/277 (100%)	275 (100%)	1 (0%)	93	97
5	E	68/71 (96%)	67 (98%)	1 (2%)	70	82
5	e	67/71 (94%)	64 (96%)	3 (4%)	32	39
6	F	27/27 (100%)	27 (100%)	0	100	100
6	f	25/27 (93%)	24 (96%)	1 (4%)	36	45
7	H	56/53 (106%)	55 (98%)	1 (2%)	64	77
7	h	54/53 (102%)	53 (98%)	1 (2%)	62	76
8	I	31/32 (97%)	30 (97%)	1 (3%)	44	56
8	i	31/32 (97%)	31 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	9	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	k	28/30 (93%)	27 (96%)	1 (4%)	40	50
11	L	33/33 (100%)	32 (97%)	1 (3%)	46	58
11	l	33/33 (100%)	32 (97%)	1 (3%)	46	58
12	O	203/206 (98%)	197 (97%)	6 (3%)	46	58
12	o	199/206 (97%)	195 (98%)	4 (2%)	60	74
13	T	24/26 (92%)	23 (96%)	1 (4%)	34	43
13	t	24/26 (92%)	22 (92%)	2 (8%)	13	13
14	U	85/84 (101%)	85 (100%)	0	100	100
14	u	82/84 (98%)	81 (99%)	1 (1%)	75	86
15	V	117/117 (100%)	113 (97%)	4 (3%)	42	53
15	v	115/117 (98%)	112 (97%)	3 (3%)	51	64
16	Y	22/22 (100%)	19 (86%)	3 (14%)	4	3
16	y	19/22 (86%)	19 (100%)	0	100	100
17	X	29/30 (97%)	27 (93%)	2 (7%)	18	19
17	x	27/30 (90%)	26 (96%)	1 (4%)	39	49
18	Z	45/52 (86%)	45 (100%)	0	100	100
18	z	40/52 (77%)	40 (100%)	0	100	100
All	All	4103/4234 (97%)	4037 (98%)	66 (2%)	68	81

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	128	THR
2	B	246	PHE
2	B	362	PHE
2	B	472	ARG
3	C	27	ASP
3	C	255	THR
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
3	C	471	SER
4	D	180	ARG
4	D	315	TYR
5	E	82	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	H	49	TYR
8	I	33	LYS
10	K	10	LYS
10	K	17	ILE
10	K	27	VAL
11	L	14	ARG
12	O	24	ASP
12	O	84	GLU
12	O	109	GLN
12	O	118	LEU
12	O	130	GLN
12	O	242	SER
13	T	25	GLU
15	V	30	LYS
15	V	110	LYS
15	V	129[A]	LYS
15	V	129[B]	LYS
16	Y	19	ILE
16	Y	25	ILE
16	Y	43	ARG
17	X	23	LEU
17	X	33	GLN
1	a	214	MET
1	a	260	PHE
2	b	246	PHE
2	b	362	PHE
2	b	467	ILE
3	c	78	GLU
3	c	156	LYS
3	c	289	PHE
3	c	334	PRO
3	c	381	LYS
3	c	418	ASN
4	d	180	ARG
5	e	7	GLU
5	e	16	SER
5	e	25	ILE
6	f	15	ILE
7	h	49	TYR
10	k	27	VAL
11	l	10	VAL
12	o	23	ASP

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Mol	Chain	Res	Type
12	o	89	SER
12	o	118	LEU
12	o	242	SER
13	t	25	GLU
13	t	28	ARG
14	u	39	ARG
15	v	6	GLU
15	v	19	ILE
15	v	28	GLU
17	x	21	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	HIS
2	B	53	ASN
2	B	331	ASN
6	F	44	GLN
12	O	58	ASN
12	O	104	GLN
12	O	130	GLN
14	U	37	GLN
15	V	34	GLN
1	a	266	ASN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
3	c	201	ASN
12	o	58	ASN
12	o	82	GLN
12	o	104	GLN
12	o	231	HIS
14	u	73	GLN
15	v	34	GLN
15	v	118	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
8	FME	I	1	8	9,9,10	0.90	0	7,9,11	1.33	2 (28%)
13	FME	T	1	13	9,9,10	0.89	1 (11%)	7,9,11	1.35	2 (28%)
8	FME	i	1	8	9,9,10	0.50	0	7,9,11	1.42	1 (14%)
13	FME	t	1	13	9,9,10	1.17	1 (11%)	7,9,11	1.78	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
13	FME	T	1	13	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
13	FME	t	1	13	-	0/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	1	FME	CA-C	2.05	1.52	1.50
13	t	1	FME	CA-C	3.10	1.54	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O-C-CA	-2.77	118.69	125.15
8	I	1	FME	O-C-CA	-2.40	119.54	125.15
13	T	1	FME	O-C-CA	-2.20	120.02	125.15
13	t	1	FME	O-C-CA	-2.11	120.23	125.15
13	T	1	FME	CE-SD-CG	2.16	108.08	100.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	CE-SD-CG	2.17	108.15	100.35
13	t	1	FME	CE-SD-CG	3.76	113.85	100.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 352 ligands modelled in this entry, 27 are unknown and 15 are monoatomic - leaving 310 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	$\# Z  > 2$
19	OEX	A	401	1,3,39	0,15,15	0.00	-	0,32,32	0.00	-
22	CLA	A	405	-	56,73,73	1.85	12 (21%)	65,113,113	1.90	18 (27%)
22	CLA	A	406	39	46,63,73	1.83	11 (23%)	53,101,113	2.53	23 (43%)
23	PHO	A	407	-	67,69,69	2.05	15 (22%)	87,99,99	1.93	22 (25%)
22	CLA	A	408	-	56,73,73	1.79	11 (19%)	65,113,113	1.88	14 (21%)
24	BCR	A	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	5 (8%)
25	LMG	A	410	-	51,51,55	0.94	2 (3%)	59,59,63	1.12	5 (8%)
26	PL9	A	411	-	55,55,55	0.95	3 (5%)	69,69,69	1.67	13 (18%)
27	LHG	A	412	-	30,30,48	1.37	2 (6%)	32,35,54	1.47	4 (12%)
28	SQD	A	413	-	48,49,54	1.06	3 (6%)	58,60,65	2.06	11 (18%)
29	LMT	A	414	-	36,36,36	0.80	0	47,47,47	1.20	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	A	416	-	3,3,3	2.65	1 (33%)	3,3,3	1.02	0
31	DMS	A	417	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
31	DMS	A	418	-	3,3,3	2.40	1 (33%)	3,3,3	1.22	0
31	DMS	A	419	-	3,3,3	2.65	1 (33%)	3,3,3	0.79	0
31	DMS	A	420	-	3,3,3	2.73	1 (33%)	3,3,3	1.31	0
32	BCT	A	421[A]	20	0,3,3	0.00	-	0,3,3	0.00	-
32	BCT	A	421[B]	20	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	602	39	56,73,73	2.05	13 (23%)	65,113,113	1.92	14 (21%)
22	CLA	B	603	-	56,73,73	1.89	13 (23%)	65,113,113	2.16	23 (35%)
22	CLA	B	604	-	56,73,73	1.80	11 (19%)	65,113,113	2.12	20 (30%)
22	CLA	B	605	-	56,73,73	1.72	12 (21%)	65,113,113	2.09	20 (30%)
22	CLA	B	606	-	56,73,73	1.71	12 (21%)	65,113,113	1.96	17 (26%)
22	CLA	B	607	-	56,73,73	1.89	11 (19%)	65,113,113	2.25	19 (29%)
22	CLA	B	608	39	56,73,73	1.77	12 (21%)	65,113,113	1.98	20 (30%)
22	CLA	B	609	-	56,73,73	1.86	12 (21%)	65,113,113	2.17	19 (29%)
22	CLA	B	610	-	56,73,73	1.77	11 (19%)	65,113,113	1.88	15 (23%)
22	CLA	B	611	39	56,73,73	1.91	12 (21%)	65,113,113	2.09	15 (23%)
22	CLA	B	612	-	56,73,73	1.84	10 (17%)	65,113,113	1.77	16 (24%)
22	CLA	B	613	-	56,73,73	1.81	11 (19%)	65,113,113	1.72	16 (24%)
22	CLA	B	614	-	52,69,73	1.90	12 (23%)	60,108,113	1.65	15 (25%)
22	CLA	B	615	-	44,61,73	2.30	14 (31%)	50,98,113	2.34	19 (38%)
22	CLA	B	616	-	56,73,73	1.89	11 (19%)	65,113,113	1.77	16 (24%)
22	CLA	B	617	-	46,63,73	1.95	11 (23%)	53,101,113	2.56	20 (37%)
24	BCR	B	618	-	18,19,41	0.86	1 (5%)	24,26,56	1.39	4 (16%)
24	BCR	B	619	-	30,30,41	0.91	0	38,39,56	1.33	7 (18%)
24	BCR	B	620	-	41,41,41	0.95	2 (4%)	56,56,56	1.48	11 (19%)
25	LMG	B	621	-	40,40,55	1.24	3 (7%)	48,48,63	1.43	9 (18%)
29	LMT	B	622	-	24,24,36	0.63	1 (4%)	29,29,47	0.85	1 (3%)
34	HTG	B	623	-	19,19,19	1.14	1 (5%)	23,24,24	2.06	3 (13%)
34	HTG	B	626	-	19,19,19	0.71	0	23,24,24	2.04	5 (21%)
34	HTG	B	627	-	19,19,19	0.98	1 (5%)	23,24,24	2.26	4 (17%)
31	DMS	B	628	-	3,3,3	2.79	1 (33%)	3,3,3	0.76	0
31	DMS	B	629	-	3,3,3	2.53	1 (33%)	3,3,3	1.15	0
31	DMS	B	630	-	3,3,3	2.80	1 (33%)	3,3,3	0.88	0
31	DMS	B	631	-	3,3,3	2.55	1 (33%)	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	B	632	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
31	DMS	B	633	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
31	DMS	B	634	-	3,3,3	2.79	1 (33%)	3,3,3	0.63	0
31	DMS	B	635	-	3,3,3	2.76	1 (33%)	3,3,3	0.67	0
31	DMS	B	636	-	3,3,3	2.59	1 (33%)	3,3,3	0.61	0
31	DMS	B	637	-	3,3,3	2.77	1 (33%)	3,3,3	0.69	0
31	DMS	B	638	-	3,3,3	2.63	1 (33%)	3,3,3	0.38	0
31	DMS	B	639	-	3,3,3	2.75	1 (33%)	3,3,3	0.69	0
31	DMS	B	640	-	3,3,3	2.62	1 (33%)	3,3,3	0.60	0
31	DMS	B	641	-	3,3,3	2.74	1 (33%)	3,3,3	0.81	0
31	DMS	B	642	-	3,3,3	2.65	1 (33%)	3,3,3	1.03	0
28	SQD	C	501	-	53,54,54	1.02	3 (5%)	63,65,65	2.22	14 (22%)
22	CLA	C	502	-	56,73,73	1.79	12 (21%)	65,113,113	2.14	17 (26%)
22	CLA	C	503	-	56,73,73	1.84	12 (21%)	65,113,113	1.79	15 (23%)
22	CLA	C	504	-	56,73,73	2.04	13 (23%)	65,113,113	1.89	19 (29%)
22	CLA	C	505	39	56,73,73	1.86	12 (21%)	65,113,113	1.76	14 (21%)
22	CLA	C	506	-	56,73,73	1.95	12 (21%)	65,113,113	1.72	16 (24%)
22	CLA	C	507	-	56,73,73	1.89	13 (23%)	65,113,113	1.83	15 (23%)
22	CLA	C	508	39	56,73,73	1.90	12 (21%)	65,113,113	1.93	15 (23%)
22	CLA	C	509	-	56,73,73	1.88	13 (23%)	65,113,113	1.75	14 (21%)
22	CLA	C	510	-	56,73,73	1.89	10 (17%)	65,113,113	2.18	18 (27%)
22	CLA	C	511	-	56,73,73	1.95	12 (21%)	65,113,113	1.93	15 (23%)
22	CLA	C	512	3	56,73,73	1.98	12 (21%)	65,113,113	1.85	17 (26%)
22	CLA	C	513	-	47,64,73	2.14	12 (25%)	54,102,113	1.99	14 (25%)
22	CLA	C	514	-	56,73,73	2.04	13 (23%)	65,113,113	1.78	15 (23%)
24	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	1.48	10 (17%)
24	BCR	C	516	-	41,41,41	0.89	0	56,56,56	1.35	8 (14%)
35	DGD	C	517	-	63,63,67	0.84	3 (4%)	77,77,81	1.37	12 (15%)
35	DGD	C	518	-	63,63,67	0.95	3 (4%)	77,77,81	1.33	11 (14%)
35	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.24	10 (12%)
25	LMG	C	520	-	51,51,55	1.06	2 (3%)	59,59,63	1.28	5 (8%)
34	HTG	C	521	-	19,19,19	0.92	2 (10%)	23,24,24	1.91	2 (8%)
27	LHG	C	522	-	29,29,48	1.28	2 (6%)	33,34,54	1.42	4 (12%)
34	HTG	C	523	-	8,8,19	0.37	0	7,7,24	1.36	1 (14%)
31	DMS	C	524	-	3,3,3	2.47	1 (33%)	3,3,3	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	C	525	-	3,3,3	2.43	1 (33%)	3,3,3	0.60	0
31	DMS	C	526	-	3,3,3	2.58	1 (33%)	3,3,3	0.54	0
31	DMS	C	527	-	3,3,3	2.64	1 (33%)	3,3,3	0.55	0
31	DMS	C	528	-	3,3,3	2.62	1 (33%)	3,3,3	0.57	0
31	DMS	C	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
31	DMS	C	530	-	3,3,3	2.66	1 (33%)	3,3,3	0.84	0
25	LMG	C	531	-	40,40,55	1.17	3 (7%)	48,48,63	1.18	4 (8%)
34	HTG	C	532	-	19,19,19	1.13	2 (10%)	23,24,24	2.31	1 (4%)
31	DMS	C	533	-	3,3,3	2.72	1 (33%)	3,3,3	0.72	0
31	DMS	C	534	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
31	DMS	C	535	-	3,3,3	2.72	1 (33%)	3,3,3	0.76	0
31	DMS	C	536	-	3,3,3	2.67	1 (33%)	3,3,3	0.44	0
31	DMS	C	537	-	3,3,3	2.74	1 (33%)	3,3,3	0.68	0
31	DMS	C	538	-	3,3,3	2.65	1 (33%)	3,3,3	0.57	0
31	DMS	C	539	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
31	DMS	C	540	-	3,3,3	2.77	1 (33%)	3,3,3	0.86	0
22	CLA	D	401	39	56,73,73	1.74	10 (17%)	65,113,113	2.28	19 (29%)
23	PHO	D	402	-	67,69,69	2.07	16 (23%)	87,99,99	2.03	20 (22%)
22	CLA	D	403	-	56,73,73	1.61	13 (23%)	65,113,113	2.46	22 (33%)
22	CLA	D	404	-	56,73,73	1.95	12 (21%)	65,113,113	1.70	15 (23%)
24	BCR	D	405	-	41,41,41	0.98	1 (2%)	56,56,56	1.97	15 (26%)
26	PL9	D	406	-	55,55,55	0.91	3 (5%)	69,69,69	1.52	15 (21%)
35	DGD	D	407	-	50,50,67	1.17	3 (6%)	58,58,81	1.35	6 (10%)
28	SQD	D	408	-	19,20,54	0.94	2 (10%)	27,29,65	2.09	8 (29%)
27	LHG	D	409	-	48,48,48	1.01	2 (4%)	49,54,54	1.42	5 (10%)
27	LHG	D	410	-	48,48,48	0.78	2 (4%)	49,54,54	1.13	5 (10%)
27	LHG	D	411	-	44,44,48	0.96	2 (4%)	45,50,54	1.09	3 (6%)
25	LMG	D	412	-	46,46,55	1.12	3 (6%)	54,54,63	1.16	2 (3%)
34	HTG	D	414	-	19,19,19	0.85	1 (5%)	23,24,24	2.23	1 (4%)
34	HTG	D	415	-	19,19,19	1.15	1 (5%)	23,24,24	2.88	8 (34%)
31	DMS	D	416	-	3,3,3	2.49	1 (33%)	3,3,3	0.62	0
31	DMS	D	417	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
31	DMS	D	418	-	3,3,3	2.39	1 (33%)	3,3,3	0.65	0
29	LMT	E	101	-	24,24,36	0.63	0	29,29,47	1.01	1 (3%)
36	HEM	E	102	5,6	28,50,50	2.14	7 (25%)	17,82,82	2.67	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	F	101	-	3,3,3	2.65	1 (33%)	3,3,3	0.59	0
37	RRX	H	101	-	42,42,42	0.80	0	56,58,58	1.49	8 (14%)
35	DGD	H	102	-	63,63,67	1.01	3 (4%)	77,77,81	1.19	6 (7%)
31	DMS	H	103	-	3,3,3	2.90	1 (33%)	3,3,3	1.15	0
31	DMS	I	101	-	3,3,3	2.70	1 (33%)	3,3,3	0.67	0
29	LMT	I	102	-	36,36,36	0.68	1 (2%)	47,47,47	1.46	5 (10%)
31	DMS	I	106	-	3,3,3	2.67	1 (33%)	3,3,3	0.73	0
25	LMG	J	101	38	45,45,55	0.97	2 (4%)	53,53,63	1.07	6 (11%)
24	BCR	K	101	-	41,41,41	0.84	0	56,56,56	1.19	4 (7%)
27	LHG	L	101	-	39,39,48	1.03	2 (5%)	40,45,54	1.25	5 (12%)
31	DMS	L	102	-	3,3,3	2.73	1 (33%)	3,3,3	0.93	0
31	DMS	O	303	-	3,3,3	2.73	1 (33%)	3,3,3	0.74	0
31	DMS	O	304	-	3,3,3	2.56	1 (33%)	3,3,3	0.41	0
31	DMS	O	305	-	3,3,3	2.88	1 (33%)	3,3,3	0.82	0
31	DMS	O	306	-	3,3,3	2.69	1 (33%)	3,3,3	0.73	0
31	DMS	O	307	-	3,3,3	2.78	1 (33%)	3,3,3	0.90	0
31	DMS	O	308	-	3,3,3	2.77	1 (33%)	3,3,3	0.61	0
31	DMS	O	309	-	3,3,3	2.52	1 (33%)	3,3,3	0.57	0
31	DMS	O	310	-	3,3,3	2.61	1 (33%)	3,3,3	0.84	0
31	DMS	O	311	-	3,3,3	2.96	1 (33%)	3,3,3	0.89	0
31	DMS	O	312	-	3,3,3	2.61	1 (33%)	3,3,3	0.93	0
31	DMS	O	313	-	3,3,3	2.61	1 (33%)	3,3,3	0.46	0
31	DMS	O	314	-	3,3,3	2.72	1 (33%)	3,3,3	0.74	0
29	LMT	T	102	-	24,24,36	0.72	1 (4%)	29,29,47	1.34	3 (10%)
31	DMS	U	202	-	3,3,3	2.76	1 (33%)	3,3,3	1.26	0
31	DMS	U	203	-	3,3,3	2.76	1 (33%)	3,3,3	1.23	0
31	DMS	V	201	-	3,3,3	2.62	1 (33%)	3,3,3	0.87	0
36	HEM	V	202	15	28,50,50	2.28	8 (28%)	17,82,82	1.80	4 (23%)
34	HTG	V	203	-	14,14,19	0.67	0	18,19,24	3.13	7 (38%)
31	DMS	V	204	-	3,3,3	2.72	1 (33%)	3,3,3	0.79	0
31	DMS	V	205	-	3,3,3	2.61	1 (33%)	3,3,3	0.63	0
31	DMS	V	206	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
31	DMS	V	207	-	3,3,3	2.74	1 (33%)	3,3,3	0.87	0
31	DMS	V	208	-	3,3,3	2.58	1 (33%)	3,3,3	0.39	0
31	DMS	V	209	-	3,3,3	2.63	1 (33%)	3,3,3	0.47	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	V	210	-	3,3,3	2.76	1 (33%)	3,3,3	0.87	0
31	DMS	V	211	-	3,3,3	2.80	1 (33%)	3,3,3	0.76	0
31	DMS	V	212	-	3,3,3	2.77	1 (33%)	3,3,3	1.15	0
24	BCR	Y	101	-	39,40,41	0.86	1 (2%)	51,54,56	1.70	16 (31%)
29	LMT	Z	101	-	36,36,36	0.67	1 (2%)	47,47,47	1.20	6 (12%)
31	DMS	a	401	-	3,3,3	2.73	1 (33%)	3,3,3	0.78	0
31	DMS	a	402	-	3,3,3	2.37	1 (33%)	3,3,3	0.71	0
19	OEX	a	403	1,3,39	0,15,15	0.00	-	0,32,32	0.00	-
22	CLA	a	407	-	56,73,73	1.88	11 (19%)	65,113,113	1.89	20 (30%)
22	CLA	a	408	39	56,73,73	1.86	10 (17%)	65,113,113	2.01	17 (26%)
22	CLA	a	409	39	52,69,73	1.79	12 (23%)	60,108,113	2.49	21 (35%)
23	PHO	a	410	-	67,69,69	1.93	16 (23%)	87,99,99	1.90	22 (25%)
23	PHO	a	411	-	67,69,69	2.01	15 (22%)	87,99,99	2.20	22 (25%)
22	CLA	a	412	-	56,73,73	1.80	10 (17%)	65,113,113	2.18	20 (30%)
24	BCR	a	413	-	41,41,41	1.12	2 (4%)	56,56,56	1.14	6 (10%)
28	SQD	a	414	-	53,54,54	1.06	3 (5%)	63,65,65	2.26	13 (20%)
26	PL9	a	415	-	55,55,55	0.93	3 (5%)	69,69,69	1.46	9 (13%)
27	LHG	a	416	-	48,48,48	1.12	2 (4%)	49,54,54	1.23	4 (8%)
28	SQD	a	418	-	50,51,54	1.14	3 (6%)	60,62,65	1.65	10 (16%)
29	LMT	a	419	-	36,36,36	0.78	0	47,47,47	1.44	8 (17%)
31	DMS	a	421	-	3,3,3	2.64	1 (33%)	3,3,3	0.59	0
32	BCT	a	422	20	0,3,3	0.00	-	0,3,3	0.00	-
27	LHG	a	423	-	44,44,48	1.00	2 (4%)	45,50,54	1.14	4 (8%)
31	DMS	a	424	-	3,3,3	2.70	1 (33%)	3,3,3	0.99	0
31	DMS	a	425	-	3,3,3	3.00	1 (33%)	3,3,3	0.87	0
22	CLA	b	602	39	56,73,73	2.18	12 (21%)	65,113,113	1.97	17 (26%)
22	CLA	b	603	-	56,73,73	1.91	11 (19%)	65,113,113	2.00	18 (27%)
22	CLA	b	604	-	56,73,73	1.72	12 (21%)	65,113,113	2.32	20 (30%)
22	CLA	b	605	-	56,73,73	1.70	12 (21%)	65,113,113	1.91	16 (24%)
22	CLA	b	606	-	56,73,73	1.61	9 (16%)	65,113,113	2.09	16 (24%)
22	CLA	b	607	-	56,73,73	1.75	12 (21%)	65,113,113	2.18	17 (26%)
22	CLA	b	608	39	56,73,73	1.86	11 (19%)	65,113,113	1.78	14 (21%)
22	CLA	b	609	-	56,73,73	1.81	10 (17%)	65,113,113	1.91	17 (26%)
22	CLA	b	610	-	56,73,73	1.91	12 (21%)	65,113,113	1.85	16 (24%)
22	CLA	b	611	39	56,73,73	1.89	12 (21%)	65,113,113	2.10	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	612	-	56,73,73	1.70	9 (16%)	65,113,113	1.83	14 (21%)
22	CLA	b	613	-	56,73,73	1.95	13 (23%)	65,113,113	2.10	21 (32%)
22	CLA	b	614	-	50,67,73	1.92	13 (26%)	57,105,113	2.00	15 (26%)
22	CLA	b	615	-	43,60,73	2.24	13 (30%)	49,97,113	2.12	18 (36%)
22	CLA	b	616	-	56,73,73	2.03	12 (21%)	65,113,113	1.81	17 (26%)
22	CLA	b	617	-	51,68,73	2.10	11 (21%)	59,107,113	2.19	19 (32%)
24	BCR	b	618	-	19,20,41	0.68	0	27,27,56	1.73	5 (18%)
24	BCR	b	619	-	31,31,41	1.08	2 (6%)	40,40,56	1.32	7 (17%)
24	BCR	b	620	-	41,41,41	0.84	0	56,56,56	1.34	8 (14%)
28	SQD	b	621	-	37,38,54	1.03	2 (5%)	46,48,65	1.72	10 (21%)
25	LMG	b	622	-	43,43,55	1.34	4 (9%)	51,51,63	1.92	12 (23%)
34	HTG	b	623	-	19,19,19	1.08	1 (5%)	23,24,24	1.30	4 (17%)
34	HTG	b	624	-	19,19,19	1.03	1 (5%)	23,24,24	2.45	6 (26%)
34	HTG	b	626	-	19,19,19	0.82	1 (5%)	23,24,24	1.81	4 (17%)
34	HTG	b	627	-	19,19,19	1.00	1 (5%)	23,24,24	2.13	3 (13%)
31	DMS	b	629	-	3,3,3	2.27	1 (33%)	3,3,3	1.07	0
31	DMS	b	630	-	3,3,3	2.65	1 (33%)	3,3,3	0.29	0
31	DMS	b	631	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
34	HTG	b	632	-	19,19,19	1.05	2 (10%)	23,24,24	2.79	7 (30%)
31	DMS	b	633	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
31	DMS	b	634	-	3,3,3	2.70	1 (33%)	3,3,3	0.57	0
31	DMS	b	635	-	3,3,3	2.74	1 (33%)	3,3,3	0.54	0
31	DMS	b	636	-	3,3,3	2.66	1 (33%)	3,3,3	0.68	0
31	DMS	b	637	-	3,3,3	2.70	1 (33%)	3,3,3	0.60	0
31	DMS	b	638	-	3,3,3	2.96	1 (33%)	3,3,3	0.67	0
22	CLA	c	902	-	56,73,73	1.84	12 (21%)	65,113,113	1.82	13 (20%)
22	CLA	c	903	-	56,73,73	1.76	11 (19%)	65,113,113	2.06	20 (30%)
22	CLA	c	904	-	56,73,73	1.92	12 (21%)	65,113,113	1.88	18 (27%)
22	CLA	c	905	39	56,73,73	1.82	11 (19%)	65,113,113	1.75	13 (20%)
22	CLA	c	906	-	56,73,73	1.98	13 (23%)	65,113,113	1.82	16 (24%)
22	CLA	c	907	-	56,73,73	1.85	11 (19%)	65,113,113	1.91	15 (23%)
22	CLA	c	908	39	56,73,73	2.09	12 (21%)	65,113,113	1.92	12 (18%)
22	CLA	c	909	-	56,73,73	2.07	15 (26%)	65,113,113	1.78	16 (24%)
22	CLA	c	910	-	56,73,73	1.98	12 (21%)	65,113,113	2.04	20 (30%)
22	CLA	c	911	-	56,73,73	1.86	11 (19%)	65,113,113	1.81	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	912	3	56,73,73	1.97	13 (23%)	65,113,113	1.59	13 (20%)
22	CLA	c	913	-	56,73,73	1.98	12 (21%)	65,113,113	1.85	17 (26%)
22	CLA	c	914	-	56,73,73	1.94	12 (21%)	65,113,113	1.88	18 (27%)
24	BCR	c	915	-	41,41,41	0.83	1 (2%)	56,56,56	1.39	7 (12%)
24	BCR	c	916	-	41,41,41	0.84	0	56,56,56	1.54	10 (17%)
35	DGD	c	917	-	63,63,67	0.96	3 (4%)	77,77,81	1.04	4 (5%)
35	DGD	c	918	-	63,63,67	0.93	4 (6%)	77,77,81	1.06	5 (6%)
35	DGD	c	919	-	63,63,67	0.97	3 (4%)	77,77,81	1.19	6 (7%)
25	LMG	c	920	-	51,51,55	0.98	2 (3%)	59,59,63	1.14	6 (10%)
29	LMT	c	921	-	36,36,36	0.67	1 (2%)	47,47,47	1.08	4 (8%)
34	HTG	c	922	-	19,19,19	0.82	1 (5%)	23,24,24	1.96	2 (8%)
31	DMS	c	923	-	3,3,3	2.49	1 (33%)	3,3,3	0.39	0
31	DMS	c	924	-	3,3,3	2.80	1 (33%)	3,3,3	1.28	1 (33%)
31	DMS	c	925	-	3,3,3	2.64	1 (33%)	3,3,3	1.07	0
31	DMS	c	926	-	3,3,3	2.59	1 (33%)	3,3,3	0.76	0
31	DMS	c	927	-	3,3,3	2.63	1 (33%)	3,3,3	0.41	0
31	DMS	c	928	-	3,3,3	2.68	1 (33%)	3,3,3	0.75	0
31	DMS	c	929	-	3,3,3	2.79	1 (33%)	3,3,3	0.82	0
25	LMG	c	930	-	49,49,55	1.09	3 (6%)	57,57,63	1.10	4 (7%)
29	LMT	c	931	-	24,24,36	0.78	1 (4%)	29,29,47	0.88	2 (6%)
31	DMS	c	933	-	3,3,3	2.82	1 (33%)	3,3,3	0.89	0
31	DMS	c	934	-	3,3,3	2.65	1 (33%)	3,3,3	0.66	0
31	DMS	c	935	-	3,3,3	2.65	1 (33%)	3,3,3	0.86	0
31	DMS	c	936	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
31	DMS	c	937	-	3,3,3	2.86	1 (33%)	3,3,3	0.80	0
31	DMS	c	938	-	3,3,3	2.75	1 (33%)	3,3,3	0.81	0
31	DMS	c	939	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
31	DMS	c	940	-	3,3,3	2.71	1 (33%)	3,3,3	0.56	0
31	DMS	c	941	-	3,3,3	2.59	1 (33%)	3,3,3	0.51	0
31	DMS	c	942	-	3,3,3	2.72	1 (33%)	3,3,3	0.70	0
31	DMS	c	943	-	3,3,3	2.68	1 (33%)	3,3,3	0.78	0
31	DMS	c	944	-	3,3,3	2.71	1 (33%)	3,3,3	0.76	0
27	LHG	d	401	-	32,32,48	1.22	2 (6%)	36,37,54	1.22	4 (11%)
22	CLA	d	402	-	56,73,73	1.83	12 (21%)	65,113,113	1.99	15 (23%)
22	CLA	d	403	-	56,73,73	2.14	13 (23%)	65,113,113	1.71	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	d	404	-	41,41,41	1.03	3 (7%)	56,56,56	1.77	13 (23%)
26	PL9	d	405	-	55,55,55	1.00	4 (7%)	69,69,69	1.43	8 (11%)
35	DGD	d	406	-	42,42,67	1.23	3 (7%)	44,45,81	1.12	3 (6%)
27	LHG	d	407	-	48,48,48	0.74	2 (4%)	49,54,54	1.10	3 (6%)
27	LHG	d	408	-	45,45,48	1.02	2 (4%)	46,51,54	0.76	0
25	LMG	d	409	-	47,47,55	1.08	3 (6%)	55,55,63	1.50	9 (16%)
31	DMS	d	411	-	3,3,3	2.70	1 (33%)	3,3,3	0.91	0
31	DMS	d	412	-	3,3,3	2.55	1 (33%)	3,3,3	0.81	0
31	DMS	d	413	-	3,3,3	2.53	1 (33%)	3,3,3	0.38	0
31	DMS	d	414	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
31	DMS	d	415	-	3,3,3	2.61	1 (33%)	3,3,3	0.60	0
36	HEM	e	101	5,6	28,50,50	2.21	12 (42%)	17,82,82	2.17	4 (23%)
28	SQD	f	101	-	13,13,54	2.04	1 (7%)	15,16,65	1.64	3 (20%)
29	LMT	f	102	-	25,25,36	1.00	1 (4%)	30,30,47	1.27	6 (20%)
31	DMS	f	103	-	3,3,3	2.69	1 (33%)	3,3,3	0.88	0
37	RRX	h	101	-	42,42,42	0.95	0	56,58,58	1.19	5 (8%)
35	DGD	h	102	-	63,63,67	0.96	2 (3%)	77,77,81	1.18	6 (7%)
25	LMG	i	101	-	51,51,55	0.97	2 (3%)	59,59,63	1.21	7 (11%)
31	DMS	i	106	-	3,3,3	2.61	1 (33%)	3,3,3	0.55	0
25	LMG	j	101	38	47,47,55	1.00	2 (4%)	55,55,63	1.23	9 (16%)
24	BCR	k	101	-	41,41,41	0.89	0	56,56,56	1.23	6 (10%)
28	SQD	l	101	-	53,54,54	1.11	4 (7%)	63,65,65	1.65	9 (14%)
27	LHG	l	102	-	48,48,48	0.92	2 (4%)	49,54,54	1.13	3 (6%)
31	DMS	l	103	-	3,3,3	2.69	1 (33%)	3,3,3	0.64	0
31	DMS	l	104	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
31	DMS	l	105	-	3,3,3	2.73	1 (33%)	3,3,3	0.70	0
34	HTG	l	106	-	19,19,19	0.99	2 (10%)	23,24,24	2.46	3 (13%)
31	DMS	o	302	-	3,3,3	2.66	1 (33%)	3,3,3	0.94	0
31	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.79	0
31	DMS	o	304	-	3,3,3	2.80	1 (33%)	3,3,3	1.11	0
31	DMS	o	305	-	3,3,3	2.59	1 (33%)	3,3,3	0.64	0
31	DMS	o	306	-	3,3,3	2.63	1 (33%)	3,3,3	0.58	0
31	DMS	o	307	-	3,3,3	2.59	1 (33%)	3,3,3	0.56	0
31	DMS	o	308	-	3,3,3	2.77	1 (33%)	3,3,3	0.81	0
29	LMT	t	101	-	24,24,36	0.45	0	29,29,47	1.38	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DMS	t	103	-	3,3,3	2.69	1 (33%)	3,3,3	0.62	0
31	DMS	t	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0
31	DMS	t	105	-	3,3,3	2.69	1 (33%)	3,3,3	0.60	0
31	DMS	u	202	-	3,3,3	2.60	1 (33%)	3,3,3	1.02	0
31	DMS	u	203	-	3,3,3	2.71	1 (33%)	3,3,3	0.74	0
31	DMS	u	204	-	3,3,3	2.78	1 (33%)	3,3,3	0.79	0
31	DMS	u	205	-	3,3,3	3.05	1 (33%)	3,3,3	1.16	0
31	DMS	v	201	-	3,3,3	2.57	1 (33%)	3,3,3	0.83	0
36	HEM	v	202	15	28,50,50	2.38	10 (35%)	17,82,82	1.82	4 (23%)
34	HTG	v	203	-	16,16,19	1.03	1 (6%)	20,21,24	3.20	7 (35%)
31	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.67	0
31	DMS	v	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.81	0
31	DMS	v	206	-	3,3,3	2.67	1 (33%)	3,3,3	0.71	0
31	DMS	v	207	-	3,3,3	2.70	1 (33%)	3,3,3	0.63	0
31	DMS	v	208	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0
31	DMS	v	209	-	3,3,3	2.62	1 (33%)	3,3,3	0.61	0
31	DMS	v	210	-	3,3,3	2.82	1 (33%)	3,3,3	0.76	0
31	DMS	v	211	-	3,3,3	2.74	1 (33%)	3,3,3	0.74	0
24	BCR	y	101	-	41,41,41	0.88	0	56,56,56	1.59	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	OEX	A	401	1,3,39	-	0/0/68/68	0/0/6/6
22	CLA	A	405	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	A	406	39	2/2/18/25	0/25/123/135	0/0/9/9
23	PHO	A	407	-	-	0/53/103/103	0/1/6/6
22	CLA	A	408	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	LMG	A	410	-	-	0/46/66/70	0/1/1/1
26	PL9	A	411	-	-	0/53/73/73	0/1/1/1
27	LHG	A	412	-	-	0/33/33/53	0/0/0/0
28	SQD	A	413	-	-	0/44/64/69	0/1/1/1
29	LMT	A	414	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	A	416	-	-	0/0/0/0	0/0/0/0
31	DMS	A	417	-	-	0/0/0/0	0/0/0/0
31	DMS	A	418	-	-	0/0/0/0	0/0/0/0
31	DMS	A	419	-	-	0/0/0/0	0/0/0/0
31	DMS	A	420	-	-	0/0/0/0	0/0/0/0
32	BCT	A	421[A]	20	-	0/0/0/0	0/0/0/0
32	BCT	A	421[B]	20	-	0/0/0/0	0/0/0/0
22	CLA	B	602	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/19/25	0/33/131/135	0/0/9/9
22	CLA	B	615	-	3/3/17/25	0/23/121/135	0/0/9/9
22	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	617	-	3/3/18/25	0/25/123/135	0/0/9/9
24	BCR	B	618	-	-	0/11/28/63	0/1/1/2
24	BCR	B	619	-	-	0/24/41/63	0/1/1/2
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	LMG	B	621	-	-	0/35/55/70	0/1/1/1
29	LMT	B	622	-	-	0/15/35/61	0/1/1/2
34	HTG	B	623	-	-	0/10/30/30	0/1/1/1
34	HTG	B	626	-	-	0/10/30/30	0/1/1/1
34	HTG	B	627	-	-	0/10/30/30	0/1/1/1
31	DMS	B	628	-	-	0/0/0/0	0/0/0/0
31	DMS	B	629	-	-	0/0/0/0	0/0/0/0
31	DMS	B	630	-	-	0/0/0/0	0/0/0/0
31	DMS	B	631	-	-	0/0/0/0	0/0/0/0
31	DMS	B	632	-	-	0/0/0/0	0/0/0/0
31	DMS	B	633	-	-	0/0/0/0	0/0/0/0
31	DMS	B	634	-	-	0/0/0/0	0/0/0/0
31	DMS	B	635	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	B	636	-	-	0/0/0/0	0/0/0/0
31	DMS	B	637	-	-	0/0/0/0	0/0/0/0
31	DMS	B	638	-	-	0/0/0/0	0/0/0/0
31	DMS	B	639	-	-	0/0/0/0	0/0/0/0
31	DMS	B	640	-	-	0/0/0/0	0/0/0/0
31	DMS	B	641	-	-	0/0/0/0	0/0/0/0
31	DMS	B	642	-	-	0/0/0/0	0/0/0/0
28	SQD	C	501	-	-	0/49/69/69	0/1/1/1
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	39	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	513	-	3/3/18/25	0/27/125/135	0/0/9/9
22	CLA	C	514	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
35	DGD	C	517	-	-	0/51/91/95	0/2/2/2
35	DGD	C	518	-	-	0/51/91/95	0/2/2/2
35	DGD	C	519	-	-	0/51/91/95	0/2/2/2
25	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
27	LHG	C	522	-	-	0/31/31/53	0/0/0/0
34	HTG	C	523	-	-	0/6/6/30	0/0/0/1
31	DMS	C	524	-	-	0/0/0/0	0/0/0/0
31	DMS	C	525	-	-	0/0/0/0	0/0/0/0
31	DMS	C	526	-	-	0/0/0/0	0/0/0/0
31	DMS	C	527	-	-	0/0/0/0	0/0/0/0
31	DMS	C	528	-	-	0/0/0/0	0/0/0/0
31	DMS	C	529	-	-	0/0/0/0	0/0/0/0
31	DMS	C	530	-	-	0/0/0/0	0/0/0/0
25	LMG	C	531	-	-	0/35/55/70	0/1/1/1
34	HTG	C	532	-	-	1/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	C	533	-	-	0/0/0/0	0/0/0/0
31	DMS	C	534	-	-	0/0/0/0	0/0/0/0
31	DMS	C	535	-	-	0/0/0/0	0/0/0/0
31	DMS	C	536	-	-	0/0/0/0	0/0/0/0
31	DMS	C	537	-	-	0/0/0/0	0/0/0/0
31	DMS	C	538	-	-	0/0/0/0	0/0/0/0
31	DMS	C	539	-	-	0/0/0/0	0/0/0/0
31	DMS	C	540	-	-	0/0/0/0	0/0/0/0
22	CLA	D	401	39	1/1/20/25	0/37/135/135	0/0/9/9
23	PHO	D	402	-	-	0/53/103/103	0/1/6/6
22	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	D	405	-	-	0/29/63/63	0/2/2/2
26	PL9	D	406	-	-	0/53/73/73	0/1/1/1
35	DGD	D	407	-	-	0/44/64/95	0/1/1/2
28	SQD	D	408	-	-	0/12/32/69	0/1/1/1
27	LHG	D	409	-	-	0/53/53/53	0/0/0/0
27	LHG	D	410	-	-	0/53/53/53	0/0/0/0
27	LHG	D	411	-	-	0/49/49/53	0/0/0/0
25	LMG	D	412	-	-	0/41/61/70	0/1/1/1
34	HTG	D	414	-	-	0/10/30/30	0/1/1/1
34	HTG	D	415	-	-	0/10/30/30	0/1/1/1
31	DMS	D	416	-	-	0/0/0/0	0/0/0/0
31	DMS	D	417	-	-	0/0/0/0	0/0/0/0
31	DMS	D	418	-	-	0/0/0/0	0/0/0/0
29	LMT	E	101	-	-	0/15/35/61	0/1/1/2
36	HEM	E	102	5,6	-	0/6/54/54	0/0/8/8
31	DMS	F	101	-	-	0/0/0/0	0/0/0/0
37	RRX	H	101	-	-	0/29/65/65	0/2/2/2
35	DGD	H	102	-	-	0/51/91/95	0/2/2/2
31	DMS	H	103	-	-	0/0/0/0	0/0/0/0
31	DMS	I	101	-	-	0/0/0/0	0/0/0/0
29	LMT	I	102	-	-	0/21/61/61	0/2/2/2
31	DMS	I	106	-	-	0/0/0/0	0/0/0/0
25	LMG	J	101	38	-	0/40/60/70	0/1/1/1
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
27	LHG	L	101	-	-	0/44/44/53	0/0/0/0
31	DMS	L	102	-	-	0/0/0/0	0/0/0/0
31	DMS	O	303	-	-	0/0/0/0	0/0/0/0
31	DMS	O	304	-	-	0/0/0/0	0/0/0/0
31	DMS	O	305	-	-	0/0/0/0	0/0/0/0
31	DMS	O	306	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	O	307	-	-	0/0/0/0	0/0/0/0
31	DMS	O	308	-	-	0/0/0/0	0/0/0/0
31	DMS	O	309	-	-	0/0/0/0	0/0/0/0
31	DMS	O	310	-	-	0/0/0/0	0/0/0/0
31	DMS	O	311	-	-	0/0/0/0	0/0/0/0
31	DMS	O	312	-	-	0/0/0/0	0/0/0/0
31	DMS	O	313	-	-	0/0/0/0	0/0/0/0
31	DMS	O	314	-	-	0/0/0/0	0/0/0/0
29	LMT	T	102	-	-	0/15/35/61	0/1/1/2
31	DMS	U	202	-	-	0/0/0/0	0/0/0/0
31	DMS	U	203	-	-	0/0/0/0	0/0/0/0
31	DMS	V	201	-	-	0/0/0/0	0/0/0/0
36	HEM	V	202	15	-	0/6/54/54	0/0/8/8
34	HTG	V	203	-	-	0/5/25/30	0/1/1/1
31	DMS	V	204	-	-	0/0/0/0	0/0/0/0
31	DMS	V	205	-	-	0/0/0/0	0/0/0/0
31	DMS	V	206	-	-	0/0/0/0	0/0/0/0
31	DMS	V	207	-	-	0/0/0/0	0/0/0/0
31	DMS	V	208	-	-	0/0/0/0	0/0/0/0
31	DMS	V	209	-	-	0/0/0/0	0/0/0/0
31	DMS	V	210	-	-	0/0/0/0	0/0/0/0
31	DMS	V	211	-	-	0/0/0/0	0/0/0/0
31	DMS	V	212	-	-	0/0/0/0	0/0/0/0
24	BCR	Y	101	-	-	0/29/60/63	0/2/2/2
29	LMT	Z	101	-	-	0/21/61/61	0/2/2/2
31	DMS	a	401	-	-	0/0/0/0	0/0/0/0
31	DMS	a	402	-	-	0/0/0/0	0/0/0/0
19	OEX	a	403	1,3,39	-	0/0/68/68	0/0/6/6
22	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	408	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	409	39	2/2/19/25	0/33/131/135	0/0/9/9
23	PHO	a	410	-	-	0/53/103/103	0/1/6/6
23	PHO	a	411	-	-	0/53/103/103	0/1/6/6
22	CLA	a	412	-	-	0/37/135/135	0/0/9/9
24	BCR	a	413	-	-	0/29/63/63	0/2/2/2
28	SQD	a	414	-	-	0/49/69/69	0/1/1/1
26	PL9	a	415	-	-	0/53/73/73	0/1/1/1
27	LHG	a	416	-	-	0/53/53/53	0/0/0/0
28	SQD	a	418	-	-	0/46/66/69	0/1/1/1
29	LMT	a	419	-	-	0/21/61/61	0/2/2/2
31	DMS	a	421	-	-	0/0/0/0	0/0/0/0
32	BCT	a	422	20	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	a	423	-	-	0/49/49/53	0/0/0/0
31	DMS	a	424	-	-	0/0/0/0	0/0/0/0
31	DMS	a	425	-	-	0/0/0/0	0/0/0/0
22	CLA	b	602	39	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	603	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	b	604	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/18/25	0/30/128/135	0/0/9/9
22	CLA	b	615	-	3/3/17/25	0/22/120/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/19/25	0/31/129/135	0/0/9/9
24	BCR	b	618	-	-	0/13/30/63	0/1/1/2
24	BCR	b	619	-	-	2/26/43/63	0/1/1/2
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
28	SQD	b	621	-	-	0/32/52/69	0/1/1/1
25	LMG	b	622	-	-	0/38/58/70	0/1/1/1
34	HTG	b	623	-	-	0/10/30/30	0/1/1/1
34	HTG	b	624	-	-	0/10/30/30	0/1/1/1
34	HTG	b	626	-	-	0/10/30/30	0/1/1/1
34	HTG	b	627	-	-	0/10/30/30	0/1/1/1
31	DMS	b	629	-	-	0/0/0/0	0/0/0/0
31	DMS	b	630	-	-	0/0/0/0	0/0/0/0
31	DMS	b	631	-	-	0/0/0/0	0/0/0/0
34	HTG	b	632	-	-	0/10/30/30	0/1/1/1
31	DMS	b	633	-	-	0/0/0/0	0/0/0/0
31	DMS	b	634	-	-	0/0/0/0	0/0/0/0
31	DMS	b	635	-	-	0/0/0/0	0/0/0/0
31	DMS	b	636	-	-	0/0/0/0	0/0/0/0
31	DMS	b	637	-	-	0/0/0/0	0/0/0/0
31	DMS	b	638	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	903	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	905	39	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	906	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	907	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	908	39	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	912	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	913	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	914	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	c	915	-	-	0/29/63/63	0/2/2/2
24	BCR	c	916	-	-	0/29/63/63	0/2/2/2
35	DGD	c	917	-	-	0/51/91/95	0/2/2/2
35	DGD	c	918	-	-	0/51/91/95	0/2/2/2
35	DGD	c	919	-	-	0/51/91/95	0/2/2/2
25	LMG	c	920	-	-	0/46/66/70	0/1/1/1
29	LMT	c	921	-	-	0/21/61/61	0/2/2/2
34	HTG	c	922	-	-	0/10/30/30	0/1/1/1
31	DMS	c	923	-	-	0/0/0/0	0/0/0/0
31	DMS	c	924	-	-	0/0/0/0	0/0/0/0
31	DMS	c	925	-	-	0/0/0/0	0/0/0/0
31	DMS	c	926	-	-	0/0/0/0	0/0/0/0
31	DMS	c	927	-	-	0/0/0/0	0/0/0/0
31	DMS	c	928	-	-	0/0/0/0	0/0/0/0
31	DMS	c	929	-	-	0/0/0/0	0/0/0/0
25	LMG	c	930	-	-	0/44/64/70	0/1/1/1
29	LMT	c	931	-	-	0/15/35/61	0/1/1/2
31	DMS	c	933	-	-	0/0/0/0	0/0/0/0
31	DMS	c	934	-	-	0/0/0/0	0/0/0/0
31	DMS	c	935	-	-	0/0/0/0	0/0/0/0
31	DMS	c	936	-	-	0/0/0/0	0/0/0/0
31	DMS	c	937	-	-	0/0/0/0	0/0/0/0
31	DMS	c	938	-	-	0/0/0/0	0/0/0/0
31	DMS	c	939	-	-	0/0/0/0	0/0/0/0
31	DMS	c	940	-	-	0/0/0/0	0/0/0/0
31	DMS	c	941	-	-	0/0/0/0	0/0/0/0
31	DMS	c	942	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	c	943	-	-	0/0/0/0	0/0/0/0
31	DMS	c	944	-	-	0/0/0/0	0/0/0/0
27	LHG	d	401	-	-	0/34/34/53	0/0/0/0
22	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	d	404	-	-	0/29/63/63	0/2/2/2
26	PL9	d	405	-	-	0/53/73/73	0/1/1/1
35	DGD	d	406	-	-	0/44/44/95	0/0/0/2
27	LHG	d	407	-	-	0/53/53/53	0/0/0/0
27	LHG	d	408	-	-	0/50/50/53	0/0/0/0
25	LMG	d	409	-	-	0/42/62/70	0/1/1/1
31	DMS	d	411	-	-	0/0/0/0	0/0/0/0
31	DMS	d	412	-	-	0/0/0/0	0/0/0/0
31	DMS	d	413	-	-	0/0/0/0	0/0/0/0
31	DMS	d	414	-	-	0/0/0/0	0/0/0/0
31	DMS	d	415	-	-	0/0/0/0	0/0/0/0
36	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
28	SQD	f	101	-	-	0/12/12/69	0/0/0/1
29	LMT	f	102	-	-	0/17/37/61	0/1/1/2
31	DMS	f	103	-	-	0/0/0/0	0/0/0/0
37	RRX	h	101	-	-	0/29/65/65	0/2/2/2
35	DGD	h	102	-	-	0/51/91/95	0/2/2/2
25	LMG	i	101	-	-	0/46/66/70	0/1/1/1
31	DMS	i	106	-	-	0/0/0/0	0/0/0/0
25	LMG	j	101	38	-	0/42/62/70	0/1/1/1
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
28	SQD	l	101	-	-	0/49/69/69	0/1/1/1
27	LHG	l	102	-	-	0/53/53/53	0/0/0/0
31	DMS	l	103	-	-	0/0/0/0	0/0/0/0
31	DMS	l	104	-	-	0/0/0/0	0/0/0/0
31	DMS	l	105	-	-	0/0/0/0	0/0/0/0
34	HTG	l	106	-	-	0/10/30/30	0/1/1/1
31	DMS	o	302	-	-	0/0/0/0	0/0/0/0
31	DMS	o	303	-	-	0/0/0/0	0/0/0/0
31	DMS	o	304	-	-	0/0/0/0	0/0/0/0
31	DMS	o	305	-	-	0/0/0/0	0/0/0/0
31	DMS	o	306	-	-	0/0/0/0	0/0/0/0
31	DMS	o	307	-	-	0/0/0/0	0/0/0/0
31	DMS	o	308	-	-	0/0/0/0	0/0/0/0
29	LMT	t	101	-	-	0/15/35/61	0/1/1/2
31	DMS	t	103	-	-	0/0/0/0	0/0/0/0
31	DMS	t	104	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	t	105	-	-	0/0/0/0	0/0/0/0
31	DMS	u	202	-	-	0/0/0/0	0/0/0/0
31	DMS	u	203	-	-	0/0/0/0	0/0/0/0
31	DMS	u	204	-	-	0/0/0/0	0/0/0/0
31	DMS	u	205	-	-	0/0/0/0	0/0/0/0
31	DMS	v	201	-	-	0/0/0/0	0/0/0/0
36	HEM	v	202	15	-	0/6/54/54	0/0/8/8
34	HTG	v	203	-	-	0/7/27/30	0/1/1/1
31	DMS	v	204	-	-	0/0/0/0	0/0/0/0
31	DMS	v	205	-	-	0/0/0/0	0/0/0/0
31	DMS	v	206	-	-	0/0/0/0	0/0/0/0
31	DMS	v	207	-	-	0/0/0/0	0/0/0/0
31	DMS	v	208	-	-	0/0/0/0	0/0/0/0
31	DMS	v	209	-	-	0/0/0/0	0/0/0/0
31	DMS	v	210	-	-	0/0/0/0	0/0/0/0
31	DMS	v	211	-	-	0/0/0/0	0/0/0/0
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

All (1215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	f	101	SQD	C6-S	-6.78	1.67	1.77
23	A	407	PHO	C1A-NA	-5.51	1.25	1.37
36	V	202	HEM	C3B-C2B	-4.66	1.34	1.40
36	v	202	HEM	C3B-C2B	-4.47	1.34	1.40
34	B	623	HTG	C1'-S1	-4.29	1.75	1.81
23	a	411	PHO	C1A-NA	-4.01	1.28	1.37
23	D	402	PHO	C1A-NA	-3.82	1.29	1.37
34	C	532	HTG	C1'-S1	-3.72	1.76	1.81
36	E	102	HEM	C3B-C2B	-3.67	1.35	1.40
22	a	409	CLA	C4C-NC	-3.67	1.32	1.37
23	a	410	PHO	C1A-NA	-3.64	1.29	1.37
34	b	623	HTG	C1'-S1	-3.64	1.76	1.81
36	v	202	HEM	C3C-C2C	-3.64	1.35	1.40
36	E	102	HEM	C3C-C2C	-3.45	1.35	1.40
36	e	101	HEM	C3B-C2B	-3.44	1.35	1.40
34	v	203	HTG	C1'-S1	-3.42	1.77	1.81
36	e	101	HEM	C3C-C2C	-3.35	1.35	1.40
34	l	106	HTG	C1'-S1	-3.31	1.77	1.81
22	A	405	CLA	C4C-NC	-3.25	1.32	1.37
22	a	407	CLA	C4C-NC	-3.19	1.32	1.37
36	V	202	HEM	C3C-C2C	-3.18	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	415	HTG	C1'-S1	-3.15	1.77	1.81
34	b	624	HTG	C1'-S1	-3.13	1.77	1.81
22	A	406	CLA	C4C-NC	-3.11	1.32	1.37
22	b	617	CLA	C1C-NC	-3.04	1.32	1.37
22	C	509	CLA	C1C-NC	-3.00	1.32	1.37
23	A	407	PHO	C3D-C4D	-2.99	1.34	1.43
22	b	605	CLA	C4C-NC	-2.97	1.33	1.37
23	D	402	PHO	C3D-C4D	-2.90	1.34	1.43
34	C	521	HTG	C1'-S1	-2.89	1.77	1.81
22	B	616	CLA	C1C-NC	-2.89	1.33	1.37
28	A	413	SQD	C6-S	-2.87	1.65	1.77
34	b	627	HTG	C1'-S1	-2.85	1.77	1.81
22	d	402	CLA	C4C-NC	-2.84	1.33	1.37
34	B	627	HTG	C1'-S1	-2.83	1.77	1.81
22	B	602	CLA	C1C-NC	-2.78	1.33	1.37
22	C	505	CLA	C1C-NC	-2.75	1.33	1.37
22	B	603	CLA	C1C-NC	-2.73	1.33	1.37
22	c	911	CLA	C1C-NC	-2.72	1.33	1.37
22	c	906	CLA	C1C-NC	-2.69	1.33	1.37
22	C	509	CLA	C4C-NC	-2.68	1.33	1.37
22	d	403	CLA	C1C-NC	-2.67	1.33	1.37
28	a	414	SQD	C6-S	-2.67	1.66	1.77
22	b	615	CLA	C1C-NC	-2.66	1.33	1.37
23	a	410	PHO	CHB-C4A	-2.63	1.33	1.40
28	a	418	SQD	C6-S	-2.62	1.66	1.77
34	b	626	HTG	C1'-S1	-2.62	1.78	1.81
22	c	910	CLA	C4C-NC	-2.61	1.33	1.37
22	B	615	CLA	C1C-NC	-2.55	1.33	1.37
34	D	414	HTG	C1'-S1	-2.55	1.78	1.81
34	c	922	HTG	C1'-S1	-2.53	1.78	1.81
22	c	904	CLA	C1C-NC	-2.53	1.33	1.37
23	a	410	PHO	C3D-C4D	-2.49	1.35	1.43
22	B	608	CLA	C4C-NC	-2.48	1.33	1.37
23	a	411	PHO	C3D-C4D	-2.47	1.35	1.43
28	C	501	SQD	C6-S	-2.45	1.67	1.77
22	D	403	CLA	C4C-NC	-2.41	1.33	1.37
22	b	609	CLA	C1C-NC	-2.41	1.33	1.37
22	c	912	CLA	C4C-NC	-2.39	1.34	1.37
34	C	532	HTG	C1-S1	-2.36	1.77	1.80
22	c	912	CLA	C1C-NC	-2.34	1.33	1.37
22	c	902	CLA	C4C-NC	-2.33	1.34	1.37
22	b	614	CLA	C1C-NC	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	BCR	C30-C25	-2.29	1.50	1.53
22	c	909	CLA	C1C-NC	-2.28	1.34	1.37
28	b	621	SQD	C6-S	-2.28	1.68	1.77
34	l	106	HTG	C1-S1	-2.28	1.77	1.80
22	b	605	CLA	C1C-NC	-2.23	1.34	1.37
22	c	906	CLA	C4C-NC	-2.23	1.34	1.37
22	B	606	CLA	C1C-NC	-2.22	1.34	1.37
28	l	101	SQD	C6-S	-2.22	1.68	1.77
22	b	613	CLA	C1C-NC	-2.21	1.34	1.37
22	A	405	CLA	C3A-C2A	-2.19	1.48	1.54
34	C	521	HTG	C1-S1	-2.18	1.77	1.80
22	b	610	CLA	C4C-NC	-2.17	1.34	1.37
34	b	632	HTG	C1'-S1	-2.16	1.78	1.81
22	C	507	CLA	C1C-NC	-2.15	1.34	1.37
22	B	615	CLA	C4C-NC	-2.15	1.34	1.37
22	b	603	CLA	C4C-NC	-2.14	1.34	1.37
22	C	506	CLA	C4C-NC	-2.13	1.34	1.37
22	c	909	CLA	C4C-NC	-2.13	1.34	1.37
22	c	905	CLA	C1C-NC	-2.12	1.34	1.37
22	C	503	CLA	C4C-NC	-2.12	1.34	1.37
22	b	607	CLA	O2A-C1	-2.10	1.39	1.46
22	B	614	CLA	C4C-NC	-2.09	1.34	1.37
22	C	504	CLA	C1C-NC	-2.09	1.34	1.37
28	D	408	SQD	C6-S	-2.08	1.69	1.77
22	B	604	CLA	C1C-NC	-2.06	1.34	1.37
22	b	610	CLA	C1C-NC	-2.05	1.34	1.37
36	e	101	HEM	C1D-ND	2.00	1.40	1.36
22	C	504	CLA	C4C-C3C	2.00	1.48	1.45
23	A	407	PHO	C1C-C2C	2.00	1.50	1.45
23	D	402	PHO	C4D-CHA	2.01	1.49	1.44
22	c	910	CLA	C4B-CHC	2.01	1.45	1.40
25	c	930	LMG	O1-C1	2.01	1.43	1.40
25	D	412	LMG	O1-C1	2.01	1.43	1.40
22	c	908	CLA	C1C-C2C	2.02	1.48	1.44
24	B	618	BCR	C26-C25	2.02	1.37	1.34
22	B	610	CLA	C4C-C3C	2.03	1.48	1.45
22	B	609	CLA	CHD-C4C	2.03	1.47	1.41
22	c	905	CLA	OBD-CAD	2.03	1.25	1.22
25	b	622	LMG	C4-C5	2.03	1.57	1.53
35	c	918	DGD	O5D-C1E	2.03	1.43	1.40
22	b	613	CLA	C4C-C3C	2.04	1.48	1.45
22	B	613	CLA	CHD-C4C	2.04	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	918	DGD	O3G-C1D	2.05	1.43	1.40
24	B	620	BCR	C19-C18	2.05	1.50	1.45
22	B	606	CLA	CHB-C4A	2.06	1.36	1.33
22	B	603	CLA	C3B-CAB	2.06	1.52	1.47
22	C	508	CLA	C4C-C3C	2.06	1.48	1.45
22	B	617	CLA	C1C-C2C	2.06	1.48	1.44
29	T	102	LMT	O1'-C1'	2.06	1.43	1.40
22	b	606	CLA	C1B-CHB	2.06	1.45	1.40
26	d	405	PL9	C23-C24	2.07	1.38	1.33
22	a	412	CLA	C4B-CHC	2.07	1.45	1.40
23	a	410	PHO	C3B-C4B	2.08	1.47	1.43
36	e	101	HEM	C1B-NB	2.08	1.39	1.36
22	B	606	CLA	C3D-C2D	2.08	1.44	1.39
22	C	514	CLA	C4C-C3C	2.09	1.48	1.45
36	v	202	HEM	C1C-NC	2.09	1.39	1.36
22	b	604	CLA	CHD-C4C	2.09	1.47	1.41
22	B	615	CLA	CHD-C4C	2.09	1.47	1.41
22	B	614	CLA	C1C-C2C	2.09	1.48	1.44
22	B	617	CLA	CHD-C4C	2.10	1.47	1.41
36	v	202	HEM	C1D-ND	2.10	1.40	1.36
22	C	513	CLA	C4C-C3C	2.10	1.48	1.45
22	D	403	CLA	C1C-C2C	2.10	1.48	1.44
36	e	101	HEM	CMB-C2B	2.11	1.56	1.51
22	b	611	CLA	CHD-C4C	2.11	1.47	1.41
22	c	906	CLA	C4C-C3C	2.12	1.48	1.45
26	D	406	PL9	C2-C3	2.12	1.40	1.34
22	c	913	CLA	CHD-C4C	2.13	1.47	1.41
22	d	402	CLA	C4B-CHC	2.13	1.45	1.40
22	b	606	CLA	CHD-C4C	2.13	1.47	1.41
24	B	620	BCR	C26-C25	2.13	1.38	1.34
22	C	508	CLA	CHD-C4C	2.14	1.47	1.41
22	A	406	CLA	CHD-C4C	2.14	1.47	1.41
24	c	915	BCR	C23-C22	2.14	1.50	1.45
22	c	908	CLA	CHD-C4C	2.14	1.47	1.41
22	c	904	CLA	CHD-C4C	2.15	1.47	1.41
26	d	405	PL9	C7-C3	2.15	1.53	1.51
22	c	913	CLA	C1C-C2C	2.16	1.48	1.44
22	B	614	CLA	C4B-CHC	2.16	1.45	1.40
22	C	502	CLA	C1C-C2C	2.16	1.48	1.44
22	c	914	CLA	C4C-C3C	2.16	1.48	1.45
22	c	903	CLA	CHD-C4C	2.17	1.47	1.41
22	a	409	CLA	CHD-C4C	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	PHO	C4C-C3C	2.17	1.49	1.45
22	B	612	CLA	CHD-C4C	2.18	1.47	1.41
24	Y	101	BCR	C5-C6	2.18	1.36	1.33
22	C	514	CLA	CHD-C4C	2.19	1.47	1.41
22	C	503	CLA	C4C-C3C	2.19	1.48	1.45
22	B	617	CLA	OBD-CAD	2.19	1.25	1.22
22	D	401	CLA	CHD-C4C	2.20	1.47	1.41
36	v	202	HEM	CMC-C2C	2.20	1.56	1.51
22	D	404	CLA	C1C-C2C	2.21	1.48	1.44
22	c	903	CLA	C4C-C3C	2.21	1.48	1.45
25	C	531	LMG	O1-C1	2.21	1.44	1.40
22	A	408	CLA	C1B-CHB	2.22	1.46	1.40
22	C	506	CLA	C1B-CHB	2.22	1.46	1.40
22	b	608	CLA	C4C-C3C	2.23	1.49	1.45
24	C	515	BCR	C19-C18	2.23	1.50	1.45
22	c	910	CLA	CHD-C4C	2.23	1.47	1.41
22	C	503	CLA	C1C-C2C	2.23	1.48	1.44
24	a	413	BCR	C12-C13	2.23	1.50	1.45
23	a	411	PHO	C3B-C4B	2.23	1.48	1.43
23	a	410	PHO	C1B-C2B	2.23	1.50	1.45
22	a	409	CLA	C4C-C3C	2.24	1.49	1.45
22	C	511	CLA	C1C-C2C	2.24	1.48	1.44
22	C	513	CLA	CHD-C4C	2.24	1.47	1.41
22	b	604	CLA	C1B-CHB	2.24	1.46	1.40
23	D	402	PHO	C1B-C2B	2.25	1.50	1.45
36	e	101	HEM	CMD-C2D	2.25	1.56	1.51
28	l	101	SQD	O6-C1	2.25	1.44	1.40
29	B	622	LMT	O1'-C1'	2.25	1.44	1.40
22	A	408	CLA	CHD-C4C	2.25	1.47	1.41
23	a	410	PHO	CHC-C4B	2.25	1.45	1.40
22	b	610	CLA	C1C-C2C	2.25	1.48	1.44
22	a	409	CLA	C4B-CHC	2.25	1.46	1.40
25	B	621	LMG	O1-C1	2.26	1.44	1.40
22	B	610	CLA	C1C-C2C	2.27	1.48	1.44
22	C	505	CLA	OBD-CAD	2.27	1.25	1.22
22	c	914	CLA	CHD-C4C	2.27	1.48	1.41
36	e	101	HEM	CAA-C2A	2.27	1.55	1.52
22	C	511	CLA	CHD-C4C	2.28	1.48	1.41
22	B	605	CLA	CHB-C4A	2.28	1.36	1.33
22	C	512	CLA	CHD-C4C	2.28	1.48	1.41
28	D	408	SQD	O6-C1	2.28	1.44	1.40
22	B	611	CLA	CHD-C4C	2.29	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	908	CLA	C4C-C3C	2.29	1.49	1.45
35	d	406	DGD	O3G-C1D	2.29	1.44	1.40
35	D	407	DGD	O3G-C1D	2.30	1.44	1.40
22	D	404	CLA	CHD-C4C	2.30	1.48	1.41
22	B	607	CLA	C4C-C3C	2.30	1.49	1.45
22	B	614	CLA	C4C-C3C	2.30	1.49	1.45
36	E	102	HEM	CMA-C3A	2.30	1.56	1.51
24	b	619	BCR	C12-C13	2.30	1.50	1.45
22	b	615	CLA	CHD-C4C	2.31	1.48	1.41
22	D	401	CLA	C1B-CHB	2.31	1.46	1.40
22	B	605	CLA	C4B-CHC	2.31	1.46	1.40
22	C	505	CLA	CHB-C4A	2.31	1.36	1.33
26	D	406	PL9	C6-C5	2.32	1.47	1.35
36	V	202	HEM	CMA-C3A	2.32	1.56	1.51
22	B	609	CLA	C4C-C3C	2.32	1.49	1.45
22	B	605	CLA	CHD-C4C	2.32	1.48	1.41
24	b	619	BCR	C8-C9	2.33	1.50	1.45
22	B	608	CLA	C4B-CHC	2.33	1.46	1.40
22	C	510	CLA	C1B-CHB	2.33	1.46	1.40
22	C	509	CLA	CHD-C4C	2.33	1.48	1.41
22	A	406	CLA	C1B-CHB	2.35	1.46	1.40
22	C	510	CLA	C4B-CHC	2.36	1.46	1.40
22	b	607	CLA	C4C-C3C	2.36	1.49	1.45
36	e	101	HEM	C4C-NC	2.36	1.39	1.36
22	B	604	CLA	CHD-C4C	2.36	1.48	1.41
22	a	412	CLA	CHD-C4C	2.36	1.48	1.41
22	C	514	CLA	CHB-C4A	2.38	1.36	1.33
22	b	605	CLA	C4C-C3C	2.38	1.49	1.45
22	c	902	CLA	C3D-C2D	2.38	1.45	1.39
23	a	410	PHO	OBD-CAD	2.38	1.26	1.22
22	B	616	CLA	CHD-C4C	2.38	1.48	1.41
22	B	612	CLA	C1B-CHB	2.39	1.46	1.40
35	c	919	DGD	O5D-C1E	2.39	1.44	1.40
23	A	407	PHO	C3D-C2D	2.39	1.45	1.38
36	V	202	HEM	CMC-C2C	2.39	1.56	1.51
36	v	202	HEM	CMD-C2D	2.39	1.56	1.51
22	B	609	CLA	C1C-C2C	2.40	1.49	1.44
22	C	508	CLA	C1C-C2C	2.40	1.49	1.44
24	d	404	BCR	C23-C22	2.40	1.51	1.45
22	a	407	CLA	CHD-C4C	2.41	1.48	1.41
22	C	502	CLA	C4C-C3C	2.41	1.49	1.45
22	D	403	CLA	C3D-C2D	2.41	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C4B-CHC	2.41	1.46	1.40
22	c	904	CLA	C4B-CHC	2.42	1.46	1.40
23	A	407	PHO	OBD-CAD	2.42	1.26	1.22
22	D	403	CLA	C4B-CHC	2.42	1.46	1.40
22	c	911	CLA	CHD-C4C	2.44	1.48	1.41
22	C	513	CLA	C1C-C2C	2.45	1.49	1.44
24	A	409	BCR	C12-C13	2.45	1.51	1.45
22	B	603	CLA	C1C-C2C	2.46	1.49	1.44
22	B	607	CLA	C1B-CHB	2.46	1.46	1.40
22	b	614	CLA	C1C-C2C	2.47	1.49	1.44
22	b	616	CLA	CHD-C4C	2.47	1.48	1.41
22	b	611	CLA	C1C-C2C	2.47	1.49	1.44
29	Z	101	LMT	O1'-C1'	2.47	1.44	1.40
22	b	608	CLA	CHD-C4C	2.47	1.48	1.41
22	c	912	CLA	C4C-C3C	2.48	1.49	1.45
22	C	509	CLA	C4C-C3C	2.48	1.49	1.45
26	d	405	PL9	C18-C19	2.48	1.39	1.33
22	b	614	CLA	CHD-C4C	2.49	1.48	1.41
22	a	408	CLA	C1B-CHB	2.49	1.46	1.40
22	C	502	CLA	CHD-C4C	2.49	1.48	1.41
22	B	610	CLA	OBD-CAD	2.50	1.25	1.22
22	B	602	CLA	C1C-C2C	2.50	1.49	1.44
22	b	613	CLA	C1A-CHA	2.50	1.53	1.43
22	c	909	CLA	CHD-C4C	2.51	1.48	1.41
22	C	507	CLA	CHD-C4C	2.51	1.48	1.41
22	b	607	CLA	OBD-CAD	2.51	1.26	1.22
26	a	415	PL9	C2-C3	2.51	1.41	1.34
22	C	504	CLA	CHD-C4C	2.52	1.48	1.41
35	C	518	DGD	O2G-C1B	2.52	1.41	1.34
22	B	603	CLA	CHD-C4C	2.53	1.48	1.41
23	a	411	PHO	C4C-C3C	2.53	1.49	1.45
22	b	604	CLA	O2A-CGA	2.54	1.40	1.33
22	C	507	CLA	C1C-C2C	2.54	1.49	1.44
22	B	602	CLA	CHD-C4C	2.55	1.48	1.41
22	A	405	CLA	C1B-CHB	2.55	1.46	1.40
22	c	907	CLA	CHD-C4C	2.55	1.48	1.41
22	B	616	CLA	C4B-CHC	2.55	1.46	1.40
22	b	602	CLA	C4C-C3C	2.55	1.49	1.45
24	a	413	BCR	C5-C6	2.56	1.38	1.34
35	c	917	DGD	O5D-C1E	2.56	1.44	1.40
29	c	931	LMT	O1'-C1'	2.57	1.44	1.40
25	d	409	LMG	O1-C1	2.57	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	921	LMT	O1'-C1'	2.57	1.44	1.40
22	c	907	CLA	C1B-CHB	2.58	1.47	1.40
22	d	402	CLA	CHD-C4C	2.59	1.48	1.41
22	c	904	CLA	C4C-C3C	2.59	1.49	1.45
26	A	411	PL9	C6-C5	2.59	1.48	1.35
22	C	507	CLA	C4C-C3C	2.60	1.49	1.45
26	a	415	PL9	C7-C3	2.60	1.54	1.51
22	a	408	CLA	C4B-CHC	2.61	1.47	1.40
22	B	609	CLA	C1B-CHB	2.61	1.47	1.40
22	c	907	CLA	C4B-CHC	2.62	1.47	1.40
35	C	517	DGD	O5D-C1E	2.62	1.44	1.40
26	d	405	PL9	C6-C5	2.63	1.49	1.35
29	I	102	LMT	O1'-C1'	2.63	1.44	1.40
22	b	617	CLA	C4B-CHC	2.63	1.47	1.40
22	b	612	CLA	C4B-CHC	2.64	1.47	1.40
23	a	411	PHO	CHD-C4C	2.64	1.46	1.40
22	c	909	CLA	CHB-C4A	2.64	1.36	1.33
22	B	607	CLA	C1C-C2C	2.64	1.49	1.44
22	b	602	CLA	CHD-C4C	2.65	1.49	1.41
22	B	609	CLA	C4B-CHC	2.65	1.47	1.40
24	D	405	BCR	C8-C9	2.65	1.51	1.45
23	D	402	PHO	C3B-C4B	2.66	1.49	1.43
22	b	605	CLA	OBD-CAD	2.66	1.26	1.22
24	d	404	BCR	C12-C13	2.66	1.51	1.45
22	c	909	CLA	C1C-C2C	2.68	1.49	1.44
22	d	402	CLA	C1B-CHB	2.68	1.47	1.40
22	d	403	CLA	C1C-C2C	2.69	1.49	1.44
22	A	408	CLA	C4B-CHC	2.69	1.47	1.40
22	B	603	CLA	C4B-CHC	2.69	1.47	1.40
22	C	511	CLA	C4B-CHC	2.69	1.47	1.40
22	B	613	CLA	C4C-C3C	2.69	1.49	1.45
26	D	406	PL9	C7-C3	2.69	1.54	1.51
22	b	617	CLA	C1C-C2C	2.70	1.49	1.44
22	B	608	CLA	C4C-C3C	2.70	1.49	1.45
34	b	632	HTG	O5-C1	2.70	1.46	1.42
22	D	403	CLA	C3B-C2B	2.71	1.43	1.40
22	d	402	CLA	C3D-C2D	2.71	1.45	1.39
22	a	407	CLA	C4B-CHC	2.71	1.47	1.40
22	b	604	CLA	C4C-C3C	2.72	1.49	1.45
26	A	411	PL9	C2-C3	2.72	1.42	1.34
22	c	913	CLA	C4C-C3C	2.72	1.49	1.45
22	C	506	CLA	CHD-C4C	2.72	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C4C-C3C	2.73	1.49	1.45
23	A	407	PHO	CHC-C4B	2.73	1.47	1.40
22	b	616	CLA	C4B-CHC	2.75	1.47	1.40
22	b	613	CLA	CHB-C4A	2.76	1.37	1.33
22	c	903	CLA	C4B-CHC	2.76	1.47	1.40
22	c	912	CLA	CHD-C4C	2.76	1.49	1.41
22	D	403	CLA	CHC-C1C	2.76	1.43	1.35
22	C	503	CLA	C1B-CHB	2.77	1.47	1.40
22	b	615	CLA	C4B-CHC	2.77	1.47	1.40
22	c	913	CLA	C4B-CHC	2.77	1.47	1.40
22	c	910	CLA	C1B-CHB	2.78	1.47	1.40
22	B	603	CLA	C3D-C2D	2.78	1.45	1.39
22	b	603	CLA	C4B-CHC	2.78	1.47	1.40
22	b	604	CLA	C4B-CHC	2.78	1.47	1.40
22	c	911	CLA	C1B-CHB	2.78	1.47	1.40
24	A	409	BCR	C19-C18	2.78	1.52	1.45
22	C	512	CLA	C4B-CHC	2.78	1.47	1.40
22	B	609	CLA	OBD-CAD	2.78	1.26	1.22
22	a	408	CLA	CHD-C4C	2.78	1.49	1.41
22	b	614	CLA	C4C-C3C	2.79	1.50	1.45
22	c	902	CLA	C1B-CHB	2.79	1.47	1.40
22	a	409	CLA	C1B-CHB	2.80	1.47	1.40
22	B	613	CLA	C1B-CHB	2.80	1.47	1.40
35	C	519	DGD	O2G-C1B	2.80	1.42	1.34
22	A	408	CLA	C3D-C2D	2.80	1.45	1.39
22	d	403	CLA	CHD-C4C	2.81	1.49	1.41
22	A	406	CLA	C3C-C2C	2.81	1.42	1.36
22	B	607	CLA	OBD-CAD	2.82	1.26	1.22
22	A	406	CLA	C3D-C2D	2.82	1.46	1.39
22	b	605	CLA	C1B-CHB	2.82	1.47	1.40
22	B	617	CLA	C1B-CHB	2.82	1.47	1.40
22	b	615	CLA	C1C-C2C	2.82	1.50	1.44
22	D	403	CLA	OBD-CAD	2.83	1.26	1.22
26	a	415	PL9	C6-C5	2.83	1.50	1.35
22	B	612	CLA	C4B-CHC	2.83	1.47	1.40
22	b	607	CLA	C1B-CHB	2.83	1.47	1.40
22	b	604	CLA	C1C-C2C	2.83	1.50	1.44
22	B	608	CLA	CHD-C4C	2.84	1.49	1.41
27	d	407	LHG	O8-C23	2.85	1.41	1.33
35	H	102	DGD	O5D-C1E	2.86	1.45	1.40
22	b	607	CLA	C3D-C2D	2.86	1.46	1.39
22	b	609	CLA	C1B-CHB	2.86	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	CLA	C4B-CHC	2.87	1.47	1.40
23	a	411	PHO	C3D-C2D	2.87	1.46	1.38
22	C	512	CLA	C1C-C2C	2.88	1.50	1.44
22	c	902	CLA	C4C-C3C	2.88	1.50	1.45
23	D	402	PHO	C3D-C2D	2.88	1.46	1.38
22	B	606	CLA	OBD-CAD	2.88	1.26	1.22
36	E	102	HEM	C4D-ND	2.89	1.40	1.36
22	b	609	CLA	C4B-CHC	2.89	1.47	1.40
22	D	404	CLA	C4B-CHC	2.89	1.47	1.40
22	D	401	CLA	O2A-CGA	2.89	1.41	1.33
22	c	914	CLA	C1C-C2C	2.89	1.50	1.44
22	A	405	CLA	C4B-CHC	2.90	1.47	1.40
22	B	605	CLA	C3D-C2D	2.91	1.46	1.39
22	b	613	CLA	C1B-CHB	2.91	1.47	1.40
29	f	102	LMT	O1'-C1'	2.92	1.45	1.40
22	c	914	CLA	C4B-CHC	2.93	1.47	1.40
22	b	602	CLA	C1C-C2C	2.94	1.50	1.44
22	A	408	CLA	C4C-C3C	2.94	1.50	1.45
23	D	402	PHO	CHD-C4C	2.94	1.47	1.40
35	C	517	DGD	O2G-C1B	2.94	1.42	1.34
22	A	405	CLA	C4C-C3C	2.94	1.50	1.45
22	C	505	CLA	C4B-CHC	2.95	1.48	1.40
35	C	518	DGD	O3G-C1D	2.95	1.45	1.40
22	C	504	CLA	C1B-CHB	2.95	1.48	1.40
22	b	608	CLA	C4B-CHC	2.96	1.48	1.40
22	c	907	CLA	C4C-C3C	2.96	1.50	1.45
22	b	607	CLA	C4B-CHC	2.96	1.48	1.40
22	B	611	CLA	C1C-C2C	2.97	1.50	1.44
27	d	407	LHG	O7-C7	2.97	1.42	1.34
22	C	509	CLA	C1B-CHB	2.97	1.48	1.40
22	b	611	CLA	C4B-CHC	2.97	1.48	1.40
22	B	615	CLA	C1C-C2C	2.97	1.50	1.44
22	A	406	CLA	C4B-CHC	2.98	1.48	1.40
22	c	902	CLA	C4B-CHC	2.99	1.48	1.40
22	C	510	CLA	C4C-C3C	2.99	1.50	1.45
22	b	607	CLA	C1C-C2C	2.99	1.50	1.44
22	B	608	CLA	O2A-CGA	2.99	1.42	1.33
22	c	903	CLA	C1B-CHB	3.00	1.48	1.40
22	c	906	CLA	CHD-C4C	3.00	1.50	1.41
36	V	202	HEM	C4C-NC	3.01	1.40	1.36
22	C	502	CLA	C4B-CHC	3.01	1.48	1.40
36	v	202	HEM	C4D-ND	3.01	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C4B-CHC	3.01	1.48	1.40
22	B	610	CLA	C4B-CHC	3.02	1.48	1.40
22	b	616	CLA	CHB-C4A	3.02	1.37	1.33
22	c	904	CLA	C1B-CHB	3.03	1.48	1.40
22	c	907	CLA	C3D-C2D	3.03	1.46	1.39
23	D	402	PHO	CHC-C4B	3.04	1.47	1.40
22	c	902	CLA	C1C-C2C	3.04	1.50	1.44
22	B	605	CLA	C4C-C3C	3.04	1.50	1.45
22	B	602	CLA	C4B-CHC	3.04	1.48	1.40
22	C	504	CLA	C1C-C2C	3.05	1.50	1.44
22	D	403	CLA	C1B-CHB	3.06	1.48	1.40
22	a	412	CLA	C3D-C2D	3.07	1.46	1.39
22	B	603	CLA	C1B-CHB	3.07	1.48	1.40
22	B	604	CLA	C3D-C2D	3.07	1.46	1.39
22	b	614	CLA	C4B-CHC	3.08	1.48	1.40
22	d	402	CLA	C4C-C3C	3.08	1.50	1.45
22	C	503	CLA	C4B-CHC	3.08	1.48	1.40
22	C	507	CLA	C4B-CHC	3.08	1.48	1.40
22	C	509	CLA	C4B-CHC	3.09	1.48	1.40
22	b	605	CLA	C4B-CHC	3.09	1.48	1.40
22	b	606	CLA	C4B-CHC	3.09	1.48	1.40
22	C	502	CLA	C1B-CHB	3.09	1.48	1.40
22	c	903	CLA	OBD-CAD	3.09	1.26	1.22
22	b	616	CLA	C4C-C3C	3.10	1.50	1.45
22	c	905	CLA	C4C-C3C	3.10	1.50	1.45
22	A	405	CLA	O2A-CGA	3.10	1.42	1.33
22	a	412	CLA	C1B-CHB	3.10	1.48	1.40
22	B	614	CLA	C1B-CHB	3.11	1.48	1.40
22	B	607	CLA	C3D-C2D	3.11	1.46	1.39
22	b	606	CLA	C3B-C2B	3.11	1.44	1.40
22	C	514	CLA	C1C-C2C	3.13	1.50	1.44
22	c	906	CLA	C1B-CHB	3.13	1.48	1.40
22	c	905	CLA	C4B-CHC	3.13	1.48	1.40
22	c	913	CLA	C1B-CHB	3.13	1.48	1.40
22	C	505	CLA	CHD-C4C	3.14	1.50	1.41
22	b	614	CLA	C3D-C2D	3.14	1.46	1.39
22	C	512	CLA	C4C-C3C	3.14	1.50	1.45
22	D	401	CLA	C3B-C2B	3.14	1.44	1.40
22	b	610	CLA	C4B-CHC	3.14	1.48	1.40
22	c	904	CLA	C3D-C2D	3.15	1.46	1.39
22	C	513	CLA	C4B-CHC	3.15	1.48	1.40
22	b	608	CLA	C1B-CHB	3.16	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	409	CLA	C3D-C2D	3.16	1.46	1.39
22	C	511	CLA	C4C-C3C	3.17	1.50	1.45
22	d	403	CLA	C1B-CHB	3.18	1.48	1.40
22	b	604	CLA	OBD-CAD	3.18	1.26	1.22
22	B	605	CLA	C1B-CHB	3.18	1.48	1.40
22	b	603	CLA	CHD-C4C	3.19	1.50	1.41
22	B	610	CLA	C1B-CHB	3.19	1.48	1.40
22	b	617	CLA	C1B-CHB	3.20	1.48	1.40
22	D	401	CLA	CHC-C1C	3.20	1.44	1.35
22	c	909	CLA	C4C-C3C	3.21	1.50	1.45
27	D	410	LHG	O7-C7	3.22	1.43	1.34
22	C	508	CLA	C1B-CHB	3.22	1.48	1.40
23	a	410	PHO	CHD-C4C	3.23	1.48	1.40
22	B	611	CLA	C4C-C3C	3.23	1.50	1.45
36	e	101	HEM	C4D-ND	3.24	1.40	1.36
22	C	507	CLA	C1B-CHB	3.24	1.48	1.40
22	b	614	CLA	C1B-CHB	3.24	1.48	1.40
27	D	410	LHG	O8-C23	3.24	1.42	1.33
22	B	606	CLA	C1C-C2C	3.24	1.50	1.44
22	B	616	CLA	OBD-CAD	3.24	1.27	1.22
22	b	603	CLA	OBD-CAD	3.24	1.27	1.22
22	B	604	CLA	OBD-CAD	3.26	1.27	1.22
22	b	603	CLA	C3D-C2D	3.26	1.46	1.39
22	c	905	CLA	C1B-CHB	3.27	1.48	1.40
22	D	403	CLA	C4C-C3C	3.27	1.50	1.45
22	C	506	CLA	C4B-CHC	3.27	1.48	1.40
22	C	505	CLA	O2A-CGA	3.27	1.43	1.33
22	B	608	CLA	C1B-CHB	3.28	1.48	1.40
22	D	401	CLA	C4B-CHC	3.28	1.48	1.40
22	b	613	CLA	C4B-CHC	3.29	1.48	1.40
22	b	606	CLA	C3D-C2D	3.29	1.47	1.39
23	a	410	PHO	C3D-C2D	3.29	1.47	1.38
22	B	608	CLA	C3D-C2D	3.30	1.47	1.39
22	c	909	CLA	C3D-C2D	3.30	1.47	1.39
22	B	606	CLA	C1B-CHB	3.31	1.48	1.40
22	B	611	CLA	C4B-CHC	3.31	1.48	1.40
22	c	909	CLA	C1B-CHB	3.31	1.48	1.40
22	b	615	CLA	C4C-C3C	3.32	1.50	1.45
22	b	611	CLA	C4C-C3C	3.32	1.50	1.45
22	d	403	CLA	C4B-CHC	3.32	1.49	1.40
22	C	511	CLA	C1B-CHB	3.33	1.49	1.40
22	b	609	CLA	C3D-C2D	3.33	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	611	CLA	C1B-CHB	3.33	1.49	1.40
22	B	616	CLA	C1B-CHB	3.34	1.49	1.40
22	C	508	CLA	C3D-C2D	3.34	1.47	1.39
23	a	410	PHO	CHD-C1D	3.34	1.45	1.38
22	D	404	CLA	C1B-CHB	3.34	1.49	1.40
22	B	602	CLA	C1B-CHB	3.34	1.49	1.40
22	b	608	CLA	O2A-CGA	3.35	1.43	1.33
22	c	912	CLA	C3D-C2D	3.35	1.47	1.39
26	A	411	PL9	C7-C3	3.36	1.54	1.51
22	c	910	CLA	C4C-C3C	3.36	1.51	1.45
22	B	612	CLA	C3D-C2D	3.37	1.47	1.39
22	b	615	CLA	OBD-CAD	3.37	1.27	1.22
22	c	912	CLA	O2A-CGA	3.37	1.43	1.33
22	b	603	CLA	C1B-CHB	3.38	1.49	1.40
22	c	912	CLA	C1B-CHB	3.38	1.49	1.40
22	C	508	CLA	C4B-CHC	3.38	1.49	1.40
22	B	613	CLA	C3D-C2D	3.38	1.47	1.39
35	C	517	DGD	O1G-C1A	3.39	1.43	1.33
22	C	508	CLA	O2A-CGA	3.39	1.43	1.33
25	b	622	LMG	O1-C1	3.39	1.46	1.40
22	b	616	CLA	C3D-C2D	3.40	1.47	1.39
22	C	513	CLA	C3D-C2D	3.41	1.47	1.39
22	B	606	CLA	C4B-CHC	3.41	1.49	1.40
23	a	411	PHO	CHC-C4B	3.41	1.48	1.40
22	C	505	CLA	C3D-C2D	3.42	1.47	1.39
22	a	407	CLA	C1B-CHB	3.43	1.49	1.40
22	b	611	CLA	OBD-CAD	3.43	1.27	1.22
27	d	408	LHG	O7-C7	3.44	1.44	1.34
22	B	611	CLA	C1B-CHB	3.44	1.49	1.40
22	c	906	CLA	C4B-CHC	3.45	1.49	1.40
22	c	912	CLA	C4B-CHC	3.45	1.49	1.40
22	C	512	CLA	C1B-CHB	3.46	1.49	1.40
22	B	606	CLA	O2A-CGA	3.46	1.43	1.33
22	b	602	CLA	C4B-CHC	3.46	1.49	1.40
22	D	403	CLA	CHB-C4A	3.46	1.38	1.33
22	c	905	CLA	O2A-CGA	3.47	1.43	1.33
22	b	615	CLA	C1B-CHB	3.47	1.49	1.40
22	c	909	CLA	C4B-CHC	3.47	1.49	1.40
22	B	605	CLA	O2A-CGA	3.48	1.43	1.33
22	C	507	CLA	C3D-C2D	3.48	1.47	1.39
22	b	611	CLA	C3D-C2D	3.48	1.47	1.39
22	B	611	CLA	O2A-CGA	3.48	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	918	DGD	O2G-C1B	3.48	1.44	1.34
22	C	506	CLA	C3D-C2D	3.49	1.47	1.39
22	b	607	CLA	O2A-CGA	3.50	1.43	1.33
22	a	408	CLA	C3D-C2D	3.50	1.47	1.39
22	B	604	CLA	C1B-CHB	3.50	1.49	1.40
22	c	903	CLA	O2A-CGA	3.50	1.43	1.33
22	b	612	CLA	OBD-CAD	3.50	1.27	1.22
22	A	406	CLA	O2A-CGA	3.50	1.43	1.33
22	b	605	CLA	O2A-CGA	3.51	1.43	1.33
23	D	402	PHO	CHD-C1D	3.51	1.45	1.38
22	C	513	CLA	C1B-CHB	3.51	1.49	1.40
23	D	402	PHO	OBD-CAD	3.51	1.28	1.22
22	C	505	CLA	C1B-CHB	3.52	1.49	1.40
22	B	615	CLA	C3D-C2D	3.53	1.47	1.39
22	c	906	CLA	OBD-CAD	3.53	1.27	1.22
22	C	511	CLA	C3D-C2D	3.53	1.47	1.39
22	c	910	CLA	CHC-C1C	3.54	1.45	1.35
22	D	403	CLA	O2D-CGD	3.54	1.42	1.33
22	A	408	CLA	O2A-CGA	3.55	1.43	1.33
22	d	403	CLA	C4C-C3C	3.55	1.51	1.45
23	a	410	PHO	O2A-CGA	3.56	1.43	1.33
22	C	514	CLA	OBD-CAD	3.56	1.27	1.22
22	a	407	CLA	O2A-CGA	3.56	1.43	1.33
22	b	604	CLA	C3B-C2B	3.57	1.45	1.40
22	B	613	CLA	C4B-CHC	3.57	1.49	1.40
22	a	409	CLA	OBD-CAD	3.58	1.27	1.22
22	B	602	CLA	C3D-C2D	3.58	1.47	1.39
22	c	902	CLA	O2A-CGA	3.58	1.43	1.33
22	C	502	CLA	OBD-CAD	3.58	1.27	1.22
22	b	610	CLA	C1B-CHB	3.59	1.49	1.40
22	b	612	CLA	C3D-C2D	3.59	1.47	1.39
22	a	407	CLA	C3D-C2D	3.60	1.47	1.39
22	C	511	CLA	O2A-CGA	3.60	1.43	1.33
22	c	911	CLA	C4B-CHC	3.60	1.49	1.40
22	b	611	CLA	O2A-CGA	3.60	1.43	1.33
22	c	911	CLA	O2A-CGA	3.60	1.43	1.33
22	b	612	CLA	C3B-C2B	3.61	1.45	1.40
35	c	919	DGD	O2G-C1B	3.62	1.44	1.34
22	B	613	CLA	O2A-CGA	3.62	1.44	1.33
22	a	409	CLA	C3C-C2C	3.62	1.44	1.36
22	B	614	CLA	C3D-C2D	3.62	1.47	1.39
23	a	411	PHO	O2A-CGA	3.62	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	C4C-C3C	3.62	1.51	1.45
22	C	509	CLA	OBD-CAD	3.63	1.27	1.22
22	D	404	CLA	C3D-C2D	3.63	1.47	1.39
27	D	411	LHG	O8-C23	3.64	1.44	1.33
22	C	514	CLA	C3D-C2D	3.64	1.47	1.39
22	B	616	CLA	C3D-C2D	3.64	1.47	1.39
22	b	614	CLA	OBD-CAD	3.64	1.27	1.22
22	A	405	CLA	C3D-C2D	3.64	1.47	1.39
36	e	101	HEM	C3C-CAC	3.64	1.55	1.47
22	C	512	CLA	C3D-C2D	3.65	1.47	1.39
35	c	917	DGD	O1G-C1A	3.65	1.44	1.33
22	b	609	CLA	O2D-CGD	3.66	1.42	1.33
25	j	101	LMG	O7-C10	3.66	1.44	1.34
22	b	614	CLA	O2A-CGA	3.66	1.44	1.33
22	C	514	CLA	C1B-CHB	3.66	1.49	1.40
22	c	914	CLA	C3D-C2D	3.67	1.47	1.39
22	c	908	CLA	C4B-CHC	3.67	1.49	1.40
23	A	407	PHO	CHD-C4C	3.67	1.49	1.40
22	B	606	CLA	O2D-CGD	3.69	1.42	1.33
22	D	401	CLA	C3D-C2D	3.69	1.47	1.39
22	b	605	CLA	C3D-C2D	3.70	1.47	1.39
22	c	914	CLA	C1B-CHB	3.70	1.50	1.40
22	b	616	CLA	C1B-CHB	3.70	1.50	1.40
22	b	617	CLA	C3D-C2D	3.71	1.47	1.39
22	b	604	CLA	C3D-C2D	3.71	1.47	1.39
22	B	612	CLA	O2A-CGA	3.72	1.44	1.33
22	B	615	CLA	C1B-CHB	3.72	1.50	1.40
22	A	406	CLA	C3B-C2B	3.72	1.45	1.40
23	a	411	PHO	OBD-CAD	3.73	1.29	1.22
22	C	507	CLA	OBD-CAD	3.73	1.27	1.22
22	B	602	CLA	C4C-C3C	3.73	1.51	1.45
27	D	409	LHG	O7-C7	3.73	1.45	1.34
22	c	908	CLA	C1B-CHB	3.74	1.50	1.40
22	a	412	CLA	OBD-CAD	3.74	1.27	1.22
27	L	101	LHG	O7-C7	3.75	1.45	1.34
31	b	629	DMS	O-S	3.75	1.75	1.50
22	b	605	CLA	C3B-C2B	3.75	1.45	1.40
22	c	906	CLA	C3D-C2D	3.76	1.48	1.39
22	B	613	CLA	OBD-CAD	3.76	1.27	1.22
22	B	611	CLA	OBD-CAD	3.76	1.27	1.22
22	C	503	CLA	O2A-CGA	3.76	1.44	1.33
22	d	402	CLA	OBD-CAD	3.76	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	423	LHG	O7-C7	3.76	1.45	1.34
22	B	614	CLA	O2D-CGD	3.76	1.42	1.33
22	C	509	CLA	O2A-CGA	3.77	1.44	1.33
22	b	610	CLA	C3D-C2D	3.77	1.48	1.39
35	c	917	DGD	O2G-C1B	3.77	1.45	1.34
22	c	909	CLA	O2A-CGA	3.78	1.44	1.33
22	B	616	CLA	O2A-CGA	3.78	1.44	1.33
27	D	411	LHG	O7-C7	3.78	1.45	1.34
22	B	603	CLA	O2D-CGD	3.79	1.42	1.33
22	C	504	CLA	C4B-CHC	3.81	1.50	1.40
22	B	605	CLA	C3B-C2B	3.81	1.45	1.40
22	B	603	CLA	O2A-CGA	3.81	1.44	1.33
28	A	413	SQD	O47-C7	3.81	1.45	1.34
22	c	905	CLA	C3B-C2B	3.81	1.45	1.40
22	c	913	CLA	C3D-C2D	3.82	1.48	1.39
22	a	407	CLA	OBD-CAD	3.83	1.27	1.22
28	C	501	SQD	O48-C23	3.83	1.44	1.33
22	b	608	CLA	OBD-CAD	3.83	1.27	1.22
22	b	612	CLA	C1B-CHB	3.84	1.50	1.40
22	D	404	CLA	O2A-CGA	3.84	1.44	1.33
22	B	610	CLA	C3D-C2D	3.85	1.48	1.39
22	a	409	CLA	O2A-CGA	3.86	1.44	1.33
22	C	502	CLA	C3D-C2D	3.86	1.48	1.39
22	a	408	CLA	O2A-CGA	3.86	1.44	1.33
27	l	102	LHG	O8-C23	3.87	1.44	1.33
25	J	101	LMG	O7-C10	3.88	1.45	1.34
35	c	918	DGD	O1G-C1A	3.88	1.44	1.33
27	L	101	LHG	O8-C23	3.89	1.44	1.33
22	B	614	CLA	O2A-CGA	3.89	1.44	1.33
35	H	102	DGD	O2G-C1B	3.89	1.45	1.34
22	c	908	CLA	C3D-C2D	3.90	1.48	1.39
22	b	602	CLA	C1B-CHB	3.90	1.50	1.40
22	C	502	CLA	O2A-CGA	3.90	1.44	1.33
22	C	511	CLA	CHC-C1C	3.90	1.46	1.35
25	J	101	LMG	O8-C28	3.91	1.44	1.33
22	B	609	CLA	C3D-C2D	3.92	1.48	1.39
22	b	613	CLA	C3D-C2D	3.92	1.48	1.39
22	b	605	CLA	CHC-C1C	3.92	1.46	1.35
22	B	605	CLA	O2D-CGD	3.94	1.43	1.33
22	c	910	CLA	C3D-C2D	3.94	1.48	1.39
22	C	513	CLA	O2A-CGA	3.95	1.44	1.33
22	C	503	CLA	C3D-C2D	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	903	CLA	C3D-C2D	3.95	1.48	1.39
31	D	418	DMS	O-S	3.95	1.77	1.50
22	c	914	CLA	OBD-CAD	3.96	1.28	1.22
31	C	525	DMS	O-S	3.96	1.77	1.50
22	a	408	CLA	O2D-CGD	3.96	1.43	1.33
36	e	101	HEM	C3B-CAB	3.96	1.55	1.47
25	A	410	LMG	O7-C10	3.96	1.45	1.34
22	a	412	CLA	O2A-CGA	3.97	1.45	1.33
22	C	502	CLA	O2D-CGD	3.97	1.43	1.33
22	B	617	CLA	CHC-C1C	3.97	1.46	1.35
31	A	418	DMS	O-S	3.97	1.77	1.50
22	b	604	CLA	CHC-C1C	3.97	1.46	1.35
22	b	612	CLA	CHC-C1C	3.98	1.46	1.35
22	c	902	CLA	O2D-CGD	3.98	1.43	1.33
31	a	402	DMS	O-S	3.99	1.77	1.50
36	E	102	HEM	C3B-CAB	3.99	1.55	1.47
22	b	616	CLA	O2A-CGA	3.99	1.45	1.33
35	C	519	DGD	O1G-C1A	4.00	1.45	1.33
22	b	606	CLA	O2A-CGA	4.00	1.45	1.33
25	d	409	LMG	O7-C10	4.00	1.45	1.34
22	C	508	CLA	OBD-CAD	4.01	1.28	1.22
22	C	506	CLA	O2A-CGA	4.01	1.45	1.33
22	c	907	CLA	CHC-C1C	4.01	1.47	1.35
22	B	605	CLA	CHC-C1C	4.01	1.47	1.35
22	a	409	CLA	CHC-C1C	4.03	1.47	1.35
22	d	402	CLA	O2D-CGD	4.03	1.43	1.33
22	b	608	CLA	CHC-C1C	4.04	1.47	1.35
25	c	920	LMG	O7-C10	4.05	1.46	1.34
22	B	608	CLA	C3C-C2C	4.05	1.45	1.36
22	B	610	CLA	O2A-CGA	4.06	1.45	1.33
22	B	608	CLA	CHC-C1C	4.06	1.47	1.35
22	C	514	CLA	C4B-CHC	4.07	1.50	1.40
22	b	612	CLA	O2A-CGA	4.07	1.45	1.33
27	l	102	LHG	O7-C7	4.07	1.46	1.34
22	A	406	CLA	CHC-C1C	4.07	1.47	1.35
22	b	615	CLA	CHC-C1C	4.07	1.47	1.35
22	B	617	CLA	O2D-CGD	4.07	1.43	1.33
28	A	413	SQD	O48-C23	4.07	1.45	1.33
22	C	504	CLA	C3D-C2D	4.07	1.48	1.39
22	b	609	CLA	O2A-CGA	4.08	1.45	1.33
22	D	403	CLA	O2A-CGA	4.09	1.45	1.33
22	B	604	CLA	CHC-C1C	4.09	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	408	CLA	CHC-C1C	4.09	1.47	1.35
23	A	407	PHO	O2A-CGA	4.09	1.45	1.33
22	A	405	CLA	C3B-C2B	4.10	1.45	1.40
22	c	906	CLA	O2A-CGA	4.10	1.45	1.33
31	C	524	DMS	O-S	4.10	1.78	1.50
28	a	414	SQD	O47-C7	4.10	1.46	1.34
22	c	905	CLA	C3D-C2D	4.11	1.48	1.39
22	B	611	CLA	C3D-C2D	4.11	1.48	1.39
35	h	102	DGD	O2G-C1B	4.12	1.46	1.34
27	d	408	LHG	O8-C23	4.12	1.45	1.33
22	D	404	CLA	C4C-C3C	4.12	1.52	1.45
22	C	502	CLA	C3B-C2B	4.12	1.45	1.40
22	C	509	CLA	O2D-CGD	4.12	1.43	1.33
22	C	503	CLA	C3B-C2B	4.13	1.45	1.40
22	b	617	CLA	O2A-CGA	4.13	1.45	1.33
22	c	907	CLA	O2A-CGA	4.13	1.45	1.33
25	i	101	LMG	O7-C10	4.13	1.46	1.34
22	B	602	CLA	OBD-CAD	4.14	1.28	1.22
27	d	401	LHG	O7-C7	4.14	1.46	1.34
22	C	512	CLA	CHC-C1C	4.14	1.47	1.35
22	C	508	CLA	O2D-CGD	4.15	1.43	1.33
22	C	503	CLA	OBD-CAD	4.15	1.28	1.22
22	B	604	CLA	O2A-CGA	4.15	1.45	1.33
22	B	607	CLA	C4B-CHC	4.15	1.51	1.40
22	B	617	CLA	C3D-C2D	4.16	1.48	1.39
22	c	912	CLA	OBD-CAD	4.16	1.28	1.22
22	b	617	CLA	OBD-CAD	4.16	1.28	1.22
22	B	603	CLA	OBD-CAD	4.17	1.28	1.22
22	B	617	CLA	O2A-CGA	4.18	1.45	1.33
22	C	513	CLA	OBD-CAD	4.18	1.28	1.22
31	D	416	DMS	O-S	4.19	1.78	1.50
22	B	612	CLA	CHC-C1C	4.19	1.47	1.35
31	c	923	DMS	O-S	4.20	1.78	1.50
31	O	309	DMS	O-S	4.20	1.78	1.50
23	a	411	PHO	CHD-C1D	4.20	1.46	1.38
22	b	615	CLA	C3D-C2D	4.20	1.49	1.39
22	a	409	CLA	O2D-CGD	4.20	1.43	1.33
22	B	609	CLA	O2A-CGA	4.21	1.45	1.33
22	A	405	CLA	CHC-C1C	4.22	1.47	1.35
31	d	412	DMS	O-S	4.22	1.78	1.50
36	E	102	HEM	C3C-CAC	4.22	1.56	1.47
23	a	410	PHO	O2D-CGD	4.23	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	631	DMS	O-S	4.23	1.78	1.50
22	b	612	CLA	C3C-C2C	4.23	1.45	1.36
22	C	511	CLA	C3C-C2C	4.23	1.45	1.36
22	b	616	CLA	CHC-C1C	4.23	1.47	1.35
22	C	507	CLA	O2A-CGA	4.24	1.45	1.33
22	c	908	CLA	O2D-CGD	4.24	1.44	1.33
22	A	405	CLA	O2D-CGD	4.24	1.44	1.33
22	B	613	CLA	CHC-C1C	4.25	1.47	1.35
22	c	911	CLA	O2D-CGD	4.25	1.44	1.33
22	c	904	CLA	O2A-CGA	4.25	1.45	1.33
31	d	413	DMS	O-S	4.25	1.79	1.50
31	v	201	DMS	O-S	4.25	1.79	1.50
22	D	401	CLA	O2D-CGD	4.26	1.44	1.33
23	D	402	PHO	O2A-CGA	4.26	1.45	1.33
22	c	904	CLA	O2D-CGD	4.26	1.44	1.33
22	b	610	CLA	O2A-CGA	4.26	1.45	1.33
22	c	910	CLA	C3C-C2C	4.28	1.45	1.36
22	B	607	CLA	O2A-CGA	4.28	1.45	1.33
31	B	629	DMS	O-S	4.28	1.79	1.50
22	B	611	CLA	O2D-CGD	4.28	1.44	1.33
22	b	603	CLA	O2A-CGA	4.28	1.45	1.33
35	h	102	DGD	O1G-C1A	4.29	1.46	1.33
31	B	636	DMS	O-S	4.29	1.79	1.50
22	b	613	CLA	O2A-CGA	4.29	1.46	1.33
22	C	503	CLA	O2D-CGD	4.30	1.44	1.33
31	O	304	DMS	O-S	4.30	1.79	1.50
25	b	622	LMG	O7-C10	4.30	1.46	1.34
22	c	908	CLA	O2A-CGA	4.30	1.46	1.33
28	C	501	SQD	O47-C7	4.30	1.46	1.34
22	B	610	CLA	O2D-CGD	4.30	1.44	1.33
35	C	518	DGD	O1G-C1A	4.30	1.46	1.33
22	C	510	CLA	CHC-C1C	4.30	1.47	1.35
31	u	202	DMS	O-S	4.30	1.79	1.50
23	a	411	PHO	O2D-CGD	4.31	1.44	1.33
31	c	941	DMS	O-S	4.31	1.79	1.50
22	C	509	CLA	C3D-C2D	4.31	1.49	1.39
31	d	415	DMS	O-S	4.31	1.79	1.50
31	V	208	DMS	O-S	4.32	1.79	1.50
27	C	522	LHG	O8-C23	4.32	1.46	1.33
22	c	903	CLA	O2D-CGD	4.32	1.44	1.33
31	V	201	DMS	O-S	4.32	1.79	1.50
22	c	913	CLA	OBD-CAD	4.32	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	C3D-C2D	4.32	1.49	1.39
22	c	906	CLA	O2D-CGD	4.32	1.44	1.33
31	B	640	DMS	O-S	4.33	1.79	1.50
22	C	504	CLA	O2D-CGD	4.33	1.44	1.33
22	c	902	CLA	OBD-CAD	4.33	1.28	1.22
23	A	407	PHO	O2D-CGD	4.33	1.44	1.33
25	c	930	LMG	O8-C28	4.33	1.46	1.33
22	B	610	CLA	C3B-C2B	4.33	1.46	1.40
22	b	602	CLA	C3D-C2D	4.34	1.49	1.39
22	b	607	CLA	CHC-C1C	4.34	1.48	1.35
22	d	403	CLA	O2D-CGD	4.34	1.44	1.33
31	o	305	DMS	O-S	4.34	1.79	1.50
22	D	403	CLA	C3C-C2C	4.34	1.46	1.36
22	B	606	CLA	C3C-C2C	4.34	1.46	1.36
22	c	905	CLA	CHC-C1C	4.34	1.48	1.35
22	b	606	CLA	O2D-CGD	4.34	1.44	1.33
22	b	614	CLA	C3B-C2B	4.35	1.46	1.40
22	C	506	CLA	O2D-CGD	4.35	1.44	1.33
28	a	418	SQD	O47-C7	4.35	1.46	1.34
31	o	307	DMS	O-S	4.36	1.79	1.50
28	l	101	SQD	O47-C7	4.36	1.46	1.34
25	A	410	LMG	O8-C28	4.36	1.46	1.33
22	C	514	CLA	O2A-CGA	4.36	1.46	1.33
31	V	205	DMS	O-S	4.36	1.79	1.50
31	v	208	DMS	O-S	4.37	1.79	1.50
22	c	907	CLA	OBD-CAD	4.37	1.28	1.22
27	a	423	LHG	O8-C23	4.37	1.46	1.33
25	C	531	LMG	O8-C28	4.37	1.46	1.33
31	c	926	DMS	O-S	4.38	1.79	1.50
31	O	313	DMS	O-S	4.38	1.79	1.50
31	v	205	DMS	O-S	4.38	1.79	1.50
31	C	528	DMS	O-S	4.38	1.79	1.50
25	d	409	LMG	O8-C28	4.38	1.46	1.33
31	C	526	DMS	O-S	4.38	1.79	1.50
22	c	903	CLA	CHC-C1C	4.38	1.48	1.35
31	O	312	DMS	O-S	4.38	1.80	1.50
22	b	605	CLA	O2D-CGD	4.38	1.44	1.33
31	v	209	DMS	O-S	4.38	1.80	1.50
22	c	913	CLA	O2A-CGA	4.38	1.46	1.33
31	i	106	DMS	O-S	4.38	1.80	1.50
31	o	306	DMS	O-S	4.38	1.80	1.50
22	B	609	CLA	O2D-CGD	4.39	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C3D-C2D	4.39	1.49	1.39
31	B	632	DMS	O-S	4.39	1.80	1.50
22	B	603	CLA	CHC-C1C	4.40	1.48	1.35
22	b	608	CLA	C3D-C2D	4.40	1.49	1.39
22	c	913	CLA	CHC-C1C	4.40	1.48	1.35
31	O	310	DMS	O-S	4.40	1.80	1.50
31	a	421	DMS	O-S	4.40	1.80	1.50
25	j	101	LMG	O8-C28	4.41	1.46	1.33
31	c	935	DMS	O-S	4.41	1.80	1.50
22	a	412	CLA	C3B-C2B	4.42	1.46	1.40
31	B	638	DMS	O-S	4.42	1.80	1.50
25	C	520	LMG	O7-C10	4.42	1.47	1.34
31	c	934	DMS	O-S	4.42	1.80	1.50
22	C	505	CLA	O2D-CGD	4.42	1.44	1.33
31	F	101	DMS	O-S	4.42	1.80	1.50
31	C	538	DMS	O-S	4.42	1.80	1.50
31	c	927	DMS	O-S	4.42	1.80	1.50
31	v	204	DMS	O-S	4.43	1.80	1.50
22	B	609	CLA	CHC-C1C	4.43	1.48	1.35
31	V	209	DMS	O-S	4.43	1.80	1.50
31	b	636	DMS	O-S	4.43	1.80	1.50
31	A	416	DMS	O-S	4.43	1.80	1.50
22	A	408	CLA	OBD-CAD	4.43	1.28	1.22
27	D	409	LHG	O8-C23	4.43	1.46	1.33
23	D	402	PHO	C3C-C2C	4.44	1.46	1.36
31	C	529	DMS	O-S	4.44	1.80	1.50
22	C	509	CLA	CHC-C1C	4.44	1.48	1.35
35	c	919	DGD	O1G-C1A	4.44	1.46	1.33
31	B	642	DMS	O-S	4.44	1.80	1.50
28	b	621	SQD	O48-C23	4.44	1.46	1.33
31	b	633	DMS	O-S	4.44	1.80	1.50
22	c	911	CLA	CHC-C1C	4.44	1.48	1.35
35	H	102	DGD	O1G-C1A	4.45	1.46	1.33
28	l	101	SQD	O48-C23	4.45	1.46	1.33
31	A	417	DMS	O-S	4.45	1.80	1.50
22	C	504	CLA	O2A-CGA	4.45	1.46	1.33
22	B	606	CLA	CHC-C1C	4.45	1.48	1.35
22	B	608	CLA	C3B-C2B	4.45	1.46	1.40
31	I	106	DMS	O-S	4.46	1.80	1.50
31	C	530	DMS	O-S	4.46	1.80	1.50
31	C	527	DMS	O-S	4.47	1.80	1.50
31	v	206	DMS	O-S	4.47	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	539	DMS	O-S	4.47	1.80	1.50
31	c	925	DMS	O-S	4.47	1.80	1.50
22	B	607	CLA	CHC-C1C	4.47	1.48	1.35
31	c	936	DMS	O-S	4.47	1.80	1.50
25	B	621	LMG	O7-C10	4.47	1.47	1.34
31	d	414	DMS	O-S	4.47	1.80	1.50
31	b	631	DMS	O-S	4.47	1.80	1.50
22	c	913	CLA	O2D-CGD	4.48	1.44	1.33
22	c	904	CLA	CHC-C1C	4.48	1.48	1.35
22	D	404	CLA	O2D-CGD	4.48	1.44	1.33
31	C	534	DMS	O-S	4.48	1.80	1.50
31	o	303	DMS	O-S	4.48	1.80	1.50
31	A	420	DMS	O-S	4.48	1.80	1.50
31	v	207	DMS	O-S	4.49	1.80	1.50
31	c	943	DMS	O-S	4.49	1.80	1.50
22	c	914	CLA	CHC-C1C	4.49	1.48	1.35
22	c	911	CLA	C3D-C2D	4.49	1.49	1.39
22	c	911	CLA	C3B-C2B	4.49	1.46	1.40
31	o	302	DMS	O-S	4.50	1.80	1.50
31	l	103	DMS	O-S	4.50	1.80	1.50
31	t	105	DMS	O-S	4.50	1.80	1.50
22	B	608	CLA	O2D-CGD	4.50	1.44	1.33
31	B	633	DMS	O-S	4.50	1.80	1.50
22	a	408	CLA	CHC-C1C	4.50	1.48	1.35
22	c	914	CLA	O2A-CGA	4.50	1.46	1.33
36	V	202	HEM	C3D-C2D	4.50	1.51	1.37
22	b	607	CLA	O2D-CGD	4.50	1.44	1.33
31	t	103	DMS	O-S	4.50	1.80	1.50
31	c	944	DMS	O-S	4.50	1.80	1.50
31	c	928	DMS	O-S	4.50	1.80	1.50
22	a	407	CLA	C3C-C2C	4.51	1.46	1.36
31	A	419	DMS	O-S	4.51	1.80	1.50
22	C	505	CLA	CHC-C1C	4.51	1.48	1.35
22	B	605	CLA	C3C-C2C	4.51	1.46	1.36
23	a	410	PHO	CHC-C1C	4.51	1.47	1.38
31	t	104	DMS	O-S	4.51	1.80	1.50
31	b	630	DMS	O-S	4.51	1.80	1.50
28	a	418	SQD	O48-C23	4.51	1.46	1.33
22	B	607	CLA	O2D-CGD	4.51	1.44	1.33
31	f	103	DMS	O-S	4.51	1.80	1.50
22	b	610	CLA	C3B-C2B	4.51	1.46	1.40
31	C	536	DMS	O-S	4.51	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	C3B-C2B	4.51	1.46	1.40
27	A	412	LHG	O8-C23	4.51	1.46	1.33
31	O	306	DMS	O-S	4.51	1.80	1.50
31	d	411	DMS	O-S	4.52	1.80	1.50
31	V	204	DMS	O-S	4.52	1.80	1.50
31	U	202	DMS	O-S	4.52	1.80	1.50
22	c	911	CLA	C3C-C2C	4.52	1.46	1.36
31	u	203	DMS	O-S	4.52	1.80	1.50
31	b	634	DMS	O-S	4.52	1.80	1.50
31	c	940	DMS	O-S	4.52	1.80	1.50
31	b	637	DMS	O-S	4.53	1.81	1.50
22	d	402	CLA	O2A-CGA	4.53	1.46	1.33
31	a	424	DMS	O-S	4.53	1.81	1.50
22	C	502	CLA	CHC-C1C	4.53	1.48	1.35
31	L	102	DMS	O-S	4.53	1.81	1.50
22	C	507	CLA	CHC-C1C	4.53	1.48	1.35
31	c	942	DMS	O-S	4.53	1.81	1.50
31	O	314	DMS	O-S	4.53	1.81	1.50
22	c	910	CLA	O2A-CGA	4.54	1.46	1.33
31	l	105	DMS	O-S	4.54	1.81	1.50
22	b	602	CLA	OBD-CAD	4.54	1.28	1.22
31	C	535	DMS	O-S	4.54	1.81	1.50
31	a	401	DMS	O-S	4.54	1.81	1.50
22	a	407	CLA	CHC-C1C	4.54	1.48	1.35
22	d	402	CLA	CHC-C1C	4.54	1.48	1.35
31	C	533	DMS	O-S	4.55	1.81	1.50
27	C	522	LHG	O7-C7	4.55	1.47	1.34
31	B	639	DMS	O-S	4.55	1.81	1.50
22	b	613	CLA	C3C-C2C	4.55	1.46	1.36
31	I	101	DMS	O-S	4.56	1.81	1.50
31	V	207	DMS	O-S	4.56	1.81	1.50
22	b	612	CLA	O2D-CGD	4.56	1.44	1.33
31	C	537	DMS	O-S	4.56	1.81	1.50
22	C	506	CLA	OBD-CAD	4.56	1.28	1.22
22	C	504	CLA	OBD-CAD	4.56	1.28	1.22
22	C	508	CLA	CHC-C1C	4.57	1.48	1.35
22	b	609	CLA	CHC-C1C	4.57	1.48	1.35
31	V	206	DMS	O-S	4.58	1.81	1.50
22	B	610	CLA	C3C-C2C	4.58	1.46	1.36
31	D	417	DMS	O-S	4.58	1.81	1.50
31	U	203	DMS	O-S	4.58	1.81	1.50
27	a	416	LHG	O7-C7	4.58	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	CHC-C1C	4.58	1.48	1.35
31	O	303	DMS	O-S	4.59	1.81	1.50
36	v	202	HEM	C3B-CAB	4.59	1.57	1.47
22	b	615	CLA	O2A-CGA	4.59	1.46	1.33
22	b	614	CLA	CHC-C1C	4.59	1.48	1.35
36	V	202	HEM	C3B-CAB	4.59	1.57	1.47
22	a	412	CLA	CHC-C1C	4.59	1.48	1.35
31	c	938	DMS	O-S	4.59	1.81	1.50
28	a	414	SQD	O48-C23	4.59	1.46	1.33
23	a	410	PHO	C3C-C2C	4.60	1.46	1.36
22	B	614	CLA	C3C-C2C	4.60	1.46	1.36
31	l	104	DMS	O-S	4.60	1.81	1.50
27	d	401	LHG	O8-C23	4.60	1.46	1.33
31	v	211	DMS	O-S	4.61	1.81	1.50
31	u	204	DMS	O-S	4.61	1.81	1.50
31	C	540	DMS	O-S	4.61	1.81	1.50
31	b	635	DMS	O-S	4.61	1.81	1.50
22	B	606	CLA	C3B-C2B	4.61	1.46	1.40
25	c	930	LMG	O7-C10	4.62	1.47	1.34
22	b	617	CLA	O2D-CGD	4.62	1.44	1.33
31	V	210	DMS	O-S	4.62	1.81	1.50
31	V	212	DMS	O-S	4.62	1.81	1.50
31	c	939	DMS	O-S	4.62	1.81	1.50
22	C	512	CLA	OBD-CAD	4.62	1.29	1.22
31	B	641	DMS	O-S	4.62	1.81	1.50
31	O	307	DMS	O-S	4.62	1.81	1.50
25	C	531	LMG	O7-C10	4.62	1.47	1.34
31	O	308	DMS	O-S	4.63	1.81	1.50
25	c	920	LMG	O8-C28	4.63	1.47	1.33
31	B	637	DMS	O-S	4.64	1.81	1.50
22	C	507	CLA	C3C-C2C	4.64	1.46	1.36
31	o	308	DMS	O-S	4.64	1.81	1.50
22	c	909	CLA	CHC-C1C	4.65	1.48	1.35
22	C	510	CLA	C3B-C2B	4.65	1.46	1.40
25	i	101	LMG	O8-C28	4.65	1.47	1.33
22	b	613	CLA	CHC-C1C	4.65	1.48	1.35
22	B	616	CLA	CHC-C1C	4.65	1.48	1.35
22	b	609	CLA	OBD-CAD	4.65	1.29	1.22
22	A	408	CLA	C3B-C2B	4.65	1.46	1.40
22	a	408	CLA	OBD-CAD	4.65	1.29	1.22
25	D	412	LMG	O7-C10	4.65	1.47	1.34
22	d	403	CLA	CHC-C1C	4.66	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	635	DMS	O-S	4.66	1.81	1.50
22	b	610	CLA	CHC-C1C	4.67	1.49	1.35
22	B	602	CLA	CHC-C1C	4.67	1.49	1.35
22	C	513	CLA	CHC-C1C	4.67	1.49	1.35
31	c	929	DMS	O-S	4.67	1.82	1.50
31	V	211	DMS	O-S	4.68	1.82	1.50
31	B	634	DMS	O-S	4.68	1.82	1.50
22	D	404	CLA	CHC-C1C	4.68	1.49	1.35
35	D	407	DGD	O1G-C1A	4.68	1.47	1.33
22	C	510	CLA	O2A-CGA	4.69	1.47	1.33
25	C	520	LMG	O8-C28	4.69	1.47	1.33
22	b	603	CLA	CHC-C1C	4.70	1.49	1.35
23	A	407	PHO	C3C-C2C	4.70	1.46	1.36
22	C	512	CLA	O2A-CGA	4.71	1.47	1.33
22	c	908	CLA	OBD-CAD	4.72	1.29	1.22
22	C	511	CLA	O2D-CGD	4.72	1.45	1.33
22	b	608	CLA	C3B-C2B	4.72	1.46	1.40
22	b	610	CLA	C3C-C2C	4.72	1.46	1.36
31	o	304	DMS	O-S	4.72	1.82	1.50
22	B	613	CLA	O2D-CGD	4.73	1.45	1.33
22	b	610	CLA	O2D-CGD	4.73	1.45	1.33
22	C	514	CLA	CHC-C1C	4.73	1.49	1.35
31	B	630	DMS	O-S	4.74	1.82	1.50
22	c	903	CLA	C3C-C2C	4.74	1.46	1.36
22	b	606	CLA	CHC-C1C	4.74	1.49	1.35
22	C	514	CLA	O2D-CGD	4.74	1.45	1.33
35	d	406	DGD	O2G-C1B	4.74	1.48	1.34
22	A	408	CLA	O2D-CGD	4.75	1.45	1.33
31	c	924	DMS	O-S	4.75	1.82	1.50
31	v	210	DMS	O-S	4.76	1.82	1.50
22	b	617	CLA	CHC-C1C	4.76	1.49	1.35
22	d	402	CLA	C3C-C2C	4.76	1.46	1.36
31	c	933	DMS	O-S	4.76	1.82	1.50
23	A	407	PHO	CHC-C1C	4.76	1.48	1.38
25	B	621	LMG	O8-C28	4.77	1.47	1.33
22	b	616	CLA	O2D-CGD	4.77	1.45	1.33
22	b	614	CLA	O2D-CGD	4.78	1.45	1.33
22	B	608	CLA	OBD-CAD	4.78	1.29	1.22
31	B	628	DMS	O-S	4.78	1.82	1.50
22	B	613	CLA	C3C-C2C	4.79	1.47	1.36
22	B	614	CLA	OBD-CAD	4.79	1.29	1.22
22	b	611	CLA	O2D-CGD	4.80	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	911	CLA	OBD-CAD	4.80	1.29	1.22
31	c	937	DMS	O-S	4.80	1.82	1.50
35	d	406	DGD	O1G-C1A	4.80	1.47	1.33
31	O	305	DMS	O-S	4.80	1.82	1.50
22	b	611	CLA	CHC-C1C	4.80	1.49	1.35
22	B	615	CLA	O2D-CGD	4.80	1.45	1.33
22	c	904	CLA	C3B-C2B	4.80	1.46	1.40
22	b	605	CLA	C3C-C2C	4.81	1.47	1.36
31	H	103	DMS	O-S	4.81	1.82	1.50
22	B	611	CLA	CHC-C1C	4.82	1.49	1.35
22	B	612	CLA	OBD-CAD	4.82	1.29	1.22
22	c	906	CLA	CHC-C1C	4.83	1.49	1.35
22	c	909	CLA	OBD-CAD	4.83	1.29	1.22
22	b	613	CLA	OBD-CAD	4.83	1.29	1.22
22	c	902	CLA	CHC-C1C	4.84	1.49	1.35
22	B	604	CLA	O2D-CGD	4.84	1.45	1.33
22	b	609	CLA	C3B-C2B	4.85	1.46	1.40
22	b	613	CLA	O2D-CGD	4.85	1.45	1.33
25	D	412	LMG	O8-C28	4.85	1.47	1.33
22	a	408	CLA	C3C-C2C	4.85	1.47	1.36
22	C	506	CLA	C3B-C2B	4.86	1.46	1.40
22	c	912	CLA	CHC-C1C	4.86	1.49	1.35
22	b	610	CLA	OBD-CAD	4.86	1.29	1.22
22	C	509	CLA	C3B-C2B	4.87	1.46	1.40
22	b	607	CLA	C3B-C2B	4.87	1.46	1.40
35	D	407	DGD	O2G-C1B	4.88	1.48	1.34
22	A	406	CLA	O2D-CGD	4.88	1.45	1.33
22	B	602	CLA	O2A-CGA	4.88	1.47	1.33
22	B	616	CLA	C3C-C2C	4.89	1.47	1.36
22	C	507	CLA	O2D-CGD	4.90	1.45	1.33
22	c	914	CLA	C3C-C2C	4.90	1.47	1.36
22	B	615	CLA	CHC-C1C	4.92	1.49	1.35
22	D	404	CLA	C3B-C2B	4.92	1.46	1.40
22	B	612	CLA	O2D-CGD	4.92	1.45	1.33
22	b	602	CLA	CHC-C1C	4.93	1.49	1.35
22	a	407	CLA	C3B-C2B	4.93	1.46	1.40
25	b	622	LMG	O8-C28	4.93	1.47	1.33
22	C	510	CLA	OBD-CAD	4.93	1.29	1.22
22	B	615	CLA	C3B-C2B	4.93	1.46	1.40
22	C	512	CLA	O2D-CGD	4.94	1.45	1.33
22	B	615	CLA	OBD-CAD	4.94	1.29	1.22
22	c	912	CLA	C3C-C2C	4.96	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	410	PHO	C3B-C2B	4.96	1.46	1.37
22	B	602	CLA	C3C-C2C	4.96	1.47	1.36
22	A	406	CLA	OBD-CAD	4.97	1.29	1.22
22	b	607	CLA	C3C-C2C	4.98	1.47	1.36
22	b	614	CLA	C3C-C2C	4.98	1.47	1.36
27	a	416	LHG	O8-C23	4.98	1.48	1.33
22	b	616	CLA	OBD-CAD	4.98	1.29	1.22
22	C	506	CLA	CHC-C1C	4.99	1.49	1.35
22	c	910	CLA	O2D-CGD	5.00	1.45	1.33
22	b	615	CLA	O2D-CGD	5.00	1.45	1.33
22	c	907	CLA	O2D-CGD	5.03	1.46	1.33
22	C	502	CLA	C3C-C2C	5.03	1.47	1.36
31	b	638	DMS	O-S	5.03	1.84	1.50
31	O	311	DMS	O-S	5.04	1.84	1.50
22	B	604	CLA	C3B-C2B	5.04	1.47	1.40
22	d	403	CLA	C3C-C2C	5.04	1.47	1.36
22	b	608	CLA	O2D-CGD	5.05	1.46	1.33
22	c	908	CLA	CHC-C1C	5.05	1.50	1.35
31	a	425	DMS	O-S	5.05	1.84	1.50
22	C	507	CLA	C3B-C2B	5.05	1.47	1.40
22	c	907	CLA	C3C-C2C	5.06	1.47	1.36
22	b	604	CLA	O2D-CGD	5.06	1.46	1.33
22	C	510	CLA	O2D-CGD	5.07	1.46	1.33
22	c	902	CLA	C3C-C2C	5.07	1.47	1.36
22	c	906	CLA	C3C-C2C	5.08	1.47	1.36
22	B	604	CLA	C3C-C2C	5.08	1.47	1.36
22	a	409	CLA	C3B-C2B	5.08	1.47	1.40
36	V	202	HEM	C3C-CAC	5.10	1.57	1.47
22	B	613	CLA	C3B-C2B	5.10	1.47	1.40
22	B	607	CLA	C3C-C2C	5.10	1.47	1.36
22	B	602	CLA	O2D-CGD	5.11	1.46	1.33
22	a	407	CLA	O2D-CGD	5.11	1.46	1.33
23	A	407	PHO	CHD-C1D	5.11	1.48	1.38
22	b	615	CLA	C3B-C2B	5.12	1.47	1.40
22	B	614	CLA	CHC-C1C	5.12	1.50	1.35
22	C	504	CLA	CHC-C1C	5.13	1.50	1.35
22	b	606	CLA	C3C-C2C	5.13	1.47	1.36
31	u	205	DMS	O-S	5.13	1.85	1.50
22	B	610	CLA	CHC-C1C	5.13	1.50	1.35
22	B	616	CLA	C3B-C2B	5.15	1.47	1.40
22	B	615	CLA	C3C-C2C	5.15	1.47	1.36
36	v	202	HEM	C3C-CAC	5.16	1.58	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	412	LHG	O7-C7	5.16	1.47	1.35
22	b	611	CLA	C3C-C2C	5.16	1.47	1.36
22	a	412	CLA	O2D-CGD	5.16	1.46	1.33
23	a	411	PHO	CHC-C1C	5.17	1.48	1.38
22	B	614	CLA	C3B-C2B	5.17	1.47	1.40
22	C	510	CLA	C3C-C2C	5.17	1.47	1.36
22	C	513	CLA	O2D-CGD	5.18	1.46	1.33
22	A	405	CLA	OBD-CAD	5.18	1.29	1.22
22	c	904	CLA	OBD-CAD	5.18	1.29	1.22
22	d	403	CLA	O2A-CGA	5.19	1.48	1.33
22	D	401	CLA	C3C-C2C	5.20	1.47	1.36
22	b	603	CLA	O2D-CGD	5.20	1.46	1.33
22	c	912	CLA	O2D-CGD	5.20	1.46	1.33
22	D	404	CLA	OBD-CAD	5.21	1.29	1.22
22	A	405	CLA	C3C-C2C	5.21	1.47	1.36
22	B	612	CLA	C3B-C2B	5.22	1.47	1.40
22	C	508	CLA	C3C-C2C	5.22	1.47	1.36
22	b	611	CLA	C3B-C2B	5.22	1.47	1.40
22	b	603	CLA	C3B-C2B	5.23	1.47	1.40
22	C	504	CLA	C3C-C2C	5.25	1.48	1.36
22	c	902	CLA	C3B-C2B	5.26	1.47	1.40
22	c	914	CLA	O2D-CGD	5.26	1.46	1.33
22	D	404	CLA	C3C-C2C	5.26	1.48	1.36
22	B	609	CLA	C3B-C2B	5.27	1.47	1.40
22	C	512	CLA	C3B-C2B	5.27	1.47	1.40
22	C	506	CLA	C3C-C2C	5.28	1.48	1.36
22	B	617	CLA	C3C-C2C	5.29	1.48	1.36
22	c	903	CLA	C3B-C2B	5.30	1.47	1.40
22	C	512	CLA	C3C-C2C	5.33	1.48	1.36
22	c	909	CLA	O2D-CGD	5.33	1.46	1.33
22	b	613	CLA	C3B-C2B	5.34	1.47	1.40
22	c	914	CLA	C3B-C2B	5.34	1.47	1.40
22	c	909	CLA	C3B-C2B	5.35	1.47	1.40
36	v	202	HEM	C3D-C2D	5.35	1.53	1.37
22	B	605	CLA	OBD-CAD	5.36	1.30	1.22
22	B	612	CLA	C3C-C2C	5.38	1.48	1.36
22	C	505	CLA	C3C-C2C	5.39	1.48	1.36
36	E	102	HEM	C3D-C2D	5.40	1.53	1.37
22	C	509	CLA	C3C-C2C	5.40	1.48	1.36
22	c	905	CLA	O2D-CGD	5.40	1.46	1.33
22	b	602	CLA	O2D-CGD	5.40	1.46	1.33
23	a	411	PHO	CHB-C1B	5.41	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e	101	HEM	C3D-C2D	5.41	1.53	1.37
23	D	402	PHO	CHC-C1C	5.41	1.49	1.38
23	D	402	PHO	O2D-CGD	5.42	1.46	1.33
22	B	617	CLA	C3B-C2B	5.42	1.47	1.40
22	c	905	CLA	C3C-C2C	5.43	1.48	1.36
22	b	602	CLA	O2A-CGA	5.44	1.49	1.33
22	d	403	CLA	C3B-C2B	5.44	1.47	1.40
22	b	615	CLA	C3C-C2C	5.45	1.48	1.36
22	C	511	CLA	C3B-C2B	5.46	1.47	1.40
22	b	604	CLA	C3C-C2C	5.47	1.48	1.36
22	B	615	CLA	O2A-CGA	5.48	1.49	1.33
22	B	609	CLA	C3C-C2C	5.49	1.48	1.36
22	C	513	CLA	C3B-C2B	5.49	1.47	1.40
23	D	402	PHO	CHB-C1B	5.50	1.49	1.38
22	b	617	CLA	C3C-C2C	5.53	1.48	1.36
23	a	411	PHO	C3C-C2C	5.53	1.48	1.36
22	C	514	CLA	C3C-C2C	5.54	1.48	1.36
22	b	616	CLA	C3C-C2C	5.55	1.48	1.36
23	A	407	PHO	CHB-C1B	5.56	1.49	1.38
22	c	910	CLA	C3B-C2B	5.57	1.47	1.40
22	c	907	CLA	C3B-C2B	5.58	1.47	1.40
22	b	609	CLA	C3C-C2C	5.59	1.48	1.36
22	A	408	CLA	C3C-C2C	5.60	1.48	1.36
22	c	912	CLA	C3B-C2B	5.61	1.47	1.40
22	B	603	CLA	C3B-C2B	5.64	1.47	1.40
22	b	608	CLA	C3C-C2C	5.65	1.48	1.36
22	c	904	CLA	C3C-C2C	5.67	1.48	1.36
22	B	603	CLA	C3C-C2C	5.67	1.48	1.36
22	C	503	CLA	C3C-C2C	5.68	1.48	1.36
23	A	407	PHO	C3B-C2B	5.68	1.47	1.37
22	d	402	CLA	C3B-C2B	5.71	1.47	1.40
22	C	513	CLA	C3C-C2C	5.71	1.49	1.36
23	a	411	PHO	C3B-C2B	5.72	1.47	1.37
22	B	616	CLA	O2D-CGD	5.74	1.47	1.33
22	c	913	CLA	C3C-C2C	5.75	1.49	1.36
22	D	401	CLA	OBD-CAD	5.75	1.30	1.22
22	B	611	CLA	C3C-C2C	5.78	1.49	1.36
22	c	908	CLA	C3C-C2C	5.80	1.49	1.36
22	c	906	CLA	C3B-C2B	5.82	1.48	1.40
22	b	602	CLA	C3C-C2C	5.82	1.49	1.36
22	C	505	CLA	C3B-C2B	5.84	1.48	1.40
22	b	603	CLA	C3C-C2C	5.89	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	408	CLA	C3B-C2B	5.91	1.48	1.40
22	B	602	CLA	C3B-C2B	5.93	1.48	1.40
22	c	909	CLA	C3C-C2C	5.96	1.49	1.36
22	c	910	CLA	OBD-CAD	5.98	1.31	1.22
23	a	410	PHO	CHB-C1B	5.98	1.50	1.38
22	C	504	CLA	C3B-C2B	6.02	1.48	1.40
22	a	412	CLA	C3C-C2C	6.03	1.49	1.36
22	c	913	CLA	C3B-C2B	6.26	1.48	1.40
22	d	403	CLA	OBD-CAD	6.28	1.31	1.22
23	D	402	PHO	C3B-C2B	6.36	1.49	1.37
22	b	602	CLA	C3B-C2B	6.37	1.48	1.40
22	B	607	CLA	C3B-C2B	6.45	1.48	1.40
22	C	508	CLA	C3B-C2B	6.46	1.48	1.40
22	C	514	CLA	C3B-C2B	6.47	1.48	1.40
22	C	511	CLA	OBD-CAD	6.60	1.31	1.22
22	b	616	CLA	C3B-C2B	6.63	1.49	1.40
22	b	617	CLA	C3B-C2B	6.65	1.49	1.40
22	c	908	CLA	C3B-C2B	7.09	1.49	1.40

All (1885) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	V	203	HTG	O5-C1-C2	-8.24	98.98	110.28
36	E	102	HEM	CBD-CAD-C3D	-7.63	97.91	112.47
22	b	606	CLA	CHD-C4C-C3C	-7.41	113.75	124.92
34	v	203	HTG	O5-C1-C2	-7.08	100.58	110.28
23	a	411	PHO	C1-C2-C3	-6.80	113.43	125.96
22	C	502	CLA	O2D-CGD-O1D	-6.76	110.22	123.82
22	D	403	CLA	C1C-C2C-C3C	-6.26	99.97	106.92
22	b	613	CLA	CHD-C4C-C3C	-6.25	115.50	124.92
22	B	615	CLA	CHD-C4C-C3C	-6.21	115.56	124.92
24	D	405	BCR	C24-C23-C22	-6.16	116.96	126.21
22	B	610	CLA	CHD-C4C-C3C	-6.15	115.65	124.92
22	b	607	CLA	CHD-C4C-C3C	-6.14	115.66	124.92
36	e	101	HEM	CBD-CAD-C3D	-6.13	100.77	112.47
34	D	415	HTG	O5-C1-C2	-6.12	101.88	110.28
22	a	409	CLA	C1C-C2C-C3C	-6.06	100.19	106.92
22	a	408	CLA	CHD-C4C-C3C	-6.05	115.81	124.92
22	D	401	CLA	C1C-C2C-C3C	-6.01	100.25	106.92
22	B	617	CLA	CHD-C4C-C3C	-6.01	115.86	124.92
22	D	403	CLA	C1C-NC-C4C	-5.99	103.61	107.06
22	A	406	CLA	C1C-C2C-C3C	-5.88	100.39	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	O2D-CGD-O1D	-5.86	112.03	123.82
28	A	413	SQD	C5-C6-S	-5.82	106.22	114.34
22	b	612	CLA	CHD-C4C-C3C	-5.82	116.15	124.92
22	A	406	CLA	C1C-NC-C4C	-5.74	103.75	107.06
23	D	402	PHO	C4C-C3C-C2C	-5.72	100.39	106.81
22	b	604	CLA	CHD-C4C-C3C	-5.64	116.41	124.92
22	D	401	CLA	CHD-C4C-C3C	-5.64	116.41	124.92
22	B	607	CLA	CHD-C4C-C3C	-5.63	116.44	124.92
22	b	607	CLA	O2D-CGD-O1D	-5.51	112.74	123.82
22	b	617	CLA	CHD-C4C-C3C	-5.46	116.69	124.92
22	B	609	CLA	CHD-C4C-C3C	-5.41	116.76	124.92
22	B	606	CLA	CHD-C4C-C3C	-5.34	116.86	124.92
24	D	405	BCR	C7-C8-C9	-5.33	118.21	126.21
22	c	914	CLA	CHD-C4C-C3C	-5.33	116.89	124.92
22	b	610	CLA	C1C-C2C-C3C	-5.19	101.16	106.92
22	c	903	CLA	CHD-C4C-C3C	-5.18	117.11	124.92
22	b	611	CLA	CHD-C4C-C3C	-5.17	117.13	124.92
24	d	404	BCR	C7-C8-C9	-5.15	118.47	126.21
22	B	616	CLA	CHD-C4C-C3C	-5.15	117.16	124.92
22	a	412	CLA	C1C-C2C-C3C	-5.14	101.22	106.92
28	a	418	SQD	C1-O5-C5	-5.13	104.05	113.72
22	c	902	CLA	CHD-C4C-C3C	-5.08	117.26	124.92
22	b	604	CLA	C1C-NC-C4C	-5.07	104.14	107.06
22	C	514	CLA	CHD-C4C-C3C	-5.03	117.34	124.92
22	c	903	CLA	C1-C2-C3	-4.99	116.77	125.96
22	C	504	CLA	CHD-C4C-C3C	-4.96	117.44	124.92
24	b	618	BCR	C28-C27-C26	-4.96	105.25	113.78
22	c	911	CLA	CHD-C4C-C3C	-4.96	117.45	124.92
28	a	418	SQD	C5-C6-S	-4.96	107.43	114.34
22	a	408	CLA	C1C-C2C-C3C	-4.95	101.42	106.92
28	C	501	SQD	C1-C2-C3	-4.92	100.83	109.98
22	c	908	CLA	CHD-C4C-C3C	-4.92	117.51	124.92
22	C	510	CLA	C1C-C2C-C3C	-4.92	101.47	106.92
22	B	605	CLA	C1C-C2C-C3C	-4.90	101.48	106.92
22	B	603	CLA	CHD-C4C-C3C	-4.90	117.54	124.92
22	D	403	CLA	C1-C2-C3	-4.89	116.95	125.96
22	B	617	CLA	O2D-CGD-O1D	-4.88	114.00	123.82
22	c	903	CLA	O2D-CGD-O1D	-4.86	114.04	123.82
22	B	611	CLA	CHD-C4C-C3C	-4.86	117.60	124.92
22	c	902	CLA	C1C-C2C-C3C	-4.85	101.53	106.92
23	D	402	PHO	C1-C2-C3	-4.85	117.02	125.96
22	A	406	CLA	CHD-C4C-C3C	-4.84	117.62	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	CHD-C4C-C3C	-4.83	117.63	124.92
22	C	513	CLA	CHD-C4C-C3C	-4.83	117.64	124.92
36	V	202	HEM	CBD-CAD-C3D	-4.81	103.28	112.47
22	c	913	CLA	C1-C2-C3	-4.81	117.10	125.96
28	a	414	SQD	C1-C2-C3	-4.78	101.10	109.98
24	C	515	BCR	C33-C5-C6	-4.76	119.17	124.51
22	C	503	CLA	O2D-CGD-O1D	-4.76	114.24	123.82
23	a	410	PHO	C4C-C3C-C2C	-4.76	101.46	106.81
23	a	411	PHO	O2D-CGD-O1D	-4.72	114.32	123.82
22	C	507	CLA	CHD-C4C-C3C	-4.70	117.83	124.92
22	B	611	CLA	O2D-CGD-O1D	-4.69	114.38	123.82
22	C	508	CLA	CHD-C4C-C3C	-4.69	117.85	124.92
23	D	402	PHO	C3D-C2D-C1D	-4.67	98.89	105.82
22	B	602	CLA	O1D-CGD-CBD	-4.66	116.23	124.60
22	B	609	CLA	C1C-NC-C4C	-4.65	104.38	107.06
22	A	405	CLA	C1C-C2C-C3C	-4.64	101.78	106.92
28	C	501	SQD	C1-O5-C5	-4.62	105.01	113.72
22	a	409	CLA	C1C-NC-C4C	-4.61	104.40	107.06
22	c	908	CLA	O2D-CGD-O1D	-4.60	114.57	123.82
22	b	607	CLA	C1-C2-C3	-4.59	117.50	125.96
22	b	610	CLA	CHD-C4C-C3C	-4.59	118.00	124.92
22	b	604	CLA	C1C-C2C-C3C	-4.59	101.83	106.92
24	Y	101	BCR	C38-C26-C25	-4.57	119.39	124.51
22	C	512	CLA	CHD-C4C-C3C	-4.57	118.03	124.92
24	y	101	BCR	C33-C5-C6	-4.57	119.39	124.51
24	d	404	BCR	C38-C26-C25	-4.55	119.41	124.51
22	B	612	CLA	CHD-C4C-C3C	-4.55	118.06	124.92
22	a	409	CLA	CHD-C4C-C3C	-4.55	118.06	124.92
23	a	410	PHO	C3D-C2D-C1D	-4.52	99.12	105.82
23	a	411	PHO	C3D-C2D-C1D	-4.49	99.16	105.82
34	v	203	HTG	C1-C2-C3	-4.49	101.08	110.69
23	A	407	PHO	C3D-C2D-C1D	-4.46	99.21	105.82
22	C	502	CLA	CHD-C4C-C3C	-4.45	118.22	124.92
22	b	614	CLA	CHD-C4C-C3C	-4.43	118.24	124.92
22	B	607	CLA	C1C-C2C-C3C	-4.42	102.01	106.92
22	C	505	CLA	C1C-C2C-C3C	-4.42	102.02	106.92
35	H	102	DGD	O1G-C1A-O1A	-4.41	112.61	123.55
22	A	408	CLA	C1C-C2C-C3C	-4.41	102.03	106.92
22	C	503	CLA	CHD-C4C-C3C	-4.39	118.30	124.92
24	c	916	BCR	C15-C14-C13	-4.39	121.04	127.31
22	C	510	CLA	C1C-NC-C4C	-4.39	104.53	107.06
28	a	414	SQD	C5-C6-S	-4.39	108.22	114.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	C1C-C2C-C3C	-4.37	102.07	106.92
22	C	511	CLA	C1C-C2C-C3C	-4.37	102.08	106.92
23	A	407	PHO	C1C-C2C-C3C	-4.35	101.47	106.51
35	C	517	DGD	O3G-C3G-C2G	-4.32	100.71	110.99
22	d	403	CLA	C1C-C2C-C3C	-4.32	102.13	106.92
23	a	411	PHO	C4C-C3C-C2C	-4.32	101.97	106.81
22	d	402	CLA	C1C-C2C-C3C	-4.31	102.14	106.92
22	C	511	CLA	CHD-C4C-C3C	-4.30	118.44	124.92
22	B	605	CLA	CHD-C4C-C3C	-4.28	118.47	124.92
24	c	915	BCR	C33-C5-C6	-4.26	119.74	124.51
22	c	909	CLA	C1C-C2C-C3C	-4.23	102.23	106.92
37	H	101	RRX	C24-C23-C22	-4.23	119.86	126.21
22	c	914	CLA	C1C-C2C-C3C	-4.23	102.23	106.92
22	B	608	CLA	C1C-C2C-C3C	-4.22	102.24	106.92
22	B	602	CLA	O2D-CGD-O1D	-4.20	115.37	123.82
22	b	617	CLA	CBC-CAC-C3C	-4.20	100.49	112.41
22	B	603	CLA	C1C-C2C-C3C	-4.17	102.30	106.92
22	c	907	CLA	C1C-C2C-C3C	-4.16	102.30	106.92
27	d	407	LHG	O8-C23-O10	-4.16	113.22	123.55
22	c	910	CLA	C1C-C2C-C3C	-4.15	102.32	106.92
22	c	907	CLA	CHD-C4C-C3C	-4.14	118.68	124.92
22	c	908	CLA	C1C-C2C-C3C	-4.14	102.33	106.92
22	B	617	CLA	C1C-C2C-C3C	-4.13	102.34	106.92
22	c	906	CLA	CHD-C4C-C3C	-4.13	118.69	124.92
22	b	602	CLA	CHD-C4C-C3C	-4.12	118.70	124.92
35	C	517	DGD	C3G-C2G-C1G	-4.12	102.56	111.86
22	C	504	CLA	O2D-CGD-O1D	-4.12	115.53	123.82
22	B	609	CLA	C1C-C2C-C3C	-4.11	102.37	106.92
22	B	613	CLA	CHD-C4C-C3C	-4.10	118.73	124.92
36	v	202	HEM	CBD-CAD-C3D	-4.09	104.67	112.47
24	b	618	BCR	C38-C26-C25	-4.08	119.94	124.51
22	B	611	CLA	C1C-C2C-C3C	-4.08	102.39	106.92
22	C	511	CLA	O2D-CGD-O1D	-4.07	115.63	123.82
22	c	905	CLA	CHD-C4C-C3C	-4.05	118.81	124.92
22	b	616	CLA	CHD-C4C-C3C	-4.04	118.83	124.92
22	b	602	CLA	C1C-C2C-C3C	-4.04	102.44	106.92
22	C	514	CLA	O2D-CGD-O1D	-4.03	115.70	123.82
22	B	617	CLA	C1C-NC-C4C	-4.03	104.74	107.06
22	b	606	CLA	O2D-CGD-O1D	-4.02	115.73	123.82
28	A	413	SQD	O48-C23-O10	-4.02	113.57	123.55
23	a	410	PHO	O2D-CGD-O1D	-4.00	115.78	123.82
22	c	905	CLA	C1C-C2C-C3C	-4.00	102.49	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C1C-C2C-C3C	-4.00	102.49	106.92
22	a	412	CLA	O2D-CGD-O1D	-3.99	115.78	123.82
22	b	615	CLA	CHD-C4C-C3C	-3.99	118.90	124.92
22	c	913	CLA	C1C-C2C-C3C	-3.99	102.50	106.92
22	B	604	CLA	CHD-C4C-C3C	-3.99	118.91	124.92
22	C	513	CLA	O1D-CGD-CBD	-3.99	117.44	124.60
22	C	508	CLA	C1C-C2C-C3C	-3.98	102.50	106.92
22	B	609	CLA	O2D-CGD-O1D	-3.98	115.81	123.82
22	b	612	CLA	C1C-C2C-C3C	-3.97	102.51	106.92
22	c	913	CLA	CHD-C4C-C3C	-3.97	118.93	124.92
22	B	606	CLA	O2D-CGD-O1D	-3.96	115.85	123.82
22	b	611	CLA	C1C-C2C-C3C	-3.95	102.54	106.92
22	a	407	CLA	C1C-C2C-C3C	-3.94	102.55	106.92
36	E	102	HEM	CBA-CAA-C2A	-3.94	104.95	112.48
37	H	101	RRX	C31-C1-C6	-3.94	103.93	110.31
22	b	608	CLA	C1C-C2C-C3C	-3.93	102.56	106.92
22	C	507	CLA	C1C-C2C-C3C	-3.93	102.56	106.92
22	B	604	CLA	O2D-CGD-O1D	-3.93	115.92	123.82
22	c	904	CLA	C1C-C2C-C3C	-3.92	102.57	106.92
22	a	412	CLA	CHD-C4C-C3C	-3.92	119.01	124.92
22	b	605	CLA	CHD-C4C-C3C	-3.92	119.02	124.92
27	D	409	LHG	O7-C7-O9	-3.90	113.94	123.68
22	c	913	CLA	O2D-CGD-O1D	-3.89	115.99	123.82
22	C	502	CLA	C1C-C2C-C3C	-3.89	102.61	106.92
22	d	402	CLA	O2D-CGD-O1D	-3.88	116.00	123.82
22	b	607	CLA	C1C-C2C-C3C	-3.88	102.62	106.92
22	b	617	CLA	O1D-CGD-CBD	-3.87	117.65	124.60
29	a	419	LMT	C4B-C3B-C2B	-3.86	104.02	110.84
22	b	611	CLA	C1C-NC-C4C	-3.85	104.84	107.06
26	d	405	PL9	O1-C4-C3	-3.84	116.36	120.71
22	B	615	CLA	C1C-C2C-C3C	-3.81	102.69	106.92
22	c	909	CLA	CHD-C4C-C3C	-3.80	119.20	124.92
22	B	607	CLA	C1C-NC-C4C	-3.79	104.88	107.06
22	b	603	CLA	O2D-CGD-O1D	-3.78	116.21	123.82
24	d	404	BCR	C30-C25-C26	-3.78	117.28	122.59
22	B	603	CLA	O2D-CGD-O1D	-3.78	116.22	123.82
22	b	605	CLA	C1C-C2C-C3C	-3.78	102.73	106.92
24	c	915	BCR	C15-C14-C13	-3.78	121.92	127.31
22	C	506	CLA	C1C-C2C-C3C	-3.78	102.73	106.92
22	c	914	CLA	O2D-CGD-O1D	-3.77	116.24	123.82
22	C	509	CLA	CHD-C4C-C3C	-3.76	119.25	124.92
22	C	508	CLA	O2D-CGD-O1D	-3.76	116.25	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	CGD-CBD-CAD	-3.76	98.13	110.71
22	D	401	CLA	C1C-NC-C4C	-3.75	104.90	107.06
22	b	611	CLA	O2D-CGD-O1D	-3.75	116.28	123.82
22	C	503	CLA	C1C-C2C-C3C	-3.75	102.76	106.92
26	D	406	PL9	C7-C8-C9	-3.73	120.47	126.71
22	c	903	CLA	C1D-CHD-C4C	-3.73	117.39	122.48
22	b	603	CLA	C1C-C2C-C3C	-3.73	102.78	106.92
22	B	612	CLA	C1C-C2C-C3C	-3.72	102.79	106.92
22	B	608	CLA	CGD-CBD-CAD	-3.71	98.27	110.71
24	Y	101	BCR	C16-C15-C14	-3.71	115.54	123.46
22	B	612	CLA	O2D-CGD-O1D	-3.71	116.36	123.82
34	v	203	HTG	O4-C4-C3	-3.70	102.30	110.36
22	A	408	CLA	CHD-C4C-C3C	-3.69	119.36	124.92
34	V	203	HTG	C1-C2-C3	-3.68	102.81	110.69
22	C	505	CLA	CHD-C4C-C3C	-3.68	119.37	124.92
27	D	411	LHG	O8-C23-O10	-3.68	114.42	123.55
28	a	414	SQD	C1-O5-C5	-3.67	106.80	113.72
22	C	513	CLA	C1C-C2C-C3C	-3.67	102.85	106.92
24	k	101	BCR	C24-C23-C22	-3.67	120.70	126.21
22	B	615	CLA	O1D-CGD-CBD	-3.66	118.02	124.60
24	B	618	BCR	C28-C27-C26	-3.66	107.48	113.78
22	B	608	CLA	CBC-CAC-C3C	-3.65	102.04	112.41
22	D	401	CLA	C1D-CHD-C4C	-3.65	117.49	122.48
22	c	903	CLA	C1C-C2C-C3C	-3.65	102.87	106.92
22	A	406	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	c	912	CLA	C1C-C2C-C3C	-3.64	102.88	106.92
24	b	620	BCR	C7-C8-C9	-3.64	120.74	126.21
22	b	606	CLA	C1C-NC-C4C	-3.64	104.96	107.06
22	B	614	CLA	CHD-C4C-C3C	-3.63	119.44	124.92
22	b	616	CLA	C1C-C2C-C3C	-3.63	102.89	106.92
24	C	515	BCR	C38-C26-C25	-3.63	120.45	124.51
22	C	509	CLA	O2D-CGD-O1D	-3.62	116.53	123.82
22	C	512	CLA	C1C-C2C-C3C	-3.61	102.91	106.92
22	c	911	CLA	O2D-CGD-O1D	-3.61	116.55	123.82
22	c	902	CLA	O2D-CGD-O1D	-3.61	116.55	123.82
22	D	401	CLA	CBC-CAC-C3C	-3.61	102.16	112.41
22	C	514	CLA	C1C-C2C-C3C	-3.61	102.92	106.92
36	v	202	HEM	C1D-C2D-C3D	-3.60	104.49	107.00
22	c	906	CLA	C1C-C2C-C3C	-3.59	102.93	106.92
22	D	403	CLA	C2A-C1A-CHA	-3.58	117.57	123.92
35	h	102	DGD	O1G-C1A-O1A	-3.58	114.66	123.55
22	b	612	CLA	C1C-NC-C4C	-3.58	105.00	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	BCR	C28-C27-C26	-3.56	107.65	113.78
22	b	602	CLA	O2D-CGD-O1D	-3.55	116.67	123.82
24	d	404	BCR	C16-C15-C14	-3.55	115.88	123.46
35	C	519	DGD	O6D-C1D-O3G	-3.55	101.59	110.02
22	b	617	CLA	O2D-CGD-O1D	-3.54	116.69	123.82
24	A	409	BCR	C15-C16-C17	-3.54	115.90	123.46
22	d	402	CLA	CHD-C4C-C3C	-3.54	119.59	124.92
22	B	611	CLA	O2A-CGA-O1A	-3.53	114.78	123.55
26	d	405	PL9	C7-C8-C9	-3.52	120.82	126.71
22	C	510	CLA	CHD-C4C-C3C	-3.51	119.63	124.92
22	D	404	CLA	C1C-C2C-C3C	-3.50	103.03	106.92
22	c	904	CLA	C1-C2-C3	-3.50	119.50	125.96
22	B	605	CLA	C1C-NC-C4C	-3.50	105.04	107.06
22	b	608	CLA	O2D-CGD-O1D	-3.50	116.78	123.82
29	t	101	LMT	C1'-C2'-C3'	-3.50	103.48	109.98
24	K	101	BCR	C24-C23-C22	-3.49	120.96	126.21
24	c	916	BCR	C33-C5-C6	-3.49	120.60	124.51
22	B	614	CLA	O2D-CGD-O1D	-3.49	116.81	123.82
22	c	910	CLA	C1C-NC-C4C	-3.48	105.05	107.06
22	c	910	CLA	C2A-C1A-CHA	-3.48	117.75	123.92
22	D	403	CLA	CHD-C4C-C3C	-3.48	119.68	124.92
22	c	904	CLA	CHD-C4C-C3C	-3.47	119.69	124.92
22	b	608	CLA	CHD-C4C-C3C	-3.46	119.70	124.92
22	c	911	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
28	b	621	SQD	O5-C1-C2	-3.46	103.61	110.30
22	b	613	CLA	C1C-NC-C4C	-3.45	105.07	107.06
22	B	614	CLA	C1C-C2C-C3C	-3.45	103.09	106.92
22	B	603	CLA	C7-C6-C5	-3.44	103.55	113.11
22	b	605	CLA	O2D-CGD-O1D	-3.44	116.90	123.82
22	C	509	CLA	C1C-C2C-C3C	-3.43	103.12	106.92
27	D	410	LHG	O8-C6-C5	-3.43	100.04	108.66
22	B	613	CLA	C2A-C1A-CHA	-3.42	117.85	123.92
22	B	613	CLA	C1C-C2C-C3C	-3.42	103.13	106.92
22	b	609	CLA	O2D-CGD-O1D	-3.42	116.94	123.82
22	c	912	CLA	O2A-CGA-O1A	-3.41	115.08	123.55
22	b	604	CLA	O2A-CGA-O1A	-3.39	115.12	123.55
22	B	616	CLA	C1C-C2C-C3C	-3.39	103.16	106.92
22	b	614	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
28	C	501	SQD	C5-C6-S	-3.37	109.64	114.34
22	d	402	CLA	O2A-CGA-O1A	-3.36	115.20	123.55
24	y	101	BCR	C21-C20-C19	-3.35	112.96	123.23
37	H	101	RRX	C7-C8-C9	-3.33	121.21	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	O2D-CGD-O1D	-3.32	117.14	123.82
24	y	101	BCR	C24-C23-C22	-3.32	121.23	126.21
22	B	606	CLA	CHC-C1C-NC	-3.31	117.86	124.08
22	C	509	CLA	O2A-CGA-O1A	-3.30	115.37	123.55
22	b	615	CLA	C1C-C2C-C3C	-3.29	103.27	106.92
22	b	614	CLA	CAA-CBA-CGA	-3.28	103.45	113.35
22	a	409	CLA	C1-C2-C3	-3.28	119.91	125.96
22	c	908	CLA	CBC-CAC-C3C	-3.28	103.09	112.41
22	b	603	CLA	CHD-C4C-C3C	-3.28	119.98	124.92
23	a	411	PHO	C3B-C2B-C1B	-3.27	99.71	106.30
22	B	612	CLA	C2A-C1A-CHA	-3.27	118.13	123.92
22	b	617	CLA	C1C-C2C-C3C	-3.26	103.30	106.92
29	A	414	LMT	C1'-C2'-C3'	-3.26	103.92	109.98
22	C	504	CLA	C1C-C2C-C3C	-3.24	103.33	106.92
22	a	408	CLA	CBC-CAC-C3C	-3.22	103.25	112.41
23	A	407	PHO	C3B-C2B-C1B	-3.22	99.79	106.30
22	C	511	CLA	C1C-NC-C4C	-3.22	105.20	107.06
22	b	613	CLA	C4C-C3C-C2C	-3.21	101.99	106.91
24	y	101	BCR	C38-C26-C25	-3.20	120.92	124.51
25	C	520	LMG	O8-C28-O10	-3.19	115.62	123.55
22	d	403	CLA	CHD-C4C-C3C	-3.19	120.11	124.92
22	B	602	CLA	CHD-C4C-C3C	-3.19	120.11	124.92
37	h	101	RRX	C7-C8-C9	-3.17	121.44	126.21
22	b	617	CLA	C4C-C3C-C2C	-3.17	102.04	106.91
22	A	408	CLA	O2D-CGD-O1D	-3.17	117.44	123.82
22	B	607	CLA	C1-C2-C3	-3.17	120.11	125.96
22	d	403	CLA	O2D-CGD-O1D	-3.17	117.45	123.82
23	a	411	PHO	C4D-ND-C1D	-3.16	101.27	106.98
22	B	616	CLA	O1D-CGD-CBD	-3.15	118.94	124.60
22	B	617	CLA	O2A-CGA-O1A	-3.15	115.72	123.55
22	b	609	CLA	C1C-C2C-C3C	-3.15	103.43	106.92
22	A	406	CLA	O1D-CGD-CBD	-3.15	118.95	124.60
23	D	402	PHO	C4D-ND-C1D	-3.15	101.30	106.98
22	C	502	CLA	C1C-NC-C4C	-3.15	105.25	107.06
22	C	511	CLA	O2A-CGA-O1A	-3.14	115.75	123.55
22	c	905	CLA	C5-C3-C2	-3.14	114.68	121.10
22	b	616	CLA	O1D-CGD-CBD	-3.14	118.97	124.60
22	a	407	CLA	O2D-CGD-O1D	-3.13	117.51	123.82
22	B	606	CLA	C1C-C2C-C3C	-3.12	103.46	106.92
27	D	409	LHG	C5-O7-C7	-3.11	110.52	117.88
36	e	101	HEM	C1D-C2D-C3D	-3.11	104.83	107.00
22	A	405	CLA	O2A-CGA-O1A	-3.11	115.83	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	413	SQD	C1-O5-C5	-3.11	107.86	113.72
22	C	512	CLA	O2D-CGD-O1D	-3.11	117.57	123.82
22	b	604	CLA	C2A-C3A-C4A	-3.10	96.86	101.87
24	d	404	BCR	C37-C22-C21	-3.10	118.58	122.92
22	C	511	CLA	O1D-CGD-CBD	-3.10	119.04	124.60
22	b	612	CLA	C7-C6-C5	-3.10	104.51	113.11
22	b	610	CLA	CBC-CAC-C3C	-3.09	103.62	112.41
22	B	607	CLA	O1D-CGD-CBD	-3.09	119.06	124.60
37	h	101	RRX	C11-C10-C9	-3.09	122.91	127.31
22	b	607	CLA	C1C-NC-C4C	-3.09	105.28	107.06
24	B	620	BCR	C38-C26-C25	-3.08	121.06	124.51
22	b	616	CLA	O2D-CGD-O1D	-3.08	117.61	123.82
22	c	914	CLA	O1D-CGD-CBD	-3.07	119.09	124.60
22	A	405	CLA	CHD-C4C-C3C	-3.06	120.30	124.92
24	C	516	BCR	C7-C8-C9	-3.06	121.61	126.21
22	a	409	CLA	C2A-C1A-CHA	-3.06	118.49	123.92
22	b	604	CLA	O1D-CGD-CBD	-3.06	119.11	124.60
28	C	501	SQD	O7-S-C6	-3.05	104.22	106.83
36	E	102	HEM	C1D-C2D-C3D	-3.04	104.88	107.00
24	d	404	BCR	C21-C20-C19	-3.04	113.90	123.23
35	c	919	DGD	O2G-C1B-O1B	-3.04	116.10	123.68
22	a	409	CLA	O2D-CGD-O1D	-3.03	117.72	123.82
22	b	606	CLA	C1C-C2C-C3C	-3.03	103.56	106.92
24	B	620	BCR	C7-C8-C9	-3.02	121.67	126.21
24	C	515	BCR	C7-C8-C9	-3.02	121.67	126.21
28	C	501	SQD	O5-C1-C2	-3.02	104.46	110.30
22	b	606	CLA	C1-C2-C3	-3.02	120.39	125.96
24	B	620	BCR	C32-C1-C6	-3.02	105.42	110.31
22	B	607	CLA	OBD-CAD-C3D	-3.02	122.47	128.03
37	H	101	RRX	C16-C17-C18	-3.01	123.01	127.31
25	i	101	LMG	O6-C1-C2	-3.01	104.49	110.30
22	B	610	CLA	C1C-NC-C4C	-3.01	105.32	107.06
28	C	501	SQD	O48-C23-O10	-3.01	116.08	123.55
22	B	603	CLA	OBD-CAD-C3D	-3.00	122.50	128.03
24	D	405	BCR	C33-C5-C6	-2.99	121.16	124.51
24	C	516	BCR	C11-C10-C9	-2.99	123.04	127.31
22	C	504	CLA	C1D-CHD-C4C	-2.99	118.40	122.48
22	b	613	CLA	C11-C12-C13	-2.99	105.92	115.73
22	b	604	CLA	O2D-CGD-O1D	-2.99	117.81	123.82
22	B	605	CLA	C6-C5-C3	-2.97	105.92	112.66
22	D	403	CLA	O2D-CGD-O1D	-2.97	117.84	123.82
22	C	505	CLA	O2D-CGD-O1D	-2.97	117.85	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	BCR	C38-C26-C25	-2.97	121.19	124.51
28	l	101	SQD	O5-C1-C2	-2.96	104.58	110.30
22	b	605	CLA	C1C-NC-C4C	-2.96	105.35	107.06
22	B	605	CLA	O2D-CGD-O1D	-2.96	117.86	123.82
25	J	101	LMG	O8-C28-O10	-2.96	116.20	123.55
26	A	411	PL9	C22-C23-C24	-2.96	120.25	127.68
24	c	915	BCR	C7-C8-C9	-2.96	121.77	126.21
22	b	609	CLA	O2A-CGA-O1A	-2.95	116.22	123.55
26	A	411	PL9	C32-C33-C34	-2.95	120.27	127.68
24	c	916	BCR	C11-C10-C9	-2.95	123.10	127.31
22	B	604	CLA	O1D-CGD-CBD	-2.95	119.31	124.60
34	b	623	HTG	C2'-C1'-S1	-2.94	102.86	112.45
37	H	101	RRX	C10-C11-C12	-2.94	114.22	123.23
22	C	502	CLA	O1D-CGD-CBD	-2.93	119.33	124.60
22	A	408	CLA	O2A-CGA-O1A	-2.93	116.27	123.55
22	b	603	CLA	C1-C2-C3	-2.93	120.56	125.96
24	y	101	BCR	C16-C15-C14	-2.93	117.21	123.46
27	L	101	LHG	C6-C5-C4	-2.93	105.25	111.86
22	D	404	CLA	O2D-CGD-O1D	-2.92	117.94	123.82
22	B	610	CLA	CBC-CAC-C3C	-2.92	104.12	112.41
22	c	904	CLA	C7-C6-C5	-2.92	105.00	113.11
24	c	916	BCR	C38-C26-C25	-2.92	121.24	124.51
35	C	517	DGD	O5D-C6D-C5D	-2.91	104.07	108.94
37	h	101	RRX	C16-C17-C18	-2.91	123.15	127.31
24	B	619	BCR	C28-C27-C26	-2.91	108.78	113.78
22	C	508	CLA	O1D-CGD-CBD	-2.90	119.39	124.60
22	b	609	CLA	C4C-C3C-C2C	-2.90	102.45	106.91
24	B	618	BCR	C29-C28-C27	-2.90	104.43	111.34
22	a	412	CLA	C1-C2-C3	-2.90	120.61	125.96
22	A	405	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
22	B	602	CLA	C1C-C2C-C3C	-2.90	103.71	106.92
22	B	611	CLA	O1D-CGD-CBD	-2.90	119.40	124.60
24	d	404	BCR	C35-C13-C14	-2.90	118.87	122.92
22	c	909	CLA	O2D-CGD-O1D	-2.89	118.00	123.82
22	c	904	CLA	OBD-CAD-C3D	-2.89	122.69	128.03
25	j	101	LMG	O2-C2-C1	-2.89	103.98	110.03
22	a	412	CLA	OBD-CAD-C3D	-2.89	122.71	128.03
35	C	517	DGD	O6E-C1E-C2E	-2.88	104.73	110.30
22	c	911	CLA	O2A-CGA-O1A	-2.88	116.39	123.55
22	B	603	CLA	C1-C2-C3	-2.88	120.65	125.96
25	d	409	LMG	C8-O7-C10	-2.88	111.08	117.88
24	B	620	BCR	C23-C24-C25	-2.87	119.20	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	402	CLA	C2A-C1A-CHA	-2.87	118.82	123.92
29	c	921	LMT	O2'-C2'-C3'	-2.87	104.10	110.36
24	K	101	BCR	C33-C5-C6	-2.87	121.30	124.51
22	C	507	CLA	C1C-NC-C4C	-2.87	105.41	107.06
22	B	617	CLA	CBC-CAC-C3C	-2.87	104.28	112.41
22	A	405	CLA	C7-C6-C5	-2.86	105.15	113.11
24	k	101	BCR	C32-C1-C6	-2.85	105.69	110.31
24	Y	101	BCR	C24-C23-C22	-2.85	121.93	126.21
22	C	510	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
34	B	623	HTG	O4-C4-C3	-2.84	104.17	110.36
22	a	412	CLA	CBC-CAC-C3C	-2.84	104.35	112.41
24	b	618	BCR	C20-C21-C22	-2.83	123.26	127.31
22	D	401	CLA	O2D-CGD-O1D	-2.83	118.12	123.82
22	B	616	CLA	O2A-CGA-O1A	-2.83	116.52	123.55
24	D	405	BCR	C16-C17-C18	-2.83	123.27	127.31
28	b	621	SQD	O48-C23-O10	-2.82	116.54	123.55
25	j	101	LMG	C7-O1-C1	-2.82	107.96	113.76
22	a	407	CLA	O1D-CGD-CBD	-2.82	119.54	124.60
24	A	409	BCR	C38-C26-C25	-2.82	121.36	124.51
22	C	502	CLA	C2A-C1A-CHA	-2.82	118.93	123.92
22	C	509	CLA	C5-C3-C2	-2.81	115.35	121.10
22	C	505	CLA	O1D-CGD-CBD	-2.81	119.55	124.60
22	a	407	CLA	CHD-C4C-C3C	-2.81	120.68	124.92
22	b	604	CLA	C1D-CHD-C4C	-2.80	118.65	122.48
25	j	101	LMG	C9-C8-C7	-2.80	105.54	111.86
22	a	407	CLA	O2A-CGA-O1A	-2.79	116.61	123.55
22	c	908	CLA	CED-O2D-CGD	-2.79	109.43	115.97
24	c	916	BCR	C35-C13-C14	-2.79	119.01	122.92
22	b	609	CLA	C1C-NC-C4C	-2.79	105.45	107.06
22	C	514	CLA	O2A-CGA-O1A	-2.79	116.62	123.55
22	b	616	CLA	O2A-CGA-O1A	-2.79	116.63	123.55
22	B	604	CLA	C2A-C3A-C4A	-2.78	97.37	101.87
22	A	406	CLA	O2A-CGA-O1A	-2.78	116.64	123.55
26	A	411	PL9	C37-C36-C34	-2.77	103.56	112.93
24	b	620	BCR	C24-C23-C22	-2.77	122.05	126.21
22	b	610	CLA	C1-C2-C3	-2.77	120.86	125.96
22	c	913	CLA	C2A-C1A-CHA	-2.77	119.01	123.92
22	b	603	CLA	O1D-CGD-CBD	-2.77	119.63	124.60
22	a	412	CLA	C2A-C1A-CHA	-2.77	119.02	123.92
22	b	607	CLA	C14-C13-C12	-2.76	101.29	111.36
25	J	101	LMG	C7-O1-C1	-2.76	108.10	113.76
22	c	903	CLA	C6-C5-C3	-2.76	106.41	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	C4C-C3C-C2C	-2.75	102.68	106.91
29	f	102	LMT	C3'-C4'-C5'	-2.75	105.03	110.88
24	D	405	BCR	C10-C11-C12	-2.75	114.80	123.23
26	a	415	PL9	C42-C43-C44	-2.75	120.78	127.68
22	c	910	CLA	CHD-C4C-C3C	-2.75	120.78	124.92
22	b	605	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
22	c	903	CLA	C2A-C1A-CHA	-2.73	119.08	123.92
22	B	608	CLA	CHD-C4C-C3C	-2.73	120.80	124.92
22	C	510	CLA	C1-C2-C3	-2.73	120.93	125.96
22	c	912	CLA	CHD-C4C-C3C	-2.73	120.81	124.92
27	a	423	LHG	O8-C23-O10	-2.72	116.79	123.55
22	B	608	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
22	B	605	CLA	CGD-CBD-CAD	-2.72	101.60	110.71
36	V	202	HEM	C1D-C2D-C3D	-2.72	105.11	107.00
22	B	610	CLA	C1-C2-C3	-2.72	120.95	125.96
22	c	903	CLA	O2A-CGA-O1A	-2.71	116.81	123.55
27	D	409	LHG	O8-C23-O10	-2.71	116.83	123.55
22	b	609	CLA	C1D-CHD-C4C	-2.70	118.79	122.48
22	B	604	CLA	C1C-NC-C4C	-2.70	105.50	107.06
22	B	608	CLA	O1D-CGD-CBD	-2.70	119.75	124.60
35	C	518	DGD	O1G-C1A-O1A	-2.70	116.85	123.55
22	a	412	CLA	C1D-CHD-C4C	-2.69	118.81	122.48
35	C	519	DGD	O3G-C3G-C2G	-2.69	104.59	110.99
22	b	613	CLA	C2A-C1A-CHA	-2.69	119.15	123.92
22	a	408	CLA	C2A-C1A-CHA	-2.68	119.16	123.92
22	b	603	CLA	OBD-CAD-C3D	-2.68	123.08	128.03
22	c	907	CLA	C1C-NC-C4C	-2.68	105.51	107.06
28	a	414	SQD	O9-S-O7	-2.68	104.57	113.86
23	a	410	PHO	C1C-C2C-C3C	-2.68	103.40	106.51
35	c	919	DGD	O1G-C1A-O1A	-2.68	116.90	123.55
22	B	612	CLA	C7-C6-C5	-2.67	105.69	113.11
22	c	906	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
22	c	907	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
22	D	404	CLA	C2A-C1A-CHA	-2.66	119.19	123.92
22	B	607	CLA	CBC-CAC-C3C	-2.66	104.85	112.41
23	a	410	PHO	C7-C6-C5	-2.66	105.73	113.11
24	d	404	BCR	C24-C23-C22	-2.65	122.22	126.21
25	i	101	LMG	C1-O6-C5	-2.65	108.71	113.72
22	c	911	CLA	CBC-CAC-C3C	-2.65	104.88	112.41
22	d	402	CLA	CMA-C3A-C2A	-2.65	103.02	113.77
24	C	516	BCR	C33-C5-C6	-2.65	121.54	124.51
22	A	408	CLA	C5-C3-C2	-2.65	115.69	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	OBD-CAD-C3D	-2.64	123.16	128.03
22	B	607	CLA	CHC-C1C-NC	-2.63	119.13	124.08
22	b	606	CLA	OBD-CAD-C3D	-2.63	123.17	128.03
24	b	620	BCR	C3-C4-C5	-2.63	109.26	113.78
22	B	603	CLA	CHC-C1C-NC	-2.63	119.14	124.08
23	D	402	PHO	C3B-C2B-C1B	-2.63	101.00	106.30
24	C	515	BCR	C8-C7-C6	-2.63	119.90	127.25
22	C	504	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
22	b	606	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
22	a	407	CLA	C2A-C1A-CHA	-2.62	119.27	123.92
35	C	517	DGD	O2G-C1B-O1B	-2.62	117.14	123.68
35	c	919	DGD	C2G-O2G-C1B	-2.62	111.70	117.88
26	D	406	PL9	C50-C49-C48	-2.61	114.78	122.65
22	C	505	CLA	C7-C6-C5	-2.61	105.86	113.11
22	B	609	CLA	C6-C5-C3	-2.61	106.75	112.66
24	b	618	BCR	C24-C23-C22	-2.60	122.30	126.21
22	b	611	CLA	O2A-CGA-O1A	-2.60	117.09	123.55
22	B	609	CLA	C11-C12-C13	-2.60	107.21	115.73
22	b	613	CLA	O2D-CGD-O1D	-2.59	118.60	123.82
26	d	405	PL9	C22-C23-C24	-2.58	121.19	127.68
24	a	413	BCR	C28-C27-C26	-2.58	109.34	113.78
24	K	101	BCR	C20-C21-C22	-2.58	123.62	127.31
22	C	511	CLA	C1D-CHD-C4C	-2.58	118.96	122.48
24	D	405	BCR	C15-C14-C13	-2.58	123.63	127.31
34	B	626	HTG	O5-C1-C2	-2.58	106.75	110.28
25	A	410	LMG	C8-O7-C10	-2.58	111.79	117.88
28	a	414	SQD	C44-O6-C1	-2.57	108.48	113.76
22	B	616	CLA	C6-C7-C8	-2.57	107.30	115.73
34	D	415	HTG	C1-C2-C3	-2.57	105.20	110.69
24	A	409	BCR	C36-C18-C17	-2.56	119.33	122.92
23	D	402	PHO	CHD-C1D-ND	-2.56	119.61	124.64
25	b	622	LMG	O7-C10-O9	-2.56	117.28	123.68
22	C	514	CLA	CHC-C1C-NC	-2.56	119.26	124.08
22	D	401	CLA	C1-C2-C3	-2.56	121.24	125.96
35	c	919	DGD	O2E-C2E-C3E	-2.56	104.79	110.36
22	B	615	CLA	C4C-C3C-C2C	-2.56	102.99	106.91
28	C	501	SQD	C45-O47-C7	-2.55	111.84	117.88
22	B	606	CLA	C1C-NC-C4C	-2.55	105.59	107.06
24	D	405	BCR	C29-C28-C27	-2.55	105.27	111.34
26	D	406	PL9	C37-C38-C39	-2.55	121.28	127.68
22	b	610	CLA	C2A-C1A-CHA	-2.55	119.40	123.92
22	b	609	CLA	C11-C12-C13	-2.55	107.37	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	610	CLA	C7-C6-C5	-2.55	106.04	113.11
23	A	407	PHO	CHB-C1B-NB	-2.54	119.65	124.64
24	y	101	BCR	C7-C6-C5	-2.54	115.48	121.54
22	B	606	CLA	C7-C6-C5	-2.54	106.05	113.11
25	J	101	LMG	O3-C3-C2	-2.54	104.83	110.36
22	B	604	CLA	O2A-CGA-O1A	-2.54	117.25	123.55
22	b	611	CLA	C4C-C3C-C2C	-2.53	103.02	106.91
22	B	602	CLA	C4C-C3C-C2C	-2.53	103.03	106.91
24	c	916	BCR	C16-C17-C18	-2.53	123.70	127.31
26	D	406	PL9	C12-C13-C14	-2.53	121.32	127.68
35	h	102	DGD	C3D-C4D-C5D	-2.53	105.76	110.22
24	Y	101	BCR	C8-C9-C10	-2.53	115.06	118.94
22	C	508	CLA	CBC-CAC-C3C	-2.53	105.23	112.41
22	B	603	CLA	C5-C3-C2	-2.53	115.93	121.10
22	c	909	CLA	C1-C2-C3	-2.53	121.30	125.96
22	c	903	CLA	C1C-NC-C4C	-2.52	105.60	107.06
24	K	101	BCR	C16-C17-C18	-2.52	123.71	127.31
22	a	409	CLA	O2A-CGA-O1A	-2.52	117.30	123.55
22	b	607	CLA	C2A-C1A-CHA	-2.51	119.46	123.92
22	b	603	CLA	CAA-CBA-CGA	-2.51	105.80	113.35
22	b	602	CLA	O1D-CGD-CBD	-2.50	120.10	124.60
22	b	608	CLA	OBD-CAD-C3D	-2.50	123.41	128.03
25	i	101	LMG	C31-C30-C29	-2.50	104.06	113.24
27	D	410	LHG	C14-C13-C12	-2.50	101.55	114.45
22	b	613	CLA	O2A-CGA-O1A	-2.50	117.33	123.55
35	C	518	DGD	C3B-C2B-C1B	-2.50	104.45	113.58
24	k	101	BCR	C11-C10-C9	-2.50	123.74	127.31
22	A	405	CLA	CAA-CBA-CGA	-2.50	105.81	113.35
22	C	513	CLA	C1-C2-C3	-2.50	121.35	125.96
22	B	610	CLA	O2D-CGD-O1D	-2.50	118.79	123.82
36	V	202	HEM	CMA-C3A-C4A	-2.50	124.63	128.46
22	C	508	CLA	O2A-CGA-O1A	-2.50	117.35	123.55
35	C	518	DGD	O2G-C1B-O1B	-2.50	117.45	123.68
24	Y	101	BCR	C7-C8-C9	-2.49	122.46	126.21
23	D	402	PHO	CHD-C4C-C3C	-2.49	119.57	124.59
22	B	613	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
25	d	409	LMG	O7-C10-O9	-2.49	117.46	123.68
22	B	612	CLA	O1D-CGD-CBD	-2.49	120.14	124.60
22	C	512	CLA	C1D-CHD-C4C	-2.48	119.09	122.48
28	a	414	SQD	O5-C1-C2	-2.48	105.50	110.30
23	A	407	PHO	C4C-C3C-C2C	-2.48	104.02	106.81
26	a	415	PL9	C32-C33-C34	-2.47	121.47	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	410	PHO	C1C-NC-C4C	-2.47	101.63	106.52
28	a	414	SQD	O47-C7-O49	-2.47	117.52	123.68
22	c	909	CLA	OBD-CAD-C3D	-2.47	123.48	128.03
24	C	516	BCR	C38-C26-C25	-2.47	121.75	124.51
22	b	614	CLA	C4C-C3C-C2C	-2.46	103.13	106.91
26	A	411	PL9	C37-C38-C39	-2.46	121.49	127.68
24	B	620	BCR	C10-C11-C12	-2.46	115.68	123.23
29	I	102	LMT	C2'-C3'-C4'	-2.46	104.51	109.61
23	a	411	PHO	CHD-C4C-NC	-2.46	120.25	124.97
22	b	612	CLA	CBC-CAC-C3C	-2.45	105.44	112.41
22	D	403	CLA	CHC-C1C-NC	-2.45	119.47	124.08
28	D	408	SQD	C1-O5-C5	-2.45	109.10	113.72
27	d	401	LHG	O8-C23-O10	-2.45	117.47	123.55
22	B	606	CLA	C4C-C3C-C2C	-2.45	103.16	106.91
28	C	501	SQD	O9-S-O7	-2.44	105.39	113.86
35	c	918	DGD	O1G-C1A-O1A	-2.44	117.49	123.55
22	c	908	CLA	C1-C2-C3	-2.44	121.46	125.96
22	c	904	CLA	CAA-CBA-CGA	-2.44	105.99	113.35
28	I	101	SQD	O47-C7-O49	-2.44	117.59	123.68
22	B	616	CLA	O2D-CGD-O1D	-2.44	118.91	123.82
22	B	603	CLA	C1C-NC-C4C	-2.44	105.65	107.06
22	c	913	CLA	O1D-CGD-CBD	-2.44	120.22	124.60
22	c	911	CLA	C2A-C1A-CHA	-2.44	119.60	123.92
22	c	904	CLA	C4C-C3C-C2C	-2.43	103.18	106.91
27	a	423	LHG	O7-C7-O9	-2.43	117.61	123.68
22	B	606	CLA	C2A-C1A-CHA	-2.43	119.61	123.92
27	L	101	LHG	O7-C7-O9	-2.43	117.61	123.68
35	C	517	DGD	O3D-C3D-C2D	-2.43	105.07	110.36
22	A	406	CLA	C1-C2-C3	-2.43	121.48	125.96
22	C	512	CLA	C4C-C3C-C2C	-2.43	103.19	106.91
37	H	101	RRX	C38-C26-C25	-2.42	121.80	124.51
22	b	607	CLA	O2A-CGA-O1A	-2.42	117.55	123.55
22	A	405	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
29	c	921	LMT	C1B-O1B-C4'	-2.42	112.11	118.00
24	B	619	BCR	C15-C16-C17	-2.41	118.31	123.46
22	c	906	CLA	CBC-CAC-C3C	-2.41	105.56	112.41
22	C	509	CLA	C4C-C3C-C2C	-2.41	103.21	106.91
22	b	609	CLA	C1-C2-C3	-2.41	121.52	125.96
22	b	613	CLA	C1-C2-C3	-2.41	121.52	125.96
23	a	411	PHO	C1C-C2C-C3C	-2.41	103.72	106.51
22	B	605	CLA	O2A-CGA-O1A	-2.40	117.58	123.55
24	a	413	BCR	C40-C30-C25	-2.40	106.41	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	620	BCR	C33-C5-C6	-2.40	121.82	124.51
23	a	411	PHO	CHD-C1D-ND	-2.40	119.93	124.64
22	C	504	CLA	C5-C3-C2	-2.40	116.19	121.10
22	a	408	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
35	C	519	DGD	O4D-C4D-C3D	-2.40	105.14	110.36
22	D	403	CLA	C4-C3-C2	-2.40	117.29	123.69
22	b	615	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
24	Y	101	BCR	C15-C14-C13	-2.40	123.89	127.31
24	a	413	BCR	C23-C24-C25	-2.39	120.56	127.25
24	c	915	BCR	C38-C26-C25	-2.39	121.84	124.51
24	Y	101	BCR	C24-C25-C26	-2.38	115.86	121.54
22	b	615	CLA	C2A-C1A-CHA	-2.38	119.69	123.92
22	D	404	CLA	O2A-CGA-O1A	-2.38	117.63	123.55
22	b	616	CLA	C2A-C1A-CHA	-2.38	119.70	123.92
24	d	404	BCR	C15-C14-C13	-2.38	123.91	127.31
24	A	409	BCR	C33-C5-C6	-2.38	121.85	124.51
22	D	404	CLA	CBC-CAC-C3C	-2.38	105.66	112.41
22	A	405	CLA	C2A-C1A-CHA	-2.38	119.70	123.92
22	b	610	CLA	CHC-C1C-NC	-2.38	119.61	124.08
24	a	413	BCR	C8-C7-C6	-2.38	120.60	127.25
22	b	617	CLA	C1C-NC-C4C	-2.36	105.69	107.06
22	B	615	CLA	O2D-CGD-O1D	-2.36	119.07	123.82
22	C	510	CLA	C11-C10-C8	-2.36	107.98	115.73
36	E	102	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
35	c	917	DGD	O2G-C1B-O1B	-2.35	117.80	123.68
22	B	603	CLA	C4C-C3C-C2C	-2.35	103.30	106.91
25	B	621	LMG	O7-C10-O9	-2.35	117.82	123.68
28	A	413	SQD	C1-C2-C3	-2.34	105.62	109.98
35	H	102	DGD	C2G-O2G-C1B	-2.34	112.34	117.88
22	b	612	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
24	B	619	BCR	C24-C23-C22	-2.33	122.71	126.21
26	D	406	PL9	C40-C39-C38	-2.33	117.47	123.69
22	B	614	CLA	C1-C2-C3	-2.33	121.66	125.96
22	B	605	CLA	CAA-C2A-C3A	-2.33	106.42	112.81
24	B	619	BCR	C23-C24-C25	-2.33	120.73	127.25
28	b	621	SQD	C1-C2-C3	-2.33	105.65	109.98
22	D	401	CLA	O2A-CGA-O1A	-2.33	117.78	123.55
22	a	407	CLA	C5-C3-C2	-2.32	116.35	121.10
35	C	519	DGD	O2G-C1B-O1B	-2.32	117.89	123.68
22	c	907	CLA	O2A-CGA-O1A	-2.32	117.80	123.55
24	B	620	BCR	C15-C14-C13	-2.31	124.01	127.31
24	B	620	BCR	C40-C30-C25	-2.31	106.56	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	CBC-CAC-C3C	-2.31	105.86	112.41
22	C	502	CLA	O2A-CGA-O1A	-2.31	117.82	123.55
25	c	930	LMG	O7-C10-O9	-2.31	117.92	123.68
24	y	101	BCR	C15-C14-C13	-2.31	124.02	127.31
22	b	610	CLA	C16-C15-C13	-2.31	108.16	115.73
35	d	406	DGD	O2G-C1B-O1B	-2.30	117.93	123.68
22	b	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	a	410	PHO	CHB-C1B-NB	-2.30	120.13	124.64
22	C	510	CLA	O2A-CGA-O1A	-2.30	117.84	123.55
24	B	619	BCR	C20-C21-C22	-2.30	124.03	127.31
23	A	407	PHO	O1D-CGD-CBD	-2.30	120.48	124.60
22	b	604	CLA	C5-C3-C2	-2.30	116.40	121.10
22	C	506	CLA	O2D-CGD-O1D	-2.29	119.20	123.82
22	c	914	CLA	CHC-C1C-NC	-2.29	119.77	124.08
22	a	412	CLA	C5-C3-C2	-2.29	116.41	121.10
34	V	203	HTG	C1-O5-C5	-2.29	108.28	112.69
25	c	920	LMG	O3-C3-C4	-2.29	105.37	110.36
22	C	503	CLA	C6-C5-C3	-2.29	107.47	112.66
22	A	406	CLA	C5-C3-C2	-2.29	116.42	121.10
22	a	412	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
22	C	514	CLA	OBD-CAD-C3D	-2.28	123.82	128.03
22	B	602	CLA	C2A-C1A-CHA	-2.28	119.87	123.92
24	b	620	BCR	C33-C5-C6	-2.28	121.95	124.51
22	A	405	CLA	C1C-NC-C4C	-2.28	105.74	107.06
22	c	907	CLA	C2A-C1A-CHA	-2.28	119.88	123.92
22	d	403	CLA	O1D-CGD-CBD	-2.28	120.50	124.60
22	c	904	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
22	B	607	CLA	O2A-CGA-O1A	-2.28	117.89	123.55
27	D	410	LHG	O8-C23-O10	-2.28	117.89	123.55
22	B	603	CLA	O2A-CGA-O1A	-2.28	117.90	123.55
22	b	617	CLA	C4-C3-C2	-2.27	117.62	123.69
22	b	605	CLA	CGD-CBD-CAD	-2.27	103.10	110.71
25	A	410	LMG	O6-C1-C2	-2.27	105.92	110.30
22	B	604	CLA	C2A-C1A-CHA	-2.27	119.90	123.92
28	A	413	SQD	C45-O47-C7	-2.27	112.52	117.88
35	H	102	DGD	C3B-C2B-C1B	-2.26	105.32	113.58
22	B	606	CLA	O2A-CGA-O1A	-2.26	117.94	123.55
22	b	610	CLA	O2A-CGA-O1A	-2.26	117.94	123.55
27	a	416	LHG	O7-C7-O9	-2.26	118.05	123.68
37	h	101	RRX	C10-C11-C12	-2.26	116.31	123.23
22	c	913	CLA	C6-C5-C3	-2.26	107.54	112.66
22	c	910	CLA	O2D-CGD-O1D	-2.26	119.28	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	O2D-CGD-O1D	-2.25	119.29	123.82
24	a	413	BCR	C24-C23-C22	-2.25	122.83	126.21
24	d	404	BCR	C10-C11-C12	-2.25	116.33	123.23
22	C	506	CLA	CHD-C4C-C3C	-2.25	121.53	124.92
28	a	418	SQD	C44-O6-C1	-2.24	109.15	113.76
34	l	106	HTG	C1-C2-C3	-2.24	105.89	110.69
23	A	407	PHO	C4D-ND-C1D	-2.24	102.94	106.98
22	B	608	CLA	C4-C3-C2	-2.24	117.71	123.69
29	Z	101	LMT	O3B-C3B-C2B	-2.24	105.49	110.36
22	c	906	CLA	C4C-C3C-C2C	-2.23	103.48	106.91
35	C	519	DGD	O1G-C1A-O1A	-2.23	118.01	123.55
22	a	409	CLA	CHC-C1C-C2C	-2.23	120.56	126.65
22	c	906	CLA	O2A-CGA-O1A	-2.23	118.01	123.55
26	d	405	PL9	C42-C43-C44	-2.23	122.08	127.68
23	A	407	PHO	CHD-C1D-ND	-2.23	120.27	124.64
25	c	920	LMG	O4-C4-C3	-2.23	105.51	110.36
24	c	916	BCR	C7-C8-C9	-2.22	122.87	126.21
22	B	617	CLA	C2A-C1A-CHA	-2.22	119.98	123.92
34	b	632	HTG	C4-C3-C2	-2.22	106.92	110.84
22	C	503	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
22	b	613	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
22	C	507	CLA	C4C-C3C-C2C	-2.22	103.50	106.91
22	a	408	CLA	C6-C5-C3	-2.22	107.63	112.66
24	c	915	BCR	C8-C7-C6	-2.22	121.04	127.25
22	c	912	CLA	O2D-CGD-O1D	-2.22	119.36	123.82
22	b	611	CLA	C9-C8-C10	-2.21	103.28	111.36
34	l	106	HTG	O5-C1-C2	-2.21	107.24	110.28
22	B	612	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
24	B	619	BCR	C11-C12-C13	-2.21	120.21	126.42
24	C	516	BCR	C37-C22-C21	-2.21	119.83	122.92
22	D	401	CLA	C6-C5-C3	-2.21	107.65	112.66
22	C	511	CLA	CBC-CAC-C3C	-2.20	106.16	112.41
22	C	503	CLA	C4C-C3C-C2C	-2.20	103.53	106.91
23	a	411	PHO	CMD-C2D-C3D	-2.20	122.53	127.86
34	b	626	HTG	C2'-C1'-S1	-2.20	105.27	112.45
22	c	906	CLA	C2A-C1A-CHA	-2.20	120.02	123.92
24	B	620	BCR	C15-C16-C17	-2.20	118.77	123.46
25	j	101	LMG	O8-C28-O10	-2.20	118.09	123.55
23	a	411	PHO	C11-C12-C13	-2.20	108.52	115.73
22	B	609	CLA	O2A-CGA-O1A	-2.19	118.10	123.55
24	k	101	BCR	C38-C26-C25	-2.19	122.05	124.51
22	a	407	CLA	C7-C6-C5	-2.19	107.01	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	404	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
35	C	517	DGD	C4E-C3E-C2E	-2.19	106.97	110.84
22	B	603	CLA	C6-C7-C8	-2.19	108.54	115.73
22	c	910	CLA	C1D-CHD-C4C	-2.19	119.49	122.48
29	I	102	LMT	C3'-C4'-C5'	-2.19	106.23	110.88
24	b	620	BCR	C16-C17-C18	-2.19	124.19	127.31
22	A	406	CLA	CHC-C1C-C2C	-2.19	120.68	126.65
24	Y	101	BCR	C21-C20-C19	-2.18	116.53	123.23
22	c	902	CLA	O1D-CGD-CBD	-2.18	120.68	124.60
24	y	101	BCR	C10-C11-C12	-2.18	116.54	123.23
24	Y	101	BCR	C10-C11-C12	-2.18	116.55	123.23
22	B	615	CLA	CAA-CBA-CGA	-2.18	106.79	113.35
23	D	402	PHO	O2D-CGD-O1D	-2.17	119.44	123.82
24	c	916	BCR	C21-C20-C19	-2.17	116.57	123.23
22	B	608	CLA	C1-C2-C3	-2.17	121.95	125.96
22	B	605	CLA	C5-C3-C2	-2.17	116.66	121.10
22	B	609	CLA	O1D-CGD-CBD	-2.17	120.70	124.60
23	a	410	PHO	CHD-C1D-ND	-2.17	120.39	124.64
22	b	607	CLA	C4C-C3C-C2C	-2.17	103.58	106.91
35	C	518	DGD	O3D-C3D-C2D	-2.17	105.64	110.36
24	y	101	BCR	C8-C9-C10	-2.17	115.61	118.94
22	c	913	CLA	CBC-CAC-C3C	-2.17	106.26	112.41
28	a	418	SQD	O48-C23-O10	-2.17	118.17	123.55
22	B	613	CLA	C4C-C3C-C2C	-2.17	103.59	106.91
24	b	619	BCR	C24-C25-C26	-2.16	116.38	121.54
22	C	504	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
22	C	512	CLA	C6-C7-C8	-2.16	108.65	115.73
22	A	408	CLA	C2A-C1A-CHA	-2.16	120.10	123.92
25	j	101	LMG	O4-C4-C5	-2.16	103.85	109.28
22	b	602	CLA	OBD-CAD-C3D	-2.15	124.06	128.03
22	B	608	CLA	O2A-CGA-O1A	-2.15	118.21	123.55
24	C	515	BCR	C24-C23-C22	-2.15	122.98	126.21
24	b	620	BCR	C15-C14-C13	-2.15	124.24	127.31
22	C	514	CLA	C2A-C1A-CHA	-2.15	120.11	123.92
22	c	905	CLA	C7-C6-C5	-2.15	107.14	113.11
35	C	517	DGD	O6D-C1D-O3G	-2.15	104.92	110.02
25	A	410	LMG	O8-C28-O10	-2.15	118.22	123.55
22	B	613	CLA	CBA-CAA-C2A	-2.15	107.37	113.80
35	H	102	DGD	C1D-O6D-C5D	-2.15	109.67	113.72
24	b	620	BCR	C32-C1-C6	-2.15	106.83	110.31
24	y	101	BCR	C23-C24-C25	-2.15	121.25	127.25
25	J	101	LMG	C9-C8-C7	-2.15	107.02	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	623	HTG	C4'-C3'-C2'	-2.14	103.41	114.45
22	A	408	CLA	C1C-NC-C4C	-2.14	105.82	107.06
36	v	202	HEM	CMA-C3A-C4A	-2.14	125.17	128.46
22	B	612	CLA	C1C-NC-C4C	-2.14	105.82	107.06
24	y	101	BCR	C35-C13-C14	-2.14	119.93	122.92
22	A	406	CLA	C2A-C1A-CHA	-2.14	120.13	123.92
24	b	619	BCR	C35-C13-C14	-2.14	119.93	122.92
22	B	615	CLA	CHC-C1C-NC	-2.13	120.07	124.08
22	B	604	CLA	CHC-C1C-NC	-2.13	120.07	124.08
22	B	616	CLA	C4C-C3C-C2C	-2.13	103.64	106.91
35	C	519	DGD	O6D-C1D-C2D	-2.13	106.18	110.30
22	a	407	CLA	C11-C10-C8	-2.13	108.74	115.73
22	B	607	CLA	C4C-C3C-C2C	-2.13	103.64	106.91
22	B	614	CLA	C2A-C1A-CHA	-2.13	120.14	123.92
22	D	403	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
22	A	405	CLA	CHC-C1C-NC	-2.13	120.08	124.08
22	b	616	CLA	C6-C7-C8	-2.12	108.76	115.73
22	c	911	CLA	C16-C15-C13	-2.12	108.76	115.73
22	a	407	CLA	CAA-C2A-C3A	-2.12	106.99	112.81
26	D	406	PL9	C22-C23-C24	-2.12	122.35	127.68
23	A	407	PHO	CMD-C2D-C3D	-2.12	122.73	127.86
22	b	611	CLA	C2A-C1A-CHA	-2.12	120.16	123.92
36	V	202	HEM	CBA-CAA-C2A	-2.11	108.45	112.48
24	Y	101	BCR	C11-C12-C13	-2.11	120.49	126.42
24	a	413	BCR	C32-C1-C31	-2.11	102.04	108.50
37	H	101	RRX	C20-C21-C22	-2.11	124.30	127.31
22	b	614	CLA	C1C-NC-C4C	-2.11	105.84	107.06
24	C	515	BCR	C11-C12-C13	-2.10	120.50	126.42
22	c	904	CLA	C6-C5-C3	-2.10	107.90	112.66
22	C	504	CLA	C2A-C1A-CHA	-2.10	120.20	123.92
22	C	512	CLA	O1D-CGD-CBD	-2.10	120.83	124.60
24	b	619	BCR	C23-C24-C25	-2.10	121.38	127.25
22	b	608	CLA	CBC-CAC-C3C	-2.10	106.46	112.41
27	D	410	LHG	C34-C33-C32	-2.09	103.67	114.45
22	c	903	CLA	OBD-CAD-C3D	-2.09	124.17	128.03
22	b	612	CLA	C1-C2-C3	-2.09	122.11	125.96
22	B	614	CLA	O2A-CGA-O1A	-2.09	118.37	123.55
26	D	406	PL9	C36-C37-C38	-2.08	104.82	111.97
22	B	611	CLA	C2A-C1A-CHA	-2.08	120.23	123.92
22	B	614	CLA	C7-C6-C5	-2.08	107.33	113.11
22	c	907	CLA	CHC-C1C-C2C	-2.08	120.98	126.65
26	D	406	PL9	C42-C43-C44	-2.08	122.46	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	414	SQD	O48-C23-O10	-2.08	118.39	123.55
22	b	602	CLA	C5-C3-C2	-2.08	116.85	121.10
22	c	914	CLA	OBD-CAD-C3D	-2.08	124.20	128.03
25	j	101	LMG	O8-C9-C8	-2.07	103.45	108.66
24	c	915	BCR	C35-C13-C14	-2.07	120.02	122.92
24	b	619	BCR	C37-C22-C21	-2.07	120.02	122.92
23	a	410	PHO	CHD-C4C-NC	-2.07	120.99	124.97
24	c	916	BCR	C37-C22-C21	-2.07	120.02	122.92
35	C	517	DGD	O1G-C1A-O1A	-2.07	118.42	123.55
22	c	903	CLA	C16-C15-C13	-2.07	108.95	115.73
22	b	603	CLA	O2A-CGA-O1A	-2.07	118.42	123.55
24	B	618	BCR	C40-C30-C25	-2.06	106.96	110.31
22	B	604	CLA	C1D-CHD-C4C	-2.06	119.67	122.48
22	a	408	CLA	CBA-CAA-C2A	-2.06	107.64	113.80
22	c	902	CLA	O2A-CGA-O1A	-2.06	118.44	123.55
34	b	626	HTG	C4'-C3'-C2'	-2.06	103.86	114.45
22	b	603	CLA	C4C-C3C-C2C	-2.05	103.76	106.91
23	a	410	PHO	C4D-ND-C1D	-2.05	103.28	106.98
24	b	619	BCR	C20-C21-C22	-2.05	124.38	127.31
22	c	914	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
22	c	907	CLA	O1D-CGD-CBD	-2.05	120.93	124.60
28	l	101	SQD	O48-C23-O10	-2.05	118.47	123.55
24	B	619	BCR	C15-C14-C13	-2.04	124.39	127.31
27	L	101	LHG	O8-C23-O10	-2.04	118.47	123.55
22	c	910	CLA	C4C-C3C-C2C	-2.04	103.77	106.91
37	H	101	RRX	C33-C5-C6	-2.04	122.22	124.51
22	B	611	CLA	CAA-CBA-CGA	-2.04	107.19	113.35
24	B	618	BCR	C30-C25-C26	-2.04	119.72	122.59
22	C	513	CLA	C4C-C3C-C2C	-2.04	103.78	106.91
22	b	603	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
22	c	904	CLA	CAA-C2A-C3A	-2.04	107.23	112.81
35	h	102	DGD	C3G-O3G-C1D	-2.04	109.58	113.76
22	c	910	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
34	B	623	HTG	C2'-C1'-S1	-2.03	105.81	112.45
35	c	918	DGD	C3A-C2A-C1A	-2.03	106.16	113.58
35	c	917	DGD	O3G-C3G-C2G	-2.03	106.15	110.99
23	A	407	PHO	C7-C6-C5	-2.03	107.46	113.11
22	C	506	CLA	O2A-CGA-O1A	-2.03	118.51	123.55
35	c	917	DGD	O4D-C4D-C5D	-2.03	104.17	109.28
22	B	604	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
24	C	516	BCR	C8-C7-C6	-2.03	121.57	127.25
22	a	409	CLA	C1B-CHB-C4A	-2.03	126.10	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	C2A-C1A-CHA	-2.03	120.33	123.92
22	B	608	CLA	C2A-C1A-CHA	-2.03	120.33	123.92
24	b	620	BCR	C23-C24-C25	-2.02	121.58	127.25
24	k	101	BCR	C15-C16-C17	-2.02	119.14	123.46
24	C	516	BCR	C23-C24-C25	-2.02	121.59	127.25
28	D	408	SQD	O5-C1-C2	-2.02	106.40	110.30
22	D	403	CLA	C10-C8-C7	-2.02	102.40	112.10
22	A	406	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
22	B	605	CLA	C6-C7-C8	-2.02	109.12	115.73
22	C	503	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
35	c	918	DGD	C2G-O2G-C1B	-2.01	113.12	117.88
24	C	515	BCR	C36-C18-C17	-2.01	120.10	122.92
34	B	627	HTG	O5-C1-S1	-2.01	104.83	110.15
27	A	412	LHG	O7-C7-O9	-2.01	118.87	122.94
25	c	920	LMG	O8-C28-O10	-2.01	118.56	123.55
23	A	407	PHO	CHC-C1C-C2C	-2.01	121.02	125.62
28	l	101	SQD	C5-C6-S	-2.00	111.55	114.34
22	A	406	CLA	CBC-CAC-C3C	-2.00	106.72	112.41
22	B	617	CLA	C1-C2-C3	-2.00	122.27	125.96
24	c	915	BCR	C24-C23-C22	-2.00	123.20	126.21
24	y	101	BCR	C35-C13-C12	2.00	121.29	118.10
22	B	605	CLA	CMD-C2D-C3D	2.00	128.61	124.89
28	b	621	SQD	C46-O48-C23	2.00	123.15	117.13
22	c	909	CLA	C3B-C4B-NB	2.00	111.80	109.21
28	a	418	SQD	C4-C3-C2	2.01	114.38	110.84
34	D	415	HTG	O3-C3-C4	2.01	114.72	110.36
22	a	412	CLA	CAC-C3C-C4C	2.01	127.66	124.83
22	B	612	CLA	C1-O2A-CGA	2.01	121.59	116.77
22	c	913	CLA	CMC-C2C-C1C	2.01	128.06	125.02
24	C	515	BCR	C33-C5-C4	2.01	117.26	113.45
28	f	101	SQD	O9-S-C6	2.01	108.52	106.79
22	b	602	CLA	C3C-C4C-NC	2.01	112.25	110.21
25	b	622	LMG	O6-C5-C4	2.02	113.38	109.66
29	T	102	LMT	O1'-C1-C2	2.02	116.87	109.68
22	b	608	CLA	CMC-C2C-C3C	2.02	131.68	126.09
22	A	406	CLA	CHB-C4A-NA	2.02	127.30	124.51
22	C	503	CLA	C3B-C4B-NB	2.02	111.82	109.21
22	B	616	CLA	C3C-C4C-NC	2.02	112.26	110.21
22	B	617	CLA	CMC-C2C-C1C	2.02	128.09	125.02
22	C	505	CLA	CMC-C2C-C3C	2.03	131.70	126.09
29	a	419	LMT	C3'-C4'-C5'	2.03	115.17	110.88
22	C	502	CLA	C3B-C4B-NB	2.03	111.83	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Z	101	LMT	C2'-C3'-C4'	2.03	113.81	109.61
22	D	404	CLA	C3B-C4B-NB	2.03	111.83	109.21
35	C	519	DGD	C6D-C5D-C4D	2.03	116.32	112.00
35	C	518	DGD	O6E-C5E-C6E	2.03	111.27	106.41
22	B	603	CLA	CAC-C3C-C2C	2.03	131.01	127.49
29	Z	101	LMT	C1'-O5'-C5'	2.03	117.54	113.72
24	Y	101	BCR	C38-C26-C27	2.03	117.31	113.45
22	c	911	CLA	C4A-NA-C1A	2.03	108.98	106.45
22	c	905	CLA	CMC-C2C-C1C	2.03	128.11	125.02
22	B	616	CLA	CMB-C2B-C3B	2.04	128.67	124.89
34	b	624	HTG	C4-C3-C2	2.04	114.43	110.84
22	A	406	CLA	O2A-CGA-CBA	2.04	117.84	111.90
22	c	909	CLA	OBD-CAD-CBD	2.04	129.02	125.94
22	A	405	CLA	C3B-C4B-NB	2.04	111.85	109.21
28	b	621	SQD	O8-S-C6	2.04	108.50	106.01
35	C	517	DGD	C6D-C5D-C4D	2.05	116.36	112.00
22	C	505	CLA	O2A-CGA-CBA	2.05	117.86	111.90
29	B	622	LMT	O5'-C5'-C4'	2.05	113.44	109.66
25	d	409	LMG	C9-O8-C28	2.05	123.30	117.13
24	D	405	BCR	C2-C1-C6	2.05	113.69	110.48
29	f	102	LMT	C6'-C5'-C4'	2.06	118.84	113.24
24	A	409	BCR	C35-C13-C12	2.06	121.38	118.10
25	J	101	LMG	O7-C10-C11	2.06	115.83	111.55
23	D	402	PHO	CED-O2D-CGD	2.06	120.80	115.97
22	d	403	CLA	CAC-C3C-C4C	2.06	127.73	124.83
29	a	419	LMT	O4'-C4B-C5B	2.06	114.48	109.28
29	Z	101	LMT	C3'-C4'-C5'	2.06	115.26	110.88
22	A	405	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	b	604	CLA	CAC-C3C-C4C	2.07	127.75	124.83
22	D	403	CLA	CED-O2D-CGD	2.07	120.82	115.97
22	a	407	CLA	C4A-NA-C1A	2.07	109.02	106.45
29	A	414	LMT	C3'-C4'-C5'	2.07	115.28	110.88
29	A	414	LMT	O1'-C1'-C2'	2.07	111.62	108.23
22	c	912	CLA	C1-O2A-CGA	2.08	121.76	116.77
25	C	531	LMG	C9-O8-C28	2.08	123.39	117.13
22	c	903	CLA	C3B-C4B-NB	2.08	111.90	109.21
22	b	610	CLA	C3C-C4C-NC	2.08	112.32	110.21
26	d	405	PL9	C22-C21-C19	2.08	119.97	112.93
22	b	607	CLA	O2A-CGA-CBA	2.09	117.97	111.90
22	C	510	CLA	C4A-NA-C1A	2.09	109.05	106.45
24	Y	101	BCR	C30-C25-C24	2.09	121.62	115.73
22	b	613	CLA	C3B-C4B-NB	2.10	111.92	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	CMD-C2D-C3D	2.10	128.78	124.89
22	D	404	CLA	C4A-NA-C1A	2.10	109.05	106.45
22	B	615	CLA	CMB-C2B-C3B	2.10	128.79	124.89
22	C	512	CLA	CHB-C4A-NA	2.10	127.42	124.51
29	a	419	LMT	O1B-C1B-C2B	2.10	112.84	108.11
23	a	410	PHO	CMC-C2C-C1C	2.10	128.31	125.04
27	C	522	LHG	P-O6-C4	2.10	124.08	118.30
34	b	624	HTG	C1-O5-C5	2.10	116.74	112.69
24	d	404	BCR	C12-C13-C14	2.10	122.17	118.94
22	c	906	CLA	C4A-NA-C1A	2.11	109.06	106.45
27	D	410	LHG	O8-C23-C24	2.11	118.03	111.90
29	f	102	LMT	C1-O1'-C1'	2.11	117.49	113.87
22	B	611	CLA	CMC-C2C-C1C	2.11	128.22	125.02
22	D	403	CLA	CAC-C3C-C4C	2.11	127.81	124.83
22	D	401	CLA	CAC-C3C-C4C	2.11	127.81	124.83
34	b	627	HTG	C1-O5-C5	2.11	116.76	112.69
24	C	515	BCR	C36-C18-C19	2.12	121.47	118.10
22	c	907	CLA	CAC-C3C-C4C	2.12	127.82	124.83
27	L	101	LHG	O8-C6-C5	2.12	113.99	108.66
22	c	913	CLA	C3C-C4C-NC	2.12	112.36	110.21
22	C	504	CLA	CED-O2D-CGD	2.12	120.95	115.97
22	c	912	CLA	C1C-NC-C4C	2.12	108.28	107.06
24	y	101	BCR	C34-C9-C8	2.13	121.49	118.10
22	C	513	CLA	CED-O2D-CGD	2.13	120.96	115.97
22	b	609	CLA	O2A-CGA-CBA	2.13	118.10	111.90
25	C	520	LMG	O6-C5-C6	2.13	111.52	106.41
22	c	911	CLA	C1-O2A-CGA	2.13	121.89	116.77
27	C	522	LHG	O4-P-O5	2.14	118.86	110.50
26	d	405	PL9	C10-C9-C11	2.14	119.00	115.29
35	C	517	DGD	O6E-C5E-C6E	2.14	111.53	106.41
29	a	419	LMT	O3B-C3B-C2B	2.14	115.01	110.36
34	B	626	HTG	O5-C5-C4	2.14	113.60	109.66
22	c	910	CLA	CED-O2D-CGD	2.14	120.98	115.97
27	l	102	LHG	O8-C23-C24	2.14	118.12	111.90
36	e	101	HEM	CMB-C2B-C3B	2.14	128.86	124.89
22	b	611	CLA	C4A-NA-C1A	2.14	109.11	106.45
22	b	603	CLA	C3B-C4B-NB	2.14	111.98	109.21
22	C	512	CLA	CED-O2D-CGD	2.14	121.00	115.97
22	D	404	CLA	CMC-C2C-C1C	2.15	128.27	125.02
34	b	623	HTG	O5-C1-C2	2.15	113.22	110.28
22	c	903	CLA	C4A-NA-C1A	2.15	109.12	106.45
29	c	921	LMT	C1B-O5B-C5B	2.15	117.77	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	418	SQD	O5-C1-O6	2.16	115.14	110.02
24	b	619	BCR	C30-C25-C24	2.16	121.79	115.73
29	A	414	LMT	O2B-C2B-C3B	2.16	115.05	110.36
22	B	613	CLA	C4A-NA-C1A	2.16	109.13	106.45
22	a	408	CLA	CMC-C2C-C3C	2.16	132.07	126.09
22	c	911	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	b	610	CLA	O2A-CGA-CBA	2.16	118.19	111.90
25	j	101	LMG	O3-C3-C4	2.16	115.06	110.36
25	i	101	LMG	C6-C5-C4	2.16	118.06	113.00
22	b	608	CLA	C3B-C4B-NB	2.17	112.01	109.21
24	Y	101	BCR	C36-C18-C19	2.17	121.55	118.10
22	B	610	CLA	C3B-C4B-NB	2.17	112.01	109.21
22	b	602	CLA	CMC-C2C-C1C	2.17	128.31	125.02
23	a	410	PHO	CAC-C3C-C2C	2.17	131.25	127.49
27	d	407	LHG	O7-C7-C8	2.17	116.06	111.55
28	A	413	SQD	O48-C46-C45	2.17	114.12	108.66
25	B	621	LMG	O6-C1-O1	2.18	115.19	110.02
22	a	408	CLA	C4-C3-C5	2.18	119.07	115.29
22	b	604	CLA	C6-C5-C3	2.18	117.59	112.66
26	a	415	PL9	C51-C49-C50	2.18	119.69	114.60
37	h	101	RRX	C2-C1-C6	2.18	113.89	110.48
22	b	616	CLA	CAC-C3C-C4C	2.18	127.91	124.83
24	B	620	BCR	C33-C5-C4	2.18	117.60	113.45
22	C	509	CLA	C1C-NC-C4C	2.19	108.31	107.06
36	v	202	HEM	CMC-C2C-C3C	2.19	128.95	124.89
22	C	508	CLA	C3B-C4B-NB	2.19	112.04	109.21
22	C	505	CLA	CMB-C2B-C3B	2.19	128.96	124.89
31	c	924	DMS	O-S-C2	2.19	118.11	106.54
36	E	102	HEM	CMB-C2B-C3B	2.20	128.97	124.89
22	B	607	CLA	O2A-CGA-CBA	2.20	118.29	111.90
34	V	203	HTG	O5-C5-C6	2.20	111.67	106.41
22	b	608	CLA	C1-O2A-CGA	2.20	122.04	116.77
22	c	909	CLA	C1C-NC-C4C	2.20	108.32	107.06
23	A	407	PHO	O2A-CGA-CBA	2.20	118.31	111.90
25	B	621	LMG	O1-C1-C2	2.20	111.83	108.23
22	c	912	CLA	CAC-C3C-C4C	2.21	127.94	124.83
22	a	409	CLA	C3C-C4C-NC	2.21	112.45	110.21
22	C	506	CLA	C3B-C4B-NB	2.21	112.06	109.21
35	h	102	DGD	O2E-C2E-C1E	2.21	114.65	110.03
22	b	615	CLA	CMB-C2B-C3B	2.21	129.00	124.89
22	B	612	CLA	CAC-C3C-C4C	2.21	127.95	124.83
22	B	614	CLA	CMB-C2B-C3B	2.21	129.00	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	909	CLA	CMD-C2D-C3D	2.22	129.00	124.89
22	b	606	CLA	C3D-CAD-CBD	2.22	110.74	107.60
23	D	402	PHO	C4D-C3D-CAD	2.22	109.53	105.41
22	c	904	CLA	C4-C3-C5	2.22	119.15	115.29
22	a	409	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	A	406	CLA	CED-O2D-CGD	2.23	121.19	115.97
22	b	605	CLA	C1-O2A-CGA	2.23	122.11	116.77
34	v	203	HTG	O2-C2-C1	2.23	114.71	110.27
34	B	626	HTG	O5-C5-C6	2.23	111.75	106.41
22	b	616	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	A	406	CLA	C3C-C4C-NC	2.23	112.47	110.21
22	C	506	CLA	C3A-C2A-C1A	2.23	104.68	101.34
22	A	406	CLA	C3B-C4B-NB	2.23	112.10	109.21
22	C	511	CLA	CMC-C2C-C1C	2.23	128.41	125.02
22	B	609	CLA	C3B-C4B-NB	2.24	112.11	109.21
26	A	411	PL9	C10-C9-C11	2.24	119.18	115.29
34	b	623	HTG	C1-O5-C5	2.24	117.01	112.69
22	C	508	CLA	CMC-C2C-C1C	2.25	128.43	125.02
35	C	518	DGD	O1G-C1A-C2A	2.25	118.44	111.90
25	i	101	LMG	O1-C1-C2	2.25	111.90	108.23
24	b	618	BCR	C30-C25-C24	2.25	122.06	115.73
22	c	914	CLA	CAC-C3C-C4C	2.25	128.01	124.83
29	a	419	LMT	O2B-C2B-C1B	2.26	114.75	110.03
22	C	506	CLA	CMB-C2B-C3B	2.26	129.08	124.89
22	B	615	CLA	CMC-C2C-C1C	2.26	128.44	125.02
29	I	102	LMT	O3'-C3'-C4'	2.26	115.01	109.87
26	D	406	PL9	C2-C1-C6	2.26	121.62	117.82
22	A	408	CLA	CAC-C3C-C4C	2.26	128.02	124.83
29	A	414	LMT	O3B-C3B-C2B	2.27	115.29	110.36
22	B	607	CLA	C1-O2A-CGA	2.27	122.22	116.77
22	b	611	CLA	C3B-C4B-NB	2.27	112.14	109.21
22	C	506	CLA	CMC-C2C-C1C	2.27	128.46	125.02
35	C	519	DGD	O6E-C5E-C6E	2.27	111.85	106.41
22	C	510	CLA	CMD-C2D-C3D	2.27	129.11	124.89
22	B	611	CLA	CMD-C2D-C3D	2.27	129.11	124.89
22	C	503	CLA	CMB-C2B-C1B	2.27	131.96	128.46
22	c	905	CLA	CED-O2D-CGD	2.28	121.30	115.97
22	c	910	CLA	CMB-C2B-C3B	2.28	129.12	124.89
25	b	622	LMG	O8-C9-C8	2.28	114.38	108.66
22	B	608	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	d	403	CLA	O2A-CGA-CBA	2.28	118.53	111.90
34	b	624	HTG	O5-C5-C6	2.28	111.87	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	909	CLA	O2A-CGA-CBA	2.28	118.53	111.90
22	C	507	CLA	CMB-C2B-C3B	2.28	129.12	124.89
22	B	602	CLA	CED-O2D-CGD	2.28	121.31	115.97
22	c	910	CLA	C4A-NA-C1A	2.28	109.28	106.45
25	B	621	LMG	C4-C3-C2	2.28	114.86	110.84
22	B	606	CLA	CMD-C2D-C3D	2.28	129.13	124.89
22	C	511	CLA	C3B-C4B-NB	2.28	112.16	109.21
22	c	909	CLA	CMC-C2C-C3C	2.29	132.42	126.09
22	c	909	CLA	CAC-C3C-C2C	2.29	131.46	127.49
22	b	614	CLA	C3B-C4B-NB	2.29	112.17	109.21
22	b	613	CLA	C4A-NA-C1A	2.29	109.29	106.45
24	c	916	BCR	C36-C18-C19	2.29	121.75	118.10
25	B	621	LMG	O6-C5-C4	2.30	113.90	109.66
25	d	409	LMG	O6-C5-C6	2.30	111.92	106.41
22	b	605	CLA	C3B-C4B-NB	2.30	112.19	109.21
22	B	610	CLA	CAC-C3C-C4C	2.30	128.08	124.83
22	d	402	CLA	CAC-C3C-C4C	2.30	128.08	124.83
23	a	410	PHO	C4D-C3D-CAD	2.30	109.68	105.41
22	C	514	CLA	CMD-C2D-C3D	2.31	129.17	124.89
22	d	403	CLA	C3B-C4B-NB	2.31	112.20	109.21
22	B	608	CLA	CMC-C2C-C1C	2.31	128.53	125.02
22	B	603	CLA	CMD-C2D-C3D	2.31	129.18	124.89
22	d	402	CLA	C3C-C4C-NC	2.31	112.56	110.21
22	C	506	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	D	401	CLA	O2A-CGA-CBA	2.32	118.65	111.90
29	c	931	LMT	O1'-C1'-C2'	2.32	112.02	108.23
22	B	607	CLA	CMC-C2C-C1C	2.33	128.55	125.02
35	d	406	DGD	O1G-C1A-C2A	2.33	118.68	111.90
22	C	512	CLA	C3A-C2A-C1A	2.33	104.83	101.34
22	a	412	CLA	CMB-C2B-C3B	2.34	129.23	124.89
26	A	411	PL9	C26-C27-C28	2.34	119.98	111.97
22	c	906	CLA	C3C-C4C-NC	2.34	112.58	110.21
22	b	604	CLA	C3B-C4B-NB	2.34	112.23	109.21
23	a	410	PHO	CMB-C2B-C1B	2.34	128.69	125.04
22	b	610	CLA	CAC-C3C-C4C	2.34	128.13	124.83
22	b	617	CLA	C3B-C4B-NB	2.35	112.24	109.21
34	b	632	HTG	O2-C2-C3	2.35	115.46	110.36
23	A	407	PHO	C4D-C3D-CAD	2.35	109.77	105.41
25	B	621	LMG	C9-O8-C28	2.36	124.24	117.13
22	b	613	CLA	CMC-C2C-C1C	2.36	128.60	125.02
29	f	102	LMT	O1B-C4'-C5'	2.37	116.04	108.14
22	b	602	CLA	CMB-C2B-C3B	2.37	129.29	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	610	CLA	CMD-C2D-C3D	2.37	129.29	124.89
22	a	407	CLA	CMD-C2D-C3D	2.37	129.29	124.89
22	d	402	CLA	CMC-C2C-C1C	2.37	128.62	125.02
22	a	409	CLA	O2A-CGA-CBA	2.37	118.81	111.90
22	B	613	CLA	CMB-C2B-C3B	2.38	129.30	124.89
22	b	617	CLA	C4-C3-C5	2.38	119.41	115.29
22	B	609	CLA	C1-O2A-CGA	2.38	122.47	116.77
22	c	904	CLA	C3B-C4B-NB	2.38	112.29	109.21
22	b	607	CLA	C4A-NA-C1A	2.38	109.41	106.45
22	C	510	CLA	C4-C3-C5	2.38	119.42	115.29
22	B	611	CLA	CMB-C2B-C3B	2.38	129.32	124.89
22	c	905	CLA	CMD-C2D-C3D	2.39	129.32	124.89
22	c	906	CLA	CAC-C3C-C4C	2.39	128.19	124.83
22	C	512	CLA	O2D-CGD-CBD	2.39	115.57	111.30
22	c	913	CLA	O2A-CGA-CBA	2.39	118.85	111.90
22	b	611	CLA	CMC-C2C-C1C	2.40	128.66	125.02
22	b	611	CLA	CMB-C2B-C3B	2.40	129.35	124.89
22	B	605	CLA	C4-C3-C5	2.40	119.46	115.29
22	B	615	CLA	C3B-C4B-NB	2.40	112.32	109.21
22	b	604	CLA	O2A-CGA-CBA	2.41	118.90	111.90
22	B	609	CLA	CMC-C2C-C1C	2.41	128.67	125.02
22	B	613	CLA	C3B-C4B-NB	2.41	112.33	109.21
22	B	603	CLA	CMB-C2B-C3B	2.42	129.37	124.89
25	c	930	LMG	C1-O6-C5	2.42	118.28	113.72
22	C	505	CLA	C3B-C4B-NB	2.42	112.34	109.21
26	D	406	PL9	C51-C49-C50	2.43	120.27	114.60
22	c	914	CLA	C4A-NA-C1A	2.43	109.47	106.45
22	B	617	CLA	C4-C3-C5	2.43	119.51	115.29
22	C	514	CLA	C1-O2A-CGA	2.43	122.61	116.77
24	D	405	BCR	C32-C1-C6	2.44	114.26	110.31
22	B	617	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	D	405	BCR	C30-C25-C24	2.44	122.58	115.73
27	C	522	LHG	O8-C23-C24	2.44	119.00	111.90
22	D	401	CLA	C4-C3-C5	2.44	119.53	115.29
24	Y	101	BCR	C34-C9-C8	2.44	121.99	118.10
22	b	605	CLA	O2A-CGA-CBA	2.44	119.01	111.90
22	c	910	CLA	CMD-C2D-C3D	2.45	129.44	124.89
22	B	605	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	c	920	LMG	O8-C9-C8	2.45	114.82	108.66
22	a	412	CLA	CED-O2D-CGD	2.45	121.72	115.97
22	d	402	CLA	CMD-C2D-C3D	2.46	129.45	124.89
25	C	531	LMG	O6-C5-C6	2.46	112.30	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C1-O2A-CGA	2.46	122.68	116.77
22	c	914	CLA	CMD-C2D-C3D	2.46	129.46	124.89
22	C	511	CLA	C3C-C4C-NC	2.46	112.71	110.21
22	B	614	CLA	C3B-C4B-NB	2.46	112.40	109.21
35	C	517	DGD	O2G-C1B-C2B	2.46	116.67	111.55
22	B	609	CLA	CMB-C2B-C3B	2.47	129.47	124.89
22	d	403	CLA	CED-O2D-CGD	2.47	121.75	115.97
22	C	511	CLA	O2A-CGA-CBA	2.47	119.08	111.90
22	c	914	CLA	CED-O2D-CGD	2.47	121.76	115.97
25	C	520	LMG	O8-C9-C8	2.47	114.86	108.66
22	B	604	CLA	CMC-C2C-C1C	2.47	128.77	125.02
22	b	614	CLA	O2A-CGA-CBA	2.48	119.12	111.90
22	c	902	CLA	C3B-C4B-NB	2.49	112.42	109.21
28	b	621	SQD	C3-C4-C5	2.49	114.60	110.22
22	b	607	CLA	CMB-C2B-C3B	2.49	129.51	124.89
26	A	411	PL9	C3-C4-C5	2.49	121.97	118.63
28	D	408	SQD	C4-C3-C2	2.49	115.23	110.84
35	C	518	DGD	C6D-C5D-C4D	2.49	117.31	112.00
26	A	411	PL9	C30-C29-C31	2.49	119.61	115.29
22	A	405	CLA	O2A-CGA-CBA	2.49	119.15	111.90
22	c	913	CLA	C1-O2A-CGA	2.49	122.75	116.77
22	B	616	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	b	608	CLA	CMD-C2D-C3D	2.50	129.53	124.89
22	B	605	CLA	O2A-CGA-CBA	2.50	119.18	111.90
22	c	913	CLA	CMD-C2D-C3D	2.51	129.54	124.89
22	C	505	CLA	C1-O2A-CGA	2.51	122.79	116.77
22	c	907	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	a	408	CLA	C3B-C4B-NB	2.51	112.45	109.21
22	C	508	CLA	C3C-C4C-NC	2.51	112.75	110.21
27	d	401	LHG	O4-P-O5	2.51	120.33	110.50
22	b	612	CLA	O2A-CGA-CBA	2.51	119.21	111.90
22	c	902	CLA	C3C-C4C-NC	2.51	112.76	110.21
22	a	407	CLA	CMC-C2C-C1C	2.52	128.84	125.02
22	b	606	CLA	CAC-C3C-C4C	2.52	128.39	124.83
22	b	614	CLA	CED-O2D-CGD	2.53	121.89	115.97
22	B	614	CLA	C4A-NA-C1A	2.53	109.59	106.45
26	a	415	PL9	C40-C39-C41	2.53	119.68	115.29
22	C	503	CLA	CMC-C2C-C1C	2.53	128.86	125.02
22	B	612	CLA	C3B-C4B-NB	2.53	112.48	109.21
22	C	506	CLA	C4-C3-C5	2.53	119.68	115.29
22	A	406	CLA	CMB-C2B-C3B	2.53	129.59	124.89
22	A	408	CLA	O2A-CGA-CBA	2.54	119.28	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	101	LMG	O8-C28-C29	2.54	119.28	111.90
24	D	405	BCR	C36-C18-C19	2.54	122.14	118.10
22	c	914	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	A	407	PHO	CED-O2D-CGD	2.54	121.94	115.97
26	D	406	PL9	C25-C24-C26	2.55	119.70	115.29
22	B	604	CLA	CMD-C2D-C3D	2.55	129.62	124.89
22	c	907	CLA	C4-C3-C5	2.55	119.71	115.29
22	a	409	CLA	CAC-C3C-C4C	2.55	128.43	124.83
22	c	912	CLA	CMC-C2C-C1C	2.55	128.89	125.02
22	D	401	CLA	CMB-C2B-C1B	2.55	132.39	128.46
22	b	603	CLA	C3C-C4C-NC	2.55	112.80	110.21
22	b	610	CLA	O2D-CGD-CBD	2.56	115.86	111.30
22	C	502	CLA	C4A-NA-C1A	2.56	109.63	106.45
22	b	615	CLA	O2A-CGA-CBA	2.56	119.36	111.90
26	a	415	PL9	C10-C9-C11	2.56	119.74	115.29
22	B	616	CLA	C3B-C4B-NB	2.57	112.53	109.21
22	b	602	CLA	C4-C3-C5	2.57	119.75	115.29
22	B	612	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	D	404	CLA	CMB-C2B-C3B	2.58	129.67	124.89
22	B	605	CLA	C3B-C4B-NB	2.58	112.54	109.21
27	l	102	LHG	C6-O8-C23	2.58	124.90	117.13
22	A	408	CLA	CMC-C2C-C1C	2.58	128.94	125.02
22	C	514	CLA	C3C-C4C-NC	2.59	112.83	110.21
22	D	401	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	d	409	LMG	O8-C28-C29	2.59	119.43	111.90
22	C	510	CLA	CAC-C3C-C4C	2.59	128.49	124.83
22	b	605	CLA	CMB-C2B-C3B	2.60	129.71	124.89
22	c	913	CLA	C4A-NA-C1A	2.60	109.67	106.45
25	d	409	LMG	C3-C4-C5	2.60	114.79	110.22
22	b	615	CLA	C6-C5-C3	2.60	119.12	114.55
23	a	410	PHO	C4A-NA-C1A	2.60	110.27	108.16
22	D	404	CLA	C4-C3-C5	2.60	119.80	115.29
29	T	102	LMT	O5'-C1'-C2'	2.60	115.32	110.30
22	a	408	CLA	O2A-CGA-CBA	2.60	119.48	111.90
22	b	615	CLA	C3B-C4B-NB	2.61	112.58	109.21
27	A	412	LHG	C6-O8-C23	2.61	124.99	117.13
22	B	614	CLA	C3C-C4C-NC	2.61	112.86	110.21
22	a	412	CLA	CMC-C2C-C1C	2.61	128.99	125.02
22	B	617	CLA	CAC-C3C-C4C	2.62	128.52	124.83
29	c	921	LMT	O1'-C1'-C2'	2.62	112.51	108.23
22	c	903	CLA	CMC-C2C-C1C	2.62	128.99	125.02
29	f	102	LMT	O5'-C5'-C6'	2.62	112.69	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	CED-O2D-CGD	2.62	122.12	115.97
22	C	504	CLA	CMC-C2C-C1C	2.63	129.00	125.02
22	B	603	CLA	C1-O2A-CGA	2.63	123.07	116.77
22	b	617	CLA	O2A-CGA-CBA	2.63	119.55	111.90
25	b	622	LMG	C9-O8-C28	2.63	125.04	117.13
22	C	507	CLA	C4-C3-C5	2.63	119.85	115.29
22	a	409	CLA	CMD-C2D-C3D	2.63	129.77	124.89
22	B	613	CLA	O2D-CGD-CBD	2.63	116.00	111.30
22	b	606	CLA	C3B-C4B-NB	2.64	112.62	109.21
22	C	502	CLA	CMC-C2C-C1C	2.64	129.02	125.02
22	b	609	CLA	CAC-C3C-C4C	2.64	128.56	124.83
24	k	101	BCR	C2-C1-C6	2.64	114.61	110.48
22	A	406	CLA	CAC-C3C-C4C	2.64	128.56	124.83
28	D	408	SQD	C3-C4-C5	2.65	114.89	110.22
22	B	609	CLA	O2A-CGA-CBA	2.65	119.62	111.90
24	C	515	BCR	C29-C30-C25	2.66	114.63	110.48
34	C	521	HTG	C1-O5-C5	2.66	117.82	112.69
22	c	902	CLA	CMC-C2C-C1C	2.66	129.06	125.02
23	a	410	PHO	O2A-CGA-CBA	2.66	119.65	111.90
22	b	617	CLA	C1-O2A-CGA	2.67	123.18	116.77
22	C	505	CLA	C6-C5-C3	2.67	118.71	112.66
22	c	902	CLA	C4A-NA-C1A	2.67	109.77	106.45
22	C	508	CLA	C4-C3-C5	2.67	119.92	115.29
22	b	617	CLA	CAC-C3C-C4C	2.67	128.60	124.83
22	b	615	CLA	CMD-C2D-C3D	2.67	129.85	124.89
22	c	905	CLA	CAC-C3C-C4C	2.68	128.62	124.83
24	y	101	BCR	C1-C6-C7	2.68	123.28	115.73
22	b	613	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	b	617	CLA	CMB-C2B-C3B	2.69	129.88	124.89
25	j	101	LMG	O7-C10-C11	2.69	117.14	111.55
25	c	930	LMG	O8-C28-C29	2.69	119.73	111.90
22	a	408	CLA	CMD-C2D-C3D	2.69	129.88	124.89
29	a	419	LMT	O5B-C5B-C6B	2.69	112.86	106.41
23	a	410	PHO	C2B-C1B-NB	2.69	113.81	109.82
34	b	632	HTG	O5-C1-S1	2.69	117.29	110.15
22	C	513	CLA	C3C-C4C-NC	2.70	112.94	110.21
24	C	516	BCR	C37-C22-C23	2.70	122.40	118.10
23	A	407	PHO	C4A-NA-C1A	2.70	110.35	108.16
22	B	613	CLA	C3C-C4C-NC	2.70	112.95	110.21
22	a	407	CLA	O2A-CGA-CBA	2.71	119.78	111.90
23	A	407	PHO	C2D-C1D-ND	2.71	113.83	109.82
34	b	626	HTG	C3-C4-C5	2.71	115.00	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	CED-O2D-CGD	2.71	122.33	115.97
22	B	610	CLA	C4A-NA-C1A	2.71	109.82	106.45
22	B	604	CLA	C6-C5-C3	2.71	118.81	112.66
22	C	503	CLA	C3C-C4C-NC	2.72	112.97	110.21
22	B	613	CLA	CMC-C2C-C1C	2.72	129.15	125.02
22	c	903	CLA	O2A-CGA-CBA	2.72	119.82	111.90
34	D	415	HTG	O2-C2-C3	2.72	116.28	110.36
36	E	102	HEM	CMC-C2C-C3C	2.73	129.95	124.89
22	B	611	CLA	C4A-NA-C1A	2.73	109.84	106.45
28	a	418	SQD	O9-S-C6	2.73	109.16	106.83
22	b	615	CLA	CED-O2D-CGD	2.73	122.38	115.97
22	B	608	CLA	C1-O2A-CGA	2.73	123.33	116.77
24	D	405	BCR	C38-C26-C27	2.73	118.64	113.45
22	D	403	CLA	CMB-C2B-C3B	2.74	129.97	124.89
22	B	604	CLA	CMB-C2B-C3B	2.74	129.97	124.89
22	B	616	CLA	O2A-CGA-CBA	2.74	119.87	111.90
25	D	412	LMG	O8-C28-C29	2.74	119.87	111.90
23	a	411	PHO	C4D-C3D-CAD	2.74	110.50	105.41
26	A	411	PL9	C25-C24-C26	2.74	120.05	115.29
22	b	612	CLA	C4A-NA-C1A	2.74	109.86	106.45
22	c	904	CLA	C3C-C4C-NC	2.75	112.99	110.21
22	b	616	CLA	CMB-C2B-C3B	2.75	129.99	124.89
22	C	510	CLA	C1-O2A-CGA	2.75	123.38	116.77
22	b	616	CLA	CMC-C2C-C1C	2.75	129.20	125.02
22	C	513	CLA	CMD-C2D-C3D	2.76	130.01	124.89
22	c	914	CLA	O2A-CGA-CBA	2.76	119.93	111.90
24	d	404	BCR	C30-C25-C24	2.77	123.50	115.73
22	b	603	CLA	C1-O2A-CGA	2.77	123.41	116.77
22	D	403	CLA	O2A-CGA-CBA	2.77	119.96	111.90
22	C	502	CLA	O2A-CGA-CBA	2.77	119.96	111.90
24	Y	101	BCR	C1-C6-C7	2.77	123.51	115.73
35	D	407	DGD	C1D-C2D-C3D	2.77	115.13	109.98
28	C	501	SQD	O48-C23-C24	2.77	119.97	111.90
34	v	203	HTG	O5-C1-S1	2.77	117.50	110.15
22	c	903	CLA	CMB-C2B-C3B	2.77	130.04	124.89
26	a	415	PL9	C20-C19-C21	2.77	120.10	115.29
22	C	511	CLA	CAC-C3C-C4C	2.78	128.75	124.83
22	c	914	CLA	C3C-C4C-NC	2.78	113.03	110.21
22	A	408	CLA	C3B-C4B-NB	2.79	112.81	109.21
29	Z	101	LMT	O5B-C5B-C4B	2.79	114.80	109.66
22	a	412	CLA	O2A-CGA-CBA	2.79	120.02	111.90
22	c	904	CLA	OBD-CAD-CBD	2.79	130.15	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	911	CLA	CAC-C3C-C4C	2.80	128.77	124.83
22	c	903	CLA	C3C-C4C-NC	2.80	113.05	110.21
34	B	626	HTG	C3-C4-C5	2.80	115.15	110.22
22	B	610	CLA	CMD-C2D-C3D	2.80	130.09	124.89
22	C	509	CLA	O2A-CGA-CBA	2.80	120.05	111.90
22	C	509	CLA	C4A-NA-C1A	2.80	109.93	106.45
34	b	627	HTG	C3-C4-C5	2.80	115.16	110.22
22	b	613	CLA	CED-O2D-CGD	2.81	122.56	115.97
22	b	612	CLA	CMC-C2C-C1C	2.81	129.29	125.02
22	C	502	CLA	C1-O2A-CGA	2.82	123.53	116.77
25	i	101	LMG	O7-C10-C11	2.82	117.40	111.55
25	j	101	LMG	O8-C28-C29	2.82	120.10	111.90
29	t	101	LMT	O1'-C1'-C2'	2.82	112.83	108.23
35	C	518	DGD	O3G-C1D-C2D	2.82	112.83	108.23
22	C	508	CLA	CMB-C2B-C3B	2.82	130.12	124.89
22	B	614	CLA	CMD-C2D-C3D	2.82	130.12	124.89
26	A	411	PL9	C20-C19-C21	2.82	120.19	115.29
22	D	403	CLA	C4-C3-C5	2.82	120.19	115.29
34	c	922	HTG	C1-O5-C5	2.82	118.13	112.69
22	B	612	CLA	C4A-NA-C1A	2.83	109.96	106.45
26	d	405	PL9	C53-C6-C1	2.83	120.85	114.84
22	B	613	CLA	O2A-CGA-CBA	2.83	120.14	111.90
27	D	411	LHG	O7-C7-C8	2.84	117.44	111.55
35	D	407	DGD	O1G-C1G-C2G	2.84	115.78	108.66
22	B	614	CLA	O2A-CGA-CBA	2.84	120.16	111.90
23	A	407	PHO	C3C-C4C-NC	2.84	114.84	110.19
22	c	904	CLA	CAC-C3C-C4C	2.84	128.84	124.83
27	a	416	LHG	C6-O8-C23	2.84	125.69	117.13
22	c	913	CLA	CMB-C2B-C3B	2.85	130.18	124.89
22	B	614	CLA	O2D-CGD-CBD	2.85	116.39	111.30
22	c	911	CLA	O2A-CGA-CBA	2.85	120.19	111.90
25	B	621	LMG	C3-C4-C5	2.85	115.24	110.22
22	c	906	CLA	O2A-CGA-CBA	2.86	120.21	111.90
24	d	404	BCR	C37-C22-C23	2.86	122.65	118.10
22	B	608	CLA	CMD-C2D-C3D	2.86	130.19	124.89
22	B	609	CLA	CHB-C4A-NA	2.86	128.46	124.51
29	c	931	LMT	O5'-C5'-C6'	2.86	113.26	106.41
34	D	415	HTG	C3-C4-C5	2.86	115.25	110.22
22	b	612	CLA	CAC-C3C-C4C	2.86	128.86	124.83
22	b	616	CLA	C4A-NA-C1A	2.86	110.00	106.45
22	B	606	CLA	C4-C3-C5	2.86	120.25	115.29
22	C	508	CLA	O2A-CGA-CBA	2.87	120.24	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	903	CLA	CMD-C2D-C3D	2.87	130.22	124.89
22	B	602	CLA	CMC-C2C-C1C	2.88	129.38	125.02
22	C	504	CLA	CMD-C2D-C3D	2.88	130.23	124.89
28	C	501	SQD	O2-C2-C1	2.88	116.05	110.03
22	C	502	CLA	CMD-C2D-C3D	2.88	130.23	124.89
23	a	411	PHO	CAC-C3C-C4C	2.88	128.59	125.21
26	D	406	PL9	C10-C9-C11	2.89	120.29	115.29
22	b	616	CLA	O2A-CGA-CBA	2.89	120.30	111.90
34	V	203	HTG	O5-C1-S1	2.89	117.80	110.15
22	C	504	CLA	O2A-CGA-CBA	2.89	120.31	111.90
22	A	405	CLA	C4-C3-C5	2.89	120.30	115.29
22	a	407	CLA	C3C-C4C-NC	2.89	113.14	110.21
22	B	607	CLA	CMB-C2B-C3B	2.90	130.27	124.89
22	D	403	CLA	C3C-C4C-NC	2.90	113.15	110.21
35	c	918	DGD	O1G-C1A-C2A	2.90	120.34	111.90
22	c	902	CLA	C1-O2A-CGA	2.91	123.75	116.77
22	c	907	CLA	O2A-CGA-CBA	2.91	120.36	111.90
22	B	610	CLA	C1-O2A-CGA	2.91	123.75	116.77
22	a	407	CLA	CMB-C2B-C3B	2.91	130.29	124.89
22	b	605	CLA	CAC-C3C-C4C	2.91	128.93	124.83
22	B	602	CLA	O2A-CGA-CBA	2.91	120.38	111.90
22	B	605	CLA	C4A-NA-C1A	2.91	110.07	106.45
23	a	411	PHO	C4A-NA-C1A	2.91	110.52	108.16
22	b	615	CLA	C4A-NA-C1A	2.92	110.07	106.45
22	C	503	CLA	CAC-C3C-C4C	2.92	128.95	124.83
22	C	512	CLA	C3B-C4B-NB	2.92	112.99	109.21
22	c	908	CLA	O2A-CGA-CBA	2.93	120.41	111.90
23	a	411	PHO	C2C-C1C-NC	2.93	114.16	109.82
22	c	910	CLA	C3C-C4C-NC	2.93	113.18	110.21
22	c	909	CLA	C1-O2A-CGA	2.93	123.81	116.77
22	B	604	CLA	O2A-CGA-CBA	2.94	120.44	111.90
22	A	405	CLA	CMB-C2B-C3B	2.94	130.35	124.89
22	d	403	CLA	C4A-NA-C1A	2.94	110.11	106.45
22	B	611	CLA	C3C-C4C-NC	2.95	113.19	110.21
22	b	608	CLA	C4-C3-C5	2.95	120.41	115.29
24	Y	101	BCR	C37-C22-C23	2.95	122.80	118.10
22	C	510	CLA	C3B-C4B-NB	2.96	113.03	109.21
26	A	411	PL9	C45-C44-C46	2.96	120.42	115.29
22	b	605	CLA	C4A-NA-C1A	2.96	110.13	106.45
22	B	613	CLA	C1-O2A-CGA	2.96	123.89	116.77
34	D	415	HTG	O5-C1-S1	2.97	118.01	110.15
22	c	912	CLA	O2A-CGA-CBA	2.97	120.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	O2A-CGA-CBA	2.97	120.55	111.90
22	b	607	CLA	C3B-C4B-NB	2.98	113.06	109.21
22	b	606	CLA	CMC-C2C-C1C	2.99	129.55	125.02
22	C	502	CLA	C3C-C4C-NC	3.00	113.25	110.21
22	b	612	CLA	C3B-C4B-NB	3.00	113.08	109.21
22	C	509	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	B	617	CLA	C3C-C4C-NC	3.00	113.25	110.21
22	b	615	CLA	C4-C3-C5	3.01	120.51	115.29
22	C	513	CLA	C4-C3-C5	3.01	120.51	115.29
22	a	412	CLA	C3B-C4B-NB	3.01	113.10	109.21
22	b	609	CLA	C4-C3-C5	3.02	120.52	115.29
22	B	604	CLA	C3C-C4C-NC	3.02	113.27	110.21
25	i	101	LMG	O8-C28-C29	3.02	120.69	111.90
27	d	401	LHG	O8-C23-C24	3.02	120.70	111.90
22	C	509	CLA	C4-C3-C5	3.03	120.54	115.29
22	b	615	CLA	C3C-C4C-NC	3.03	113.28	110.21
28	b	621	SQD	O6-C1-C2	3.04	113.19	108.23
34	b	632	HTG	C3-C4-C5	3.05	115.59	110.22
22	B	610	CLA	C3C-C4C-NC	3.05	113.30	110.21
25	d	409	LMG	O2-C2-C1	3.05	116.41	110.03
22	c	910	CLA	C3B-C4B-NB	3.05	113.16	109.21
22	B	610	CLA	CMC-C2C-C1C	3.05	129.65	125.02
22	D	403	CLA	C4A-NA-C1A	3.06	110.25	106.45
22	a	408	CLA	CHB-C4A-NA	3.06	128.74	124.51
23	D	402	PHO	C2B-C1B-NB	3.06	114.35	109.82
22	c	905	CLA	C4-C3-C5	3.06	120.60	115.29
35	D	407	DGD	O1G-C1A-C2A	3.06	120.81	111.90
22	B	612	CLA	C3C-C4C-NC	3.06	113.31	110.21
22	A	405	CLA	C3C-C4C-NC	3.06	113.31	110.21
29	t	101	LMT	O5'-C5'-C4'	3.06	115.30	109.66
22	D	401	CLA	C3B-C4B-NB	3.07	113.17	109.21
22	C	508	CLA	C4A-NA-C1A	3.07	110.26	106.45
22	C	506	CLA	CMD-C2D-C3D	3.07	130.59	124.89
22	b	602	CLA	CMD-C2D-C3D	3.08	130.60	124.89
25	b	622	LMG	O8-C28-C29	3.08	120.86	111.90
22	B	608	CLA	CAC-C3C-C4C	3.08	129.17	124.83
22	B	609	CLA	CMD-C2D-C3D	3.08	130.61	124.89
22	B	612	CLA	O2D-CGD-CBD	3.08	116.81	111.30
22	b	604	CLA	CMB-C2B-C3B	3.08	130.61	124.89
22	C	504	CLA	C4-C3-C5	3.09	120.65	115.29
22	C	509	CLA	CMD-C2D-C3D	3.09	130.62	124.89
22	b	614	CLA	C4A-NA-C1A	3.10	110.29	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	H	102	DGD	O2G-C1B-C2B	3.10	117.98	111.55
36	e	101	HEM	CAD-CBD-CGD	3.10	117.96	112.66
23	a	410	PHO	C2D-C1D-ND	3.10	114.41	109.82
22	b	603	CLA	O2A-CGA-CBA	3.10	120.93	111.90
22	c	911	CLA	CMB-C2B-C3B	3.11	130.66	124.89
28	a	414	SQD	O2-C2-C1	3.11	116.53	110.03
22	B	617	CLA	CMB-C2B-C3B	3.11	130.66	124.89
22	C	502	CLA	CAC-C3C-C4C	3.11	129.22	124.83
22	B	616	CLA	CMD-C2D-C3D	3.11	130.67	124.89
22	b	612	CLA	C3C-C4C-NC	3.12	113.37	110.21
22	b	615	CLA	CAC-C3C-C4C	3.12	129.24	124.83
22	a	409	CLA	C1-O2A-CGA	3.12	124.27	116.77
27	A	412	LHG	O8-C23-C24	3.13	121.00	111.90
22	C	512	CLA	C4A-NA-C1A	3.13	110.34	106.45
26	a	415	PL9	C35-C34-C36	3.13	120.73	115.29
22	b	609	CLA	CMB-C2B-C3B	3.13	130.71	124.89
22	b	606	CLA	CMD-C2D-C3D	3.13	130.71	124.89
23	a	411	PHO	C3C-C4C-NC	3.14	115.32	110.19
22	c	910	CLA	CMC-C2C-C1C	3.14	129.78	125.02
22	b	615	CLA	C1-O2A-CGA	3.14	124.30	116.77
22	a	408	CLA	CMB-C2B-C3B	3.14	130.72	124.89
22	c	912	CLA	C4-C3-C5	3.14	120.75	115.29
28	A	413	SQD	O3-C3-C2	3.16	117.22	110.36
22	b	614	CLA	C3C-C4C-NC	3.16	113.41	110.21
22	B	608	CLA	C3B-C4B-NB	3.16	113.30	109.21
22	b	616	CLA	CED-O2D-CGD	3.17	123.40	115.97
22	D	404	CLA	C1-O2A-CGA	3.17	124.38	116.77
28	D	408	SQD	O6-C44-C45	3.17	114.96	108.82
22	b	603	CLA	C4-C3-C5	3.18	120.80	115.29
25	A	410	LMG	O8-C28-C29	3.18	121.15	111.90
22	C	510	CLA	C3C-C4C-NC	3.18	113.44	110.21
23	D	402	PHO	C2C-C1C-NC	3.18	114.53	109.82
24	b	619	BCR	C29-C30-C25	3.19	115.46	110.48
22	c	902	CLA	C4-C3-C5	3.19	120.82	115.29
22	c	914	CLA	C1-O2A-CGA	3.19	124.43	116.77
25	C	531	LMG	O8-C28-C29	3.19	121.19	111.90
22	A	406	CLA	O2D-CGD-CBD	3.20	117.02	111.30
28	a	414	SQD	O48-C23-C24	3.21	121.23	111.90
22	B	617	CLA	C3B-C4B-NB	3.21	113.36	109.21
22	c	905	CLA	O2D-CGD-CBD	3.21	117.04	111.30
22	C	506	CLA	C1-O2A-CGA	3.22	124.49	116.77
22	c	914	CLA	O2D-CGD-CBD	3.22	117.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	CAC-C3C-C4C	3.22	129.37	124.83
22	C	504	CLA	CMB-C2B-C3B	3.22	130.87	124.89
22	d	402	CLA	C3B-C4B-NB	3.23	113.39	109.21
23	a	411	PHO	CMB-C2B-C1B	3.23	130.08	125.04
27	a	416	LHG	O8-C23-C24	3.24	121.32	111.90
22	D	403	CLA	CMC-C2C-C1C	3.24	129.93	125.02
22	B	615	CLA	CED-O2D-CGD	3.24	123.56	115.97
22	B	603	CLA	OBD-CAD-CBD	3.24	130.83	125.94
22	C	513	CLA	C4A-NA-C1A	3.24	110.48	106.45
25	c	920	LMG	O7-C10-C11	3.25	118.29	111.55
22	C	507	CLA	CMD-C2D-C3D	3.25	130.92	124.89
28	b	621	SQD	O48-C23-C24	3.25	121.36	111.90
29	f	102	LMT	O1'-C1'-C2'	3.26	113.55	108.23
22	C	504	CLA	C4A-NA-C1A	3.26	110.50	106.45
28	l	101	SQD	O48-C23-C24	3.26	121.39	111.90
22	B	606	CLA	O2D-CGD-CBD	3.26	117.13	111.30
22	C	505	CLA	C4A-NA-C1A	3.27	110.51	106.45
22	B	603	CLA	C3B-C4B-NB	3.27	113.44	109.21
22	C	512	CLA	C3C-C4C-NC	3.27	113.53	110.21
34	b	624	HTG	C1-C2-C3	3.29	117.72	110.69
22	C	506	CLA	O2D-CGD-CBD	3.29	117.17	111.30
22	B	616	CLA	C4A-NA-C1A	3.29	110.54	106.45
22	b	617	CLA	C4A-NA-C1A	3.30	110.54	106.45
23	D	402	PHO	CMB-C2B-C1B	3.30	130.18	125.04
22	C	510	CLA	CHB-C4A-NA	3.30	129.08	124.51
22	C	507	CLA	CMC-C2C-C1C	3.30	130.03	125.02
24	D	405	BCR	C29-C30-C25	3.31	115.65	110.48
35	D	407	DGD	C3D-C4D-C5D	3.31	114.88	109.68
22	b	614	CLA	C4-C3-C5	3.31	121.03	115.29
23	A	407	PHO	CMB-C2B-C1B	3.33	130.23	125.04
25	B	621	LMG	O8-C28-C29	3.33	121.59	111.90
22	C	510	CLA	O2A-CGA-CBA	3.34	121.61	111.90
22	b	613	CLA	O2A-CGA-CBA	3.34	121.62	111.90
35	C	518	DGD	O6E-C1E-C2E	3.35	116.75	110.30
34	v	203	HTG	O3-C3-C2	3.35	117.64	110.36
22	B	615	CLA	CMD-C2D-C3D	3.36	131.12	124.89
22	c	907	CLA	C3B-C4B-NB	3.36	113.55	109.21
22	B	615	CLA	C4A-NA-C1A	3.36	110.62	106.45
26	D	406	PL9	C20-C19-C21	3.36	121.12	115.29
22	B	605	CLA	CAC-C3C-C4C	3.36	129.57	124.83
22	C	507	CLA	C4A-NA-C1A	3.36	110.63	106.45
22	D	401	CLA	CMC-C2C-C1C	3.36	130.12	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	912	CLA	O2D-CGD-CBD	3.37	117.32	111.30
22	b	617	CLA	CMD-C2D-C3D	3.38	131.16	124.89
22	b	604	CLA	C3C-C4C-NC	3.38	113.63	110.21
22	c	911	CLA	CMD-C2D-C3D	3.38	131.16	124.89
34	C	523	HTG	C1-S1-C1'	3.38	112.50	100.35
27	d	407	LHG	O8-C23-C24	3.39	121.76	111.90
22	B	603	CLA	O2A-CGA-CBA	3.40	121.78	111.90
22	D	403	CLA	O2D-CGD-CBD	3.40	117.38	111.30
22	c	910	CLA	C1-O2A-CGA	3.40	124.94	116.77
29	Z	101	LMT	C3B-C4B-C5B	3.41	116.22	110.22
22	B	606	CLA	C4A-NA-C1A	3.41	110.68	106.45
22	c	908	CLA	CMB-C2B-C3B	3.42	131.24	124.89
25	b	622	LMG	C4-C3-C2	3.43	116.88	110.84
22	c	910	CLA	O2A-CGA-CBA	3.43	121.88	111.90
26	D	406	PL9	C53-C6-C1	3.43	122.13	114.84
35	c	919	DGD	O1G-C1A-C2A	3.44	121.90	111.90
22	B	603	CLA	C3C-C4C-NC	3.45	113.70	110.21
35	C	519	DGD	O2G-C1B-C2B	3.47	118.75	111.55
27	a	423	LHG	O8-C23-C24	3.47	122.00	111.90
22	B	609	CLA	CAC-C3C-C4C	3.48	129.73	124.83
22	A	405	CLA	CMD-C2D-C3D	3.48	131.35	124.89
22	b	608	CLA	O2D-CGD-CBD	3.48	117.52	111.30
22	c	908	CLA	C4-C3-C5	3.48	121.33	115.29
22	B	606	CLA	CAC-C3C-C4C	3.49	129.75	124.83
22	c	906	CLA	CMB-C2B-C3B	3.49	131.37	124.89
22	D	403	CLA	CMD-C2D-C3D	3.49	131.37	124.89
22	b	613	CLA	C4-C3-C5	3.50	121.36	115.29
22	D	401	CLA	O2D-CGD-CBD	3.50	117.55	111.30
22	a	409	CLA	CMC-C2C-C1C	3.51	130.34	125.02
25	b	622	LMG	O6-C5-C6	3.51	114.82	106.41
22	b	605	CLA	CMD-C2D-C3D	3.51	131.41	124.89
22	C	507	CLA	C3C-C4C-NC	3.52	113.77	110.21
22	C	507	CLA	O2D-CGD-CBD	3.52	117.59	111.30
22	C	514	CLA	CMC-C2C-C1C	3.52	130.36	125.02
22	B	615	CLA	C4-C3-C5	3.52	121.40	115.29
22	d	402	CLA	C4-C3-C5	3.52	121.40	115.29
35	C	518	DGD	O2G-C1B-C2B	3.52	118.87	111.55
22	B	615	CLA	O2A-CGA-CBA	3.53	122.18	111.90
22	C	514	CLA	C2C-C1C-NC	3.53	112.65	110.22
25	b	622	LMG	O6-C1-O1	3.53	118.41	110.02
22	c	905	CLA	C4A-NA-C1A	3.55	110.85	106.45
36	E	102	HEM	CAD-CBD-CGD	3.55	118.73	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	O2D-CGD-CBD	3.55	117.64	111.30
22	b	606	CLA	C4-C3-C5	3.55	121.45	115.29
25	A	410	LMG	O7-C10-C11	3.55	118.93	111.55
23	D	402	PHO	O2D-CGD-CBD	3.57	117.67	111.30
22	B	617	CLA	CMD-C2D-C3D	3.57	131.51	124.89
22	a	409	CLA	CMB-C2B-C3B	3.58	131.53	124.89
22	B	615	CLA	C3C-C4C-NC	3.58	113.84	110.21
29	E	101	LMT	O5'-C5'-C6'	3.58	114.98	106.41
22	B	608	CLA	C4-C3-C5	3.59	121.51	115.29
22	b	604	CLA	CMD-C2D-C3D	3.59	131.56	124.89
34	B	627	HTG	O5-C1-C2	3.60	115.21	110.28
23	D	402	PHO	CAC-C3C-C4C	3.60	129.44	125.21
28	a	418	SQD	O48-C23-C24	3.62	122.43	111.90
23	A	407	PHO	C2B-C1B-NB	3.62	115.18	109.82
34	b	624	HTG	O5-C1-C2	3.63	115.25	110.28
35	C	519	DGD	O1G-C1A-C2A	3.63	122.47	111.90
22	D	403	CLA	C3B-C4B-NB	3.64	113.92	109.21
27	L	101	LHG	O7-C7-C8	3.65	119.14	111.55
35	h	102	DGD	O2G-C1B-C2B	3.66	119.16	111.55
28	l	101	SQD	O9-S-C6	3.67	109.96	106.83
22	b	614	CLA	CMB-C2B-C1B	3.67	134.11	128.46
27	D	409	LHG	O8-C23-C24	3.68	122.60	111.90
27	d	401	LHG	O7-C7-C8	3.68	119.19	111.55
22	B	602	CLA	C1-O2A-CGA	3.68	125.61	116.77
35	c	918	DGD	O2G-C1B-C2B	3.69	119.22	111.55
22	b	602	CLA	O2A-CGA-CBA	3.70	122.66	111.90
27	D	411	LHG	O8-C23-C24	3.70	122.67	111.90
22	C	514	CLA	C4A-NA-C1A	3.71	111.06	106.45
22	B	613	CLA	CAC-C3C-C4C	3.71	130.07	124.83
34	B	627	HTG	C1-O5-C5	3.71	119.84	112.69
22	c	908	CLA	C4A-NA-C1A	3.71	111.06	106.45
22	b	614	CLA	O2D-CGD-CBD	3.72	117.94	111.30
22	a	408	CLA	CED-O2D-CGD	3.72	124.69	115.97
22	a	407	CLA	C4-C3-C5	3.72	121.75	115.29
22	c	906	CLA	CMD-C2D-C3D	3.72	131.80	124.89
22	C	504	CLA	O2D-CGD-CBD	3.73	117.96	111.30
26	a	415	PL9	C7-C3-C4	3.74	119.92	116.88
22	c	911	CLA	C2C-C1C-NC	3.75	112.80	110.22
22	b	608	CLA	C4A-NA-C1A	3.75	111.11	106.45
22	c	905	CLA	C3B-C4B-NB	3.75	114.06	109.21
22	c	904	CLA	C4A-NA-C1A	3.76	111.12	106.45
22	B	610	CLA	O2D-CGD-CBD	3.76	118.03	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	404	CLA	CAC-C3C-C4C	3.77	130.14	124.83
24	B	620	BCR	C2-C1-C6	3.77	116.37	110.48
28	a	418	SQD	O47-C7-C8	3.77	119.39	111.55
28	f	101	SQD	O7-S-C6	3.77	110.03	106.79
22	C	514	CLA	O2A-CGA-CBA	3.77	122.88	111.90
22	C	511	CLA	O2D-CGD-CBD	3.78	118.05	111.30
22	C	503	CLA	CMD-C2D-C3D	3.78	131.91	124.89
25	b	622	LMG	C7-O1-C1	3.79	121.53	113.76
22	B	609	CLA	C3C-C4C-NC	3.80	114.06	110.21
22	B	608	CLA	O2D-CGD-CBD	3.80	118.09	111.30
23	a	411	PHO	C2D-C1D-ND	3.80	115.45	109.82
22	b	604	CLA	CMC-C2C-C1C	3.81	130.80	125.02
22	c	910	CLA	O2D-CGD-CBD	3.81	118.11	111.30
22	c	909	CLA	C4A-NA-C1A	3.81	111.19	106.45
22	c	906	CLA	C1-O2A-CGA	3.81	125.92	116.77
22	a	409	CLA	C4-C3-C5	3.82	121.91	115.29
22	B	602	CLA	CAC-C3C-C4C	3.82	130.22	124.83
26	a	415	PL9	C53-C6-C1	3.83	122.96	114.84
22	b	611	CLA	CMD-C2D-C3D	3.84	132.02	124.89
22	C	506	CLA	CAC-C3C-C4C	3.84	130.25	124.83
25	b	622	LMG	C3-C4-C5	3.86	117.02	110.22
22	A	408	CLA	O2D-CGD-CBD	3.86	118.19	111.30
22	A	406	CLA	CMC-C2C-C1C	3.88	130.90	125.02
22	b	606	CLA	C3C-C4C-NC	3.88	114.14	110.21
22	C	514	CLA	O2D-CGD-CBD	3.88	118.23	111.30
28	b	621	SQD	O9-S-C6	3.88	110.14	106.83
34	b	632	HTG	C1-O5-C5	3.89	120.17	112.69
22	c	904	CLA	O2A-CGA-CBA	3.89	123.22	111.90
29	a	419	LMT	C2'-C3'-C4'	3.89	117.68	109.61
22	C	504	CLA	C3C-C4C-NC	3.89	114.16	110.21
22	b	607	CLA	C3C-C4C-NC	3.90	114.16	110.21
22	B	607	CLA	C4-C3-C5	3.91	122.08	115.29
23	a	411	PHO	C2B-C1B-NB	3.92	115.62	109.82
22	B	605	CLA	CMC-C2C-C1C	3.92	130.97	125.02
22	B	615	CLA	C1-O2A-CGA	3.92	126.19	116.77
23	D	402	PHO	C3C-C4C-NC	3.93	116.61	110.19
22	B	616	CLA	O2D-CGD-CBD	3.94	118.33	111.30
22	c	912	CLA	C4A-NA-C1A	3.95	111.36	106.45
23	a	411	PHO	C4-C3-C5	3.95	122.15	115.29
22	c	903	CLA	O2D-CGD-CBD	3.97	118.39	111.30
22	b	611	CLA	C3C-C4C-NC	3.97	114.24	110.21
22	a	409	CLA	C3B-C4B-NB	3.98	114.35	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	911	CLA	O2D-CGD-CBD	3.98	118.41	111.30
22	b	613	CLA	C3C-C4C-NC	3.99	114.25	110.21
26	d	405	PL9	C35-C34-C36	3.99	122.22	115.29
23	D	402	PHO	C2D-C1D-ND	4.00	115.73	109.82
22	b	616	CLA	CMD-C2D-C3D	4.00	132.31	124.89
22	B	607	CLA	C3C-C4C-NC	4.00	114.26	110.21
28	f	101	SQD	O8-S-C6	4.00	110.97	106.06
28	D	408	SQD	O8-S-C6	4.00	110.89	106.01
22	b	610	CLA	CMC-C2C-C1C	4.00	131.09	125.02
22	d	403	CLA	O2D-CGD-CBD	4.00	118.45	111.30
26	D	406	PL9	C40-C39-C41	4.01	122.24	115.29
22	B	611	CLA	O2A-CGA-CBA	4.01	123.56	111.90
27	a	423	LHG	O7-C7-C8	4.01	119.88	111.55
25	c	930	LMG	O7-C10-C11	4.02	119.90	111.55
22	c	914	CLA	CMC-C2C-C1C	4.03	131.14	125.02
35	C	518	DGD	O5D-C6D-C5D	4.06	115.73	108.94
22	b	609	CLA	C3C-C4C-NC	4.06	114.33	110.21
25	c	920	LMG	O8-C28-C29	4.06	123.72	111.90
22	c	910	CLA	CAC-C3C-C4C	4.06	130.56	124.83
22	b	603	CLA	CMB-C2B-C3B	4.07	132.44	124.89
22	a	407	CLA	CAC-C3C-C4C	4.07	130.57	124.83
22	b	607	CLA	C1-O2A-CGA	4.07	126.55	116.77
35	H	102	DGD	O1G-C1A-C2A	4.08	123.76	111.90
22	b	605	CLA	C3C-C4C-NC	4.09	114.36	110.21
25	C	531	LMG	O7-C10-C11	4.10	120.07	111.55
35	h	102	DGD	O1G-C1A-C2A	4.10	123.84	111.90
22	b	614	CLA	CAC-C3C-C4C	4.11	130.63	124.83
26	A	411	PL9	C53-C6-C1	4.12	123.60	114.84
23	D	402	PHO	C4A-NA-C1A	4.13	111.50	108.16
34	V	203	HTG	O2-C2-C1	4.14	118.51	110.27
22	a	408	CLA	O2D-CGD-CBD	4.14	118.70	111.30
22	B	606	CLA	C3C-C4C-NC	4.15	114.41	110.21
22	c	912	CLA	C2C-C1C-NC	4.15	113.08	110.22
22	A	408	CLA	C4-C3-C5	4.17	122.52	115.29
22	B	602	CLA	C4A-NA-C1A	4.17	111.63	106.45
22	B	603	CLA	O2D-CGD-CBD	4.17	118.76	111.30
22	b	609	CLA	O2D-CGD-CBD	4.20	118.80	111.30
34	D	415	HTG	O5-C5-C4	4.20	117.40	109.66
22	d	402	CLA	O2A-CGA-CBA	4.21	124.14	111.90
22	C	504	CLA	C2C-C1C-NC	4.22	113.12	110.22
22	D	401	CLA	CMD-C2D-C3D	4.23	132.74	124.89
22	c	911	CLA	CMC-C2C-C1C	4.24	131.44	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	410	PHO	C2C-C1C-NC	4.24	116.10	109.82
22	C	506	CLA	C4A-NA-C1A	4.26	111.74	106.45
22	b	605	CLA	O2D-CGD-CBD	4.26	118.92	111.30
25	C	520	LMG	O7-C10-C11	4.26	120.41	111.55
22	b	615	CLA	O2D-CGD-CBD	4.27	118.94	111.30
22	C	513	CLA	C2C-C1C-NC	4.29	113.17	110.22
22	b	613	CLA	O2D-CGD-CBD	4.29	118.97	111.30
22	B	606	CLA	CMC-C2C-C1C	4.30	131.53	125.02
28	A	413	SQD	O6-C1-C2	4.30	115.25	108.23
35	c	917	DGD	O2G-C1B-C2B	4.30	120.49	111.55
23	D	402	PHO	C4-C3-C5	4.30	122.76	115.29
22	b	613	CLA	CMD-C2D-C3D	4.31	132.88	124.89
22	c	902	CLA	O2D-CGD-CBD	4.31	119.00	111.30
35	D	407	DGD	C4D-C3D-C2D	4.31	118.44	110.84
28	A	413	SQD	O47-C7-C8	4.34	120.57	111.55
29	T	102	LMT	C1'-C2'-C3'	4.35	118.06	109.98
28	C	501	SQD	O47-C7-C8	4.36	120.60	111.55
22	D	404	CLA	O2D-CGD-CBD	4.36	119.10	111.30
22	c	909	CLA	O2D-CGD-CBD	4.37	119.11	111.30
25	B	621	LMG	O7-C10-C11	4.38	120.65	111.55
23	a	410	PHO	C3C-C4C-NC	4.40	117.39	110.19
22	C	513	CLA	C1-O2A-CGA	4.42	127.36	116.77
22	a	412	CLA	CMD-C2D-C3D	4.42	133.09	124.89
22	b	603	CLA	C2C-C1C-NC	4.42	113.27	110.22
25	d	409	LMG	O7-C10-C11	4.43	120.75	111.55
28	a	418	SQD	O6-C1-C2	4.43	115.47	108.23
25	D	412	LMG	O7-C10-C11	4.44	120.76	111.55
27	l	102	LHG	O7-C7-C8	4.44	120.78	111.55
22	b	602	CLA	C4A-NA-C1A	4.45	111.97	106.45
23	A	407	PHO	O2D-CGD-CBD	4.46	119.27	111.30
35	D	407	DGD	O2G-C1B-C2B	4.47	120.82	111.55
22	A	406	CLA	C4-C3-C5	4.50	123.09	115.29
22	B	617	CLA	C1-O2A-CGA	4.51	127.59	116.77
22	B	605	CLA	O2D-CGD-CBD	4.51	119.36	111.30
22	b	602	CLA	C1-O2A-CGA	4.52	127.61	116.77
23	A	407	PHO	C2C-C1C-NC	4.52	116.52	109.82
22	B	617	CLA	O2A-CGA-CBA	4.54	125.11	111.90
22	B	615	CLA	O2D-CGD-CBD	4.55	119.43	111.30
22	C	505	CLA	O2D-CGD-CBD	4.56	119.44	111.30
23	a	410	PHO	O2D-CGD-CBD	4.56	119.45	111.30
22	a	412	CLA	C4-C3-C5	4.57	123.21	115.29
22	B	606	CLA	C2C-C1C-NC	4.57	113.37	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	O2D-CGD-CBD	4.58	119.48	111.30
22	C	513	CLA	O2D-CGD-CBD	4.59	119.49	111.30
22	a	407	CLA	O2D-CGD-CBD	4.61	119.54	111.30
25	C	520	LMG	O8-C28-C29	4.62	125.33	111.90
22	b	613	CLA	CAC-C3C-C4C	4.62	131.35	124.83
22	C	509	CLA	C2C-C1C-NC	4.64	113.41	110.22
22	C	503	CLA	C2C-C1C-NC	4.66	113.43	110.22
22	d	403	CLA	C1-O2A-CGA	4.66	127.95	116.77
22	a	409	CLA	O2D-CGD-CBD	4.67	119.64	111.30
22	b	602	CLA	C2C-C1C-NC	4.69	113.45	110.22
22	B	614	CLA	C2C-C1C-NC	4.69	113.45	110.22
28	D	408	SQD	O6-C1-C2	4.69	115.89	108.23
22	c	908	CLA	C2C-C1C-NC	4.70	113.45	110.22
28	D	408	SQD	O7-S-C6	4.71	110.85	106.83
22	C	510	CLA	O2D-CGD-CBD	4.71	119.71	111.30
22	C	512	CLA	C1-O2A-CGA	4.71	128.08	116.77
29	I	102	LMT	C1'-O5'-C5'	4.74	122.64	113.72
22	b	617	CLA	C3C-C4C-NC	4.74	115.02	110.21
22	b	604	CLA	C4-C3-C5	4.75	123.53	115.29
26	A	411	PL9	C7-C3-C4	4.79	120.77	116.88
22	b	606	CLA	O2D-CGD-CBD	4.80	119.87	111.30
22	c	907	CLA	O2D-CGD-CBD	4.90	120.06	111.30
35	c	919	DGD	O2G-C1B-C2B	4.91	121.74	111.55
22	C	503	CLA	O2D-CGD-CBD	4.91	120.08	111.30
28	l	101	SQD	O47-C7-C8	4.93	121.80	111.55
22	c	906	CLA	O2D-CGD-CBD	4.96	120.16	111.30
22	c	909	CLA	C2C-C1C-NC	4.99	113.66	110.22
28	l	101	SQD	O6-C1-C2	5.00	116.40	108.23
22	b	604	CLA	O2D-CGD-CBD	5.02	120.28	111.30
22	b	616	CLA	C2C-C1C-NC	5.03	113.68	110.22
22	c	913	CLA	O2D-CGD-CBD	5.03	120.30	111.30
22	B	602	CLA	C2C-C1C-NC	5.04	113.69	110.22
27	C	522	LHG	O7-C7-C8	5.05	122.04	111.55
28	A	413	SQD	O48-C23-C24	5.09	126.72	111.90
22	c	906	CLA	C2C-C1C-NC	5.14	113.76	110.22
34	b	632	HTG	O5-C5-C4	5.15	119.15	109.66
22	B	616	CLA	C2C-C1C-NC	5.18	113.78	110.22
22	D	404	CLA	C2C-C1C-NC	5.21	113.81	110.22
22	b	613	CLA	C2C-C1C-NC	5.22	113.81	110.22
22	C	508	CLA	C2C-C1C-NC	5.30	113.87	110.22
28	a	414	SQD	O47-C7-C8	5.30	122.56	111.55
29	I	102	LMT	O1B-C4'-C3'	5.32	119.99	107.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	406	DGD	O2G-C1B-C2B	5.33	122.63	111.55
22	c	913	CLA	C2C-C1C-NC	5.35	113.90	110.22
22	b	617	CLA	C2C-C1C-NC	5.35	113.90	110.22
22	a	407	CLA	C2C-C1C-NC	5.36	113.91	110.22
22	d	402	CLA	O2D-CGD-CBD	5.38	120.91	111.30
25	d	409	LMG	O1-C1-C2	5.38	117.01	108.23
22	c	908	CLA	O2D-CGD-CBD	5.39	120.93	111.30
22	C	506	CLA	C2C-C1C-NC	5.40	113.94	110.22
22	c	914	CLA	C2C-C1C-NC	5.47	113.99	110.22
22	B	615	CLA	C2C-C1C-NC	5.58	114.06	110.22
23	a	411	PHO	O2D-CGD-CBD	5.60	121.31	111.30
22	b	611	CLA	O2D-CGD-CBD	5.64	121.38	111.30
22	B	612	CLA	C2C-C1C-NC	5.66	114.12	110.22
27	a	416	LHG	O7-C7-C8	5.67	123.33	111.55
25	b	622	LMG	O7-C10-C11	5.69	123.37	111.55
28	b	621	SQD	O7-S-C6	5.72	111.72	106.83
22	B	610	CLA	C2C-C1C-NC	5.74	114.17	110.22
22	B	607	CLA	O2D-CGD-CBD	5.74	121.55	111.30
27	A	412	LHG	O7-C7-C8	5.74	121.88	111.10
25	b	622	LMG	O1-C1-C2	5.78	117.66	108.23
28	C	501	SQD	O8-S-C6	5.78	113.06	106.01
22	c	905	CLA	C2C-C1C-NC	5.79	114.20	110.22
22	B	602	CLA	O2D-CGD-CBD	5.84	121.74	111.30
22	b	617	CLA	O2D-CGD-CBD	5.85	121.75	111.30
22	b	615	CLA	C2C-C1C-NC	5.86	114.25	110.22
22	B	611	CLA	C2C-C1C-NC	5.86	114.25	110.22
22	C	512	CLA	C2C-C1C-NC	5.87	114.26	110.22
22	B	613	CLA	C2C-C1C-NC	5.87	114.26	110.22
22	b	609	CLA	C2C-C1C-NC	5.88	114.26	110.22
27	D	409	LHG	O7-C7-C8	5.90	123.81	111.55
22	a	412	CLA	O2D-CGD-CBD	5.98	121.99	111.30
22	b	607	CLA	C2C-C1C-NC	5.99	114.34	110.22
22	b	606	CLA	C2C-C1C-NC	6.01	114.36	110.22
22	b	607	CLA	O2D-CGD-CBD	6.02	122.06	111.30
22	B	617	CLA	O2D-CGD-CBD	6.08	122.17	111.30
22	c	902	CLA	C2C-C1C-NC	6.10	114.42	110.22
22	d	403	CLA	C2C-C1C-NC	6.10	114.42	110.22
22	b	614	CLA	C2C-C1C-NC	6.13	114.44	110.22
22	c	903	CLA	C2C-C1C-NC	6.16	114.46	110.22
22	B	609	CLA	O2D-CGD-CBD	6.17	122.32	111.30
22	b	612	CLA	C2C-C1C-NC	6.33	114.58	110.22
22	c	904	CLA	C2C-C1C-NC	6.36	114.59	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	O2D-CGD-CBD	6.43	122.79	111.30
22	C	502	CLA	C2C-C1C-NC	6.45	114.66	110.22
28	l	101	SQD	O7-S-C6	6.50	112.38	106.83
22	C	508	CLA	O2D-CGD-CBD	6.51	122.94	111.30
22	b	608	CLA	C2C-C1C-NC	6.51	114.70	110.22
28	C	501	SQD	O6-C1-C2	6.54	118.90	108.23
22	C	507	CLA	C2C-C1C-NC	6.58	114.75	110.22
22	C	505	CLA	C2C-C1C-NC	6.63	114.78	110.22
22	b	602	CLA	O2D-CGD-CBD	6.67	123.22	111.30
22	d	402	CLA	C2C-C1C-NC	6.68	114.82	110.22
22	b	605	CLA	C2C-C1C-NC	6.68	114.82	110.22
34	b	626	HTG	C1'-S1-C1	6.79	110.35	100.28
22	a	412	CLA	C2C-C1C-NC	6.81	114.91	110.22
22	b	610	CLA	C2C-C1C-NC	6.85	114.94	110.22
22	B	603	CLA	C2C-C1C-NC	6.98	115.02	110.22
22	a	408	CLA	C2C-C1C-NC	6.99	115.03	110.22
22	B	609	CLA	C2C-C1C-NC	7.01	115.04	110.22
23	D	402	PHO	CMD-C2D-C1D	7.04	136.01	125.04
22	B	604	CLA	C2C-C1C-NC	7.13	115.12	110.22
23	a	410	PHO	CMD-C2D-C1D	7.16	136.19	125.04
22	b	603	CLA	O2D-CGD-CBD	7.16	124.10	111.30
22	B	607	CLA	C2C-C1C-NC	7.19	115.17	110.22
22	B	617	CLA	C2C-C1C-NC	7.23	115.20	110.22
22	B	604	CLA	O2D-CGD-CBD	7.24	124.23	111.30
22	B	608	CLA	C2C-C1C-NC	7.27	115.22	110.22
22	A	408	CLA	C2C-C1C-NC	7.27	115.22	110.22
34	V	203	HTG	C1'-S1-C1	7.30	110.71	100.42
22	A	405	CLA	C2C-C1C-NC	7.37	115.29	110.22
22	b	611	CLA	C2C-C1C-NC	7.45	115.34	110.22
28	A	413	SQD	O9-S-C6	7.50	113.24	106.83
22	C	511	CLA	C2C-C1C-NC	7.57	115.43	110.22
22	c	907	CLA	C2C-C1C-NC	7.71	115.53	110.22
34	B	626	HTG	C1'-S1-C1	7.72	111.73	100.28
22	B	611	CLA	O2D-CGD-CBD	7.85	125.33	111.30
22	c	910	CLA	C2C-C1C-NC	7.89	115.65	110.22
34	C	521	HTG	C1'-S1-C1	8.05	112.23	100.28
34	c	922	HTG	C1'-S1-C1	8.07	112.25	100.28
22	B	605	CLA	C2C-C1C-NC	8.12	115.81	110.22
28	a	414	SQD	O6-C1-C2	8.16	121.56	108.23
22	b	604	CLA	C2C-C1C-NC	8.18	115.84	110.22
34	B	623	HTG	C1'-S1-C1	8.31	112.61	100.28
23	A	407	PHO	CMD-C2D-C1D	8.36	138.06	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	SQD	O9-S-C6	8.50	114.09	106.83
23	a	411	PHO	CMD-C2D-C1D	8.50	138.28	125.04
22	D	401	CLA	C2C-C1C-NC	8.76	116.24	110.22
22	A	406	CLA	C2C-C1C-NC	8.80	116.27	110.22
22	C	510	CLA	C2C-C1C-NC	8.80	116.28	110.22
34	b	627	HTG	C1'-S1-C1	8.81	113.35	100.28
34	B	627	HTG	C1'-S1-C1	8.91	113.50	100.28
34	v	203	HTG	C1'-S1-C1	9.19	113.91	100.28
34	D	415	HTG	C1'-S1-C1	9.43	114.27	100.28
34	b	624	HTG	C1'-S1-C1	9.57	114.47	100.28
28	a	414	SQD	O9-S-C6	9.70	115.12	106.83
34	b	632	HTG	C1'-S1-C1	9.90	114.97	100.28
22	a	409	CLA	C2C-C1C-NC	10.00	117.10	110.22
34	D	414	HTG	C1'-S1-C1	10.16	115.35	100.28
22	D	403	CLA	C2C-C1C-NC	10.20	117.24	110.22
34	C	532	HTG	C1'-S1-C1	10.46	115.79	100.28
34	l	106	HTG	C1'-S1-C1	10.69	116.14	100.28

All (172) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	NA
22	C	510	CLA	ND
22	A	406	CLA	NC
22	A	406	CLA	NA
22	d	402	CLA	ND
22	d	402	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	c	906	CLA	ND
22	c	905	CLA	NC
22	c	905	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	NA
22	C	506	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	506	CLA	NA
22	b	602	CLA	ND
22	b	602	CLA	NA
22	c	912	CLA	NC
22	c	912	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	A	408	CLA	NC
22	A	408	CLA	ND
22	b	613	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	C	513	CLA	NC
22	C	513	CLA	ND
22	C	513	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	514	CLA	NC
22	C	514	CLA	NA
22	D	403	CLA	ND
22	D	403	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	D	404	CLA	NC
22	D	404	CLA	ND
22	D	404	CLA	NA
22	d	403	CLA	NC
22	d	403	CLA	NA
22	a	408	CLA	NC
22	a	408	CLA	ND
22	a	408	CLA	NA
22	B	604	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	604	CLA	ND
22	B	604	CLA	NA
22	B	613	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	a	407	CLA	NC
22	a	407	CLA	ND
22	a	407	CLA	NA
22	c	914	CLA	NC
22	c	914	CLA	NA
22	c	902	CLA	NC
22	c	902	CLA	ND
22	c	902	CLA	NA
22	b	610	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	c	908	CLA	NC
22	c	908	CLA	ND
22	c	908	CLA	NA
22	B	616	CLA	NC
22	B	616	CLA	ND
22	B	616	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	b	603	CLA	ND
22	B	609	CLA	NC
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	a	409	CLA	NC
22	a	409	CLA	NA

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Mol	Chain	Res	Type	Atom
22	c	909	CLA	NC
22	c	909	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	c	910	CLA	NC
22	c	910	CLA	ND
22	c	910	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	C	511	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	c	904	CLA	NC
22	c	913	CLA	NC
22	c	913	CLA	ND
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	NA
22	b	617	CLA	ND
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	c	911	CLA	NC
22	c	911	CLA	ND
22	c	911	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	C	504	CLA	NC
22	B	608	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	608	CLA	ND
22	B	608	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	c	903	CLA	NC
22	c	903	CLA	ND
22	c	903	CLA	NA
22	D	401	CLA	NA
22	c	907	CLA	NC
22	c	907	CLA	ND
22	c	907	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	NA
22	B	617	CLA	NC
22	B	617	CLA	ND
22	B	617	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	C	532	HTG	O5-C1-S1-C1'
24	b	619	BCR	C7-C8-C9-C34
24	b	619	BCR	C7-C8-C9-C10

There are no ring outliers.

103 monomers are involved in 305 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	405	CLA	3	0
22	A	406	CLA	3	0
23	A	407	PHO	1	0
22	A	408	CLA	9	0
25	A	410	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	411	PL9	11	0
27	A	412	LHG	1	0
28	A	413	SQD	2	0
29	A	414	LMT	6	0
31	A	419	DMS	2	0
32	A	421[B]	BCT	1	0
22	B	602	CLA	6	0
22	B	603	CLA	3	0
22	B	604	CLA	2	0
22	B	605	CLA	5	0
22	B	606	CLA	11	0
22	B	607	CLA	4	0
22	B	608	CLA	9	0
22	B	609	CLA	6	0
22	B	610	CLA	8	0
22	B	611	CLA	9	0
22	B	612	CLA	2	0
22	B	613	CLA	4	0
22	B	614	CLA	6	0
22	B	615	CLA	5	0
22	B	616	CLA	3	0
22	B	617	CLA	2	0
24	B	618	BCR	4	0
24	B	619	BCR	1	0
24	B	620	BCR	3	0
25	B	621	LMG	3	0
29	B	622	LMT	3	0
34	B	623	HTG	3	0
34	B	626	HTG	1	0
31	B	628	DMS	2	0
31	B	629	DMS	1	0
31	B	631	DMS	3	0
31	B	638	DMS	7	0
31	B	641	DMS	1	0
31	B	642	DMS	1	0
28	C	501	SQD	6	0
22	C	502	CLA	2	0
22	C	503	CLA	6	0
22	C	504	CLA	3	0
22	C	505	CLA	4	0
22	C	506	CLA	1	0
22	C	507	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	508	CLA	3	0
22	C	509	CLA	3	0
22	C	510	CLA	3	0
22	C	511	CLA	5	0
22	C	512	CLA	1	0
22	C	513	CLA	5	0
22	C	514	CLA	5	0
24	C	515	BCR	4	0
24	C	516	BCR	1	0
35	C	518	DGD	1	0
35	C	519	DGD	2	0
25	C	520	LMG	1	0
34	C	521	HTG	1	0
27	C	522	LHG	1	0
31	C	530	DMS	1	0
25	C	531	LMG	2	0
34	C	532	HTG	1	0
31	C	536	DMS	1	0
31	C	540	DMS	1	0
22	D	401	CLA	4	0
23	D	402	PHO	5	0
22	D	403	CLA	2	0
22	D	404	CLA	1	0
24	D	405	BCR	1	0
26	D	406	PL9	5	0
27	D	409	LHG	7	0
27	D	410	LHG	3	0
27	D	411	LHG	8	0
25	D	412	LMG	5	0
34	D	414	HTG	2	0
34	D	415	HTG	8	0
29	E	101	LMT	1	0
36	E	102	HEM	1	0
37	H	101	RRX	12	0
35	H	102	DGD	4	0
25	J	101	LMG	2	0
24	K	101	BCR	2	0
27	L	101	LHG	7	0
31	O	303	DMS	3	0
31	O	304	DMS	9	0
31	O	305	DMS	3	0
31	O	306	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	O	307	DMS	1	0
31	O	310	DMS	4	0
31	O	312	DMS	3	0
29	T	102	LMT	1	0
31	U	203	DMS	1	0
31	V	201	DMS	1	0
36	V	202	HEM	1	0
31	V	205	DMS	1	0
31	V	206	DMS	3	0
31	V	207	DMS	2	0
31	V	210	DMS	2	0
31	V	212	DMS	10	0
24	Y	101	BCR	4	0
29	Z	101	LMT	1	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	A	334/334 (100%)	-0.33	15 (4%) 34 32	21, 28, 66, 87	0
1	a	334/334 (100%)	-0.02	34 (10%) 7 7	22, 30, 96, 135	0
2	B	505/505 (100%)	-0.21	36 (7%) 17 16	22, 33, 67, 109	0
2	b	483/505 (95%)	-0.35	21 (4%) 36 34	24, 35, 57, 124	0
3	C	451/455 (99%)	-0.32	12 (2%) 55 52	24, 37, 55, 106	0
3	c	455/455 (100%)	-0.34	2 (0%) 92 91	27, 41, 57, 89	0
4	D	342/342 (100%)	-0.52	5 (1%) 74 72	21, 29, 51, 86	0
4	d	341/342 (99%)	-0.25	14 (4%) 38 36	22, 32, 59, 85	0
5	E	79/80 (98%)	0.53	10 (12%) 4 4	30, 53, 77, 89	0
5	e	79/80 (98%)	0.80	12 (15%) 2 2	35, 54, 91, 96	0
6	F	33/33 (100%)	-0.39	4 (12%) 5 4	32, 38, 68, 87	0
6	f	31/33 (93%)	-0.19	1 (3%) 48 46	34, 42, 62, 95	0
7	H	63/63 (100%)	-0.33	1 (1%) 72 70	32, 42, 52, 104	0
7	h	62/63 (98%)	0.27	8 (12%) 4 3	34, 48, 62, 74	0
8	I	34/36 (94%)	-0.50	1 (2%) 52 50	33, 42, 60, 78	0
8	i	35/36 (97%)	-0.64	0 100 100	34, 43, 71, 95	0
9	J	36/40 (90%)	-0.52	2 (5%) 25 24	29, 46, 73, 82	0
9	j	40/40 (100%)	0.08	6 (15%) 3 2	34, 47, 81, 92	0
10	K	37/37 (100%)	-0.42	0 100 100	36, 44, 55, 70	0
10	k	37/37 (100%)	-0.19	1 (2%) 55 52	39, 47, 68, 81	0
11	L	35/35 (100%)	-0.14	7 (20%) 1 1	23, 32, 66, 78	0
11	l	35/35 (100%)	-0.15	4 (11%) 6 5	25, 35, 75, 92	0
12	O	243/243 (100%)	-0.28	8 (3%) 47 44	23, 39, 69, 104	0
12	o	243/243 (100%)	-0.29	15 (6%) 21 20	24, 42, 71, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	T	29/30 (96%)	-0.59	0 100 100	26, 32, 59, 89	0
13	t	29/30 (96%)	-0.51	2 (6%) 18 16	27, 34, 66, 98	0
14	U	97/97 (100%)	-0.19	0 100 100	26, 36, 58, 89	0
14	u	97/97 (100%)	-0.66	0 100 100	28, 37, 51, 76	0
15	V	137/137 (100%)	-0.62	0 100 100	25, 34, 50, 70	0
15	v	137/137 (100%)	-0.22	3 (2%) 62 60	29, 44, 61, 84	0
16	Y	29/29 (100%)	0.46	4 (13%) 3 3	40, 54, 69, 81	0
16	y	29/29 (100%)	0.52	4 (13%) 3 3	51, 62, 70, 74	0
17	X	37/37 (100%)	0.21	4 (10%) 6 6	41, 50, 72, 83	0
17	x	36/37 (97%)	0.94	9 (25%) 1 1	41, 54, 88, 89	0
18	Z	62/62 (100%)	0.40	13 (20%) 1 1	42, 54, 88, 106	0
18	z	61/62 (98%)	0.90	13 (21%) 1 1	49, 64, 98, 102	0
All	All	5147/5190 (99%)	-0.23	271 (5%) 27 26	21, 37, 70, 135	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	z	3	ILE	7.2
2	B	486	LEU	6.5
1	a	235	TYR	6.4
1	a	228	THR	6.2
2	B	488	PRO	6.2
17	x	2	THR	6.1
1	a	229	GLU	6.0
1	A	230	THR	6.0
1	A	246	TYR	5.8
18	z	4	LEU	5.7
1	a	230	THR	5.7
3	C	24	THR	5.6
1	a	260	PHE	5.5
2	b	484	PRO	5.5
18	z	2	THR	5.5
2	b	483	ASP	5.3
2	B	2	GLY	5.2
7	H	64	ALA	5.2
2	B	485	GLU	5.1
18	Z	33	TRP	5.0
1	a	11	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	a	227	THR	4.9
1	a	225	ARG	4.9
2	B	484	PRO	4.9
1	A	245	THR	4.9
2	B	496	TYR	4.9
2	B	479	PHE	4.8
18	Z	32	ASP	4.7
12	o	36	GLN	4.6
18	z	60	PHE	4.6
12	o	132	ASN	4.5
18	z	1	MET	4.5
2	B	495	PHE	4.5
2	B	503	THR	4.4
2	b	480	SER	4.4
18	z	5	PHE	4.4
1	A	11	ALA	4.4
1	a	245	THR	4.3
2	B	483	ASP	4.3
1	a	256	GLY	4.2
2	b	482	ILE	4.2
18	z	61	VAL	4.2
12	o	134	THR	4.2
12	o	246	ALA	4.1
6	F	15	ILE	4.1
2	B	487	SER	4.1
4	d	27	PHE	4.1
1	a	224	ILE	4.0
12	o	38	TYR	4.0
2	b	293	ALA	4.0
15	v	16	GLY	3.9
1	a	246	TYR	3.9
9	j	1	MET	3.9
2	B	506	ARG	3.9
1	a	242	GLU	3.8
3	c	143	TYR	3.8
1	a	259	ILE	3.8
18	z	6	GLN	3.8
1	a	237	TYR	3.7
6	F	16	PHE	3.7
18	Z	3	ILE	3.7
2	B	501	ASP	3.7
5	E	21	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	b	481	GLY	3.7
5	E	83	LEU	3.7
11	L	5	PRO	3.7
13	t	29	ILE	3.7
9	j	4	GLU	3.6
7	h	22	ALA	3.6
1	a	262	TYR	3.6
12	o	133	VAL	3.6
1	a	226	GLU	3.6
2	B	293	ALA	3.6
17	x	37	VAL	3.6
16	y	22	LEU	3.5
9	J	5	GLY	3.5
1	a	263	ALA	3.5
1	a	236	GLY	3.4
18	Z	30	PRO	3.4
1	a	250	ALA	3.3
2	b	126	PRO	3.3
3	C	257	PHE	3.3
2	b	295	GLY	3.3
11	L	9	PRO	3.3
18	Z	36	SER	3.3
13	t	30	THR	3.3
12	o	35	SER	3.3
1	A	228	THR	3.3
17	x	34	ILE	3.3
1	A	249	VAL	3.3
1	a	231	GLU	3.3
6	F	13	TYR	3.3
11	l	9	PRO	3.2
10	k	18	PHE	3.2
2	B	504	THR	3.2
5	e	72	ALA	3.2
1	a	261	GLN	3.2
11	L	7	ARG	3.2
6	F	14	PRO	3.2
5	E	25	ILE	3.2
2	B	161[A]	LEU	3.2
1	A	229	GLU	3.1
2	B	489	GLU	3.1
17	x	3	ILE	3.1
5	e	10	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	a	232	SER	3.1
5	e	20	TRP	3.1
1	a	240	GLY	3.1
4	D	240	ALA	3.1
5	e	21	VAL	3.1
4	d	238	THR	3.0
2	B	295	GLY	3.0
4	d	237	PRO	3.0
2	b	129	GLY	3.0
4	D	12	ARG	3.0
4	d	240	ALA	3.0
2	B	480	SER	3.0
3	C	145	SER	3.0
5	E	79	PHE	3.0
3	C	434	ALA	3.0
18	Z	34	ASP	3.0
2	B	502	VAL	3.0
5	e	79	PHE	2.9
2	b	218	LEU	2.9
18	Z	31	GLN	2.9
2	B	494	GLY	2.9
1	A	225	ARG	2.9
11	L	8	GLN	2.9
1	a	233	ALA	2.9
1	A	12	ASN	2.9
12	o	32	ILE	2.9
2	b	294	SER	2.9
18	Z	29	SER	2.9
5	E	17	VAL	2.9
17	X	38	GLN	2.9
17	x	29	ILE	2.8
4	d	236	ASN	2.8
5	E	10	PHE	2.8
4	d	12	ARG	2.8
9	j	3	SER	2.8
1	a	252	HIS	2.8
7	h	23	PRO	2.8
2	B	505	ARG	2.7
4	D	238	THR	2.7
9	j	2	MET	2.7
3	C	25	ASN	2.7
1	A	235	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
12	O	133	VAL	2.7
5	E	20	TRP	2.7
9	j	5	GLY	2.7
1	a	255	PHE	2.7
3	C	433	LEU	2.7
18	Z	38	GLN	2.7
5	e	19	TYR	2.7
4	d	287	VAL	2.7
2	b	127	ARG	2.6
12	O	135	SER	2.6
16	Y	46	LEU	2.6
3	C	255	THR	2.6
4	d	158	LEU	2.6
17	x	32	SER	2.6
4	d	17	ILE	2.6
2	B	85	GLY	2.6
17	x	36	LYS	2.6
4	d	25	ASP	2.6
2	B	162	PHE	2.6
18	Z	7	LEU	2.6
7	h	2	ALA	2.6
12	O	130	GLN	2.6
5	e	25	ILE	2.6
11	L	3	PRO	2.5
1	a	264	SER	2.5
7	h	58	VAL	2.5
1	a	257	ARG	2.5
12	O	60	ARG	2.5
16	y	20	ALA	2.5
5	E	74	GLN	2.5
18	Z	35	ARG	2.5
17	x	30	ALA	2.5
12	o	25	THR	2.5
4	d	159	ILE	2.5
17	X	34	ILE	2.5
11	l	3	PRO	2.4
12	O	27	ARG	2.4
18	Z	39	LEU	2.4
12	o	37	THR	2.4
17	X	2	THR	2.4
5	e	71	GLU	2.4
17	X	37	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
12	o	33	ASP	2.4
2	B	490	GLN	2.4
11	l	4	ASN	2.4
16	Y	18	VAL	2.4
1	a	241	GLN	2.4
18	z	7	LEU	2.4
1	A	236	GLY	2.4
7	h	57	GLY	2.4
2	B	481	GLY	2.4
5	E	78	THR	2.3
5	E	82	GLN	2.3
2	B	250	PHE	2.3
2	b	291	SER	2.3
2	b	251	VAL	2.3
3	C	261	ARG	2.3
3	c	200	THR	2.3
16	Y	19	ILE	2.3
18	z	8	ALA	2.3
2	B	246	PHE	2.3
11	L	10	VAL	2.3
4	D	237	PRO	2.3
16	y	37	PHE	2.2
3	C	256	PRO	2.2
12	O	131	PRO	2.2
3	C	23	ALA	2.2
4	d	234	ALA	2.2
12	O	132	ASN	2.2
2	b	250	PHE	2.2
2	B	290	ALA	2.2
2	b	456	ALA	2.2
1	A	243	GLU	2.2
12	o	245	PRO	2.2
1	a	238	LYS	2.2
3	C	144	SER	2.2
12	o	135	SER	2.2
1	a	14	TRP	2.2
18	z	33	TRP	2.2
1	a	234	ASN	2.2
4	d	150	ILE	2.2
7	h	24	GLY	2.2
15	v	15	GLU	2.2
6	f	15	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	2	GLY	2.2
2	b	298	LEU	2.2
12	o	34	SER	2.2
7	h	63	LYS	2.1
2	B	248	ALA	2.1
18	Z	26	ALA	2.1
12	O	136	ILE	2.1
2	b	125	ASP	2.1
1	A	266	ASN	2.1
9	J	6	GLY	2.1
5	e	59	GLU	2.1
1	a	249	VAL	2.1
2	B	251	VAL	2.1
2	B	459	ALA	2.1
2	B	244	ALA	2.1
1	A	247	ASN	2.1
7	h	56	ASP	2.1
2	B	249	ALA	2.1
5	e	17	VAL	2.1
4	d	228	GLY	2.1
18	z	9	LEU	2.1
9	j	6	GLY	2.1
2	B	126	PRO	2.1
11	l	8	GLN	2.0
2	B	292	LEU	2.0
2	b	292	LEU	2.0
5	e	61	ARG	2.0
16	Y	43	ARG	2.0
3	C	201	ASN	2.0
15	v	14	SER	2.0
16	y	41	VAL	2.0
2	b	246	PHE	2.0
5	e	14	ILE	2.0
4	D	11	GLU	2.0
18	z	38	GLN	2.0
8	I	34	ARG	2.0
12	o	24	ASP	2.0
17	x	35	ASP	2.0
11	L	4	ASN	2.0
1	A	231	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
13	FME	T	1	10/11	0.95	0.19	-	38,42,72,75	0
8	FME	I	1	10/11	0.95	0.14	-	33,37,40,41	0
8	FME	i	1	10/11	0.97	0.11	-	36,41,45,48	0
13	FME	t	1	10/11	0.97	0.09	-	33,38,80,91	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
30	UNL	a	420	6/-	0.73	0.35	62.60	56,59,60,60	0
30	UNL	t	102	16/-	0.68	0.32	24.65	59,71,78,80	0
29	LMT	A	414	35/35	0.71	0.35	23.58	59,86,109,114	0
30	UNL	A	415	5/-	0.88	0.35	12.87	68,72,73,75	0
31	DMS	o	303	4/4	0.90	0.21	11.25	60,77,80,83	0
24	BCR	b	618	20/40	0.86	0.25	10.06	57,65,70,71	0
29	LMT	T	102	24/35	0.70	0.23	9.55	42,80,98,101	0
30	UNL	T	101	13/-	0.74	0.34	9.00	63,71,77,79	0
31	DMS	O	313	4/4	0.90	0.25	8.78	89,100,100,107	0
31	DMS	C	540	4/4	0.85	0.33	8.55	82,83,91,97	0
30	UNL	i	104	16/-	0.69	0.34	8.36	67,76,87,89	0
31	DMS	u	205	4/4	0.88	0.32	8.30	64,67,73,83	0
35	DGD	d	406	43/66	0.66	0.32	7.91	58,85,139,146	0
30	UNL	B	624	7/-	0.86	0.17	7.78	30,45,51,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	C	536	4/4	0.83	0.22	7.35	77,80,94,95	0
35	DGD	D	407	50/66	0.71	0.29	7.10	60,87,120,123	0
29	LMT	a	419	35/35	0.73	0.27	6.92	46,69,93,100	0
31	DMS	c	934	4/4	0.98	0.24	6.91	64,73,74,77	0
31	DMS	L	102	4/4	0.79	0.23	6.59	79,80,91,100	0
31	DMS	b	630	4/4	0.96	0.15	6.55	56,63,63,64	0
31	DMS	c	935	4/4	0.90	0.33	6.49	71,78,81,84	0
34	HTG	b	632	19/19	0.61	0.27	6.39	56,74,91,92	0
29	LMT	E	101	24/35	0.80	0.27	6.19	61,82,97,113	0
31	DMS	C	530	4/4	0.95	0.31	6.09	71,79,82,83	0
29	LMT	f	102	25/35	0.57	0.44	5.91	61,93,105,108	0
31	DMS	b	638	4/4	0.88	0.24	5.91	49,52,54,70	0
31	DMS	U	203	4/4	0.87	0.24	5.79	62,73,74,76	0
31	DMS	c	925	4/4	0.97	0.14	5.32	51,58,60,61	0
31	DMS	C	535	4/4	0.91	0.38	5.16	70,79,83,86	0
31	DMS	c	927	4/4	0.89	0.22	5.02	87,89,91,97	0
31	DMS	C	528	4/4	0.95	0.28	5.00	88,89,90,90	0
24	BCR	B	618	19/40	0.82	0.18	4.91	50,59,74,77	0
31	DMS	O	307	4/4	0.86	0.26	4.89	84,97,98,104	0
25	LMG	C	531	40/55	0.72	0.24	4.74	37,81,103,107	0
34	HTG	D	414	19/19	0.66	0.32	4.70	63,103,114,115	0
31	DMS	O	310	4/4	0.97	0.14	4.50	66,68,68,73	0
22	CLA	b	602	65/65	0.81	0.31	4.46	49,67,89,98	0
31	DMS	a	424	4/4	0.96	0.15	4.39	38,47,50,65	0
31	DMS	o	307	4/4	0.99	0.30	4.34	48,56,62,64	0
30	UNL	D	413	16/-	0.88	0.23	4.33	38,46,52,58	0
31	DMS	O	312	4/4	0.97	0.18	4.30	37,51,56,59	0
31	DMS	o	305	4/4	0.92	0.36	4.24	78,82,86,87	0
31	DMS	V	209	4/4	0.95	0.32	4.21	76,87,89,93	0
31	DMS	v	211	4/4	0.92	0.18	4.12	65,77,82,90	0
31	DMS	o	302	4/4	0.95	0.17	4.00	59,64,71,75	0
31	DMS	B	631	4/4	0.90	0.27	3.94	78,80,84,87	0
30	UNL	a	417	10/-	0.66	0.41	3.89	75,80,84,87	0
30	UNL	j	103	16/-	0.81	0.17	3.87	59,67,71,74	0
29	LMT	t	101	24/35	0.76	0.20	3.76	50,71,109,119	0
31	DMS	i	106	4/4	0.95	0.22	3.59	72,76,79,89	0
31	DMS	V	211	4/4	0.83	0.23	3.51	77,84,85,85	0
31	DMS	c	926	4/4	0.97	0.17	3.51	63,64,67,68	0
34	HTG	V	203	14/19	0.91	0.23	3.43	48,52,79,84	0
31	DMS	f	103	4/4	0.88	0.28	3.32	87,89,90,100	0
29	LMT	c	921	35/35	0.84	0.36	3.21	74,90,99,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	LMG	J	101	45/55	0.95	0.13	3.19	28,36,71,79	0
31	DMS	c	929	4/4	0.89	0.31	3.14	69,73,76,78	0
30	UNL	U	201	14/-	0.82	0.25	3.04	44,57,65,66	0
22	CLA	B	602	65/65	0.92	0.17	3.00	39,56,101,107	0
31	DMS	D	417	4/4	0.91	0.19	2.98	72,72,77,86	0
31	DMS	B	628	4/4	0.99	0.14	2.85	27,29,32,38	0
34	HTG	B	626	19/19	0.83	0.20	2.80	42,69,81,87	0
27	LHG	A	412	31/49	0.74	0.27	2.74	66,83,107,117	0
31	DMS	c	939	4/4	0.95	0.31	2.72	88,92,95,102	0
31	DMS	F	101	4/4	0.93	0.20	2.68	69,70,74,77	0
29	LMT	c	931	24/35	0.69	0.26	2.64	50,84,95,98	0
31	DMS	c	924	4/4	0.98	0.14	2.63	37,42,47,49	0
25	LMG	b	622	43/55	0.63	0.28	2.63	48,78,88,98	0
31	DMS	O	304	4/4	0.94	0.38	2.60	74,80,84,88	0
29	LMT	Z	101	35/35	0.71	0.36	2.59	40,105,123,128	0
34	HTG	D	415	19/19	0.68	0.28	2.51	39,69,80,87	0
30	UNL	I	104	16/-	0.86	0.27	2.51	60,71,84,86	0
30	UNL	J	103	16/-	0.89	0.20	2.49	44,57,77,77	0
24	BCR	b	619	31/40	0.92	0.15	2.49	47,54,63,67	0
24	BCR	D	405	40/40	0.95	0.12	2.43	26,35,62,66	0
25	LMG	B	621	40/55	0.67	0.24	2.43	47,82,108,112	0
31	DMS	a	425	4/4	0.88	0.15	2.38	39,47,51,62	0
31	DMS	v	210	4/4	0.87	0.24	2.29	63,71,80,91	0
31	DMS	V	204	4/4	0.88	0.24	2.27	66,73,76,76	0
31	DMS	b	629	4/4	0.97	0.14	2.14	29,31,36,45	0
30	UNL	u	201	11/-	0.65	0.27	2.14	47,53,69,69	0
35	DGD	C	519	62/66	0.95	0.15	2.12	23,36,76,85	0
29	LMT	I	102	35/35	0.81	0.30	2.09	76,88,100,102	0
31	DMS	B	640	4/4	0.96	0.30	2.05	47,53,57,63	0
28	SQD	A	413	49/54	0.84	0.20	2.00	46,65,91,95	0
31	DMS	V	201	4/4	0.96	0.20	1.99	46,48,54,58	0
26	PL9	A	411	55/55	0.78	0.23	1.99	61,73,87,92	0
27	LHG	a	416	49/49	0.71	0.28	1.98	60,84,100,108	0
31	DMS	C	527	4/4	0.96	0.17	1.97	74,80,80,81	0
31	DMS	u	202	4/4	0.96	0.15	1.97	47,53,55,68	0
25	LMG	d	409	47/55	0.85	0.18	1.94	49,76,113,114	0
31	DMS	O	306	4/4	0.98	0.19	1.94	69,69,70,81	0
31	DMS	I	106	4/4	0.95	0.28	1.93	64,74,78,80	0
31	DMS	O	311	4/4	0.95	0.13	1.85	48,56,59,61	0
28	SQD	l	101	54/54	0.70	0.25	1.83	53,82,119,123	0
31	DMS	C	539	4/4	0.94	0.23	1.72	88,90,93,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	d	415	4/4	0.90	0.15	1.71	60,63,67,79	0
31	DMS	b	631	4/4	0.94	0.17	1.65	68,72,79,80	0
28	SQD	a	418	51/54	0.87	0.15	1.64	47,70,91,97	0
31	DMS	A	420	4/4	0.91	0.15	1.61	37,39,39,57	0
31	DMS	A	416	4/4	0.95	0.12	1.60	60,67,69,72	0
31	DMS	d	413	4/4	0.98	0.19	1.59	67,69,73,80	0
26	PL9	D	406	55/55	0.94	0.12	1.57	21,30,37,51	0
30	UNL	d	410	16/-	0.94	0.16	1.57	40,49,57,60	0
26	PL9	a	415	55/55	0.76	0.27	1.57	64,84,106,111	0
34	HTG	C	523	9/19	0.91	0.22	1.56	63,69,81,86	0
31	DMS	U	202	4/4	0.93	0.15	1.55	42,49,58,67	0
31	DMS	o	304	4/4	0.94	0.17	1.54	70,70,70,74	0
24	BCR	B	619	30/40	0.92	0.14	1.52	44,51,61,63	0
25	LMG	c	930	49/55	0.74	0.20	1.49	44,78,96,106	0
31	DMS	o	306	4/4	0.96	0.21	1.48	66,71,74,83	0
34	HTG	b	623	19/19	0.95	0.10	1.47	42,46,54,63	0
31	DMS	B	630	4/4	0.94	0.16	1.44	63,67,68,75	0
28	SQD	D	408	20/54	0.89	0.30	1.39	65,97,105,108	0
25	LMG	D	412	46/55	0.69	0.25	1.38	41,68,138,142	0
34	HTG	b	626	19/19	0.90	0.13	1.38	47,69,86,90	0
30	UNL	O	301	16/-	0.93	0.13	1.34	39,47,73,74	0
35	DGD	C	518	62/66	0.92	0.17	1.34	29,40,89,109	0
27	LHG	d	408	46/49	0.94	0.15	1.27	29,41,93,97	0
31	DMS	B	629	4/4	0.96	0.15	1.26	48,52,58,65	0
27	LHG	d	401	33/49	0.81	0.16	1.22	62,94,138,142	0
34	HTG	b	624	19/19	0.78	0.28	1.19	69,97,109,110	0
22	CLA	c	904	65/65	0.94	0.22	1.18	32,44,50,54	0
27	LHG	D	411	45/49	0.96	0.13	1.16	31,39,90,94	0
26	PL9	d	405	55/55	0.96	0.11	1.13	23,32,39,43	0
22	CLA	b	606	65/65	0.97	0.14	1.12	24,28,40,40	0
31	DMS	O	303	4/4	0.93	0.17	1.11	68,71,78,79	0
25	LMG	A	410	51/55	0.84	0.19	1.10	47,62,83,91	0
31	DMS	d	412	4/4	0.94	0.18	1.09	58,59,66,66	0
22	CLA	c	903	65/65	0.94	0.21	1.08	27,34,54,65	0
31	DMS	V	212	4/4	0.91	0.18	1.07	51,54,55,72	0
22	CLA	B	611	65/65	0.96	0.17	1.07	26,33,41,46	0
31	DMS	b	633	4/4	0.97	0.09	1.05	68,68,70,78	0
23	PHO	a	410	64/64	0.97	0.13	1.03	21,28,32,36	0
28	SQD	b	621	38/54	0.84	0.17	1.01	58,90,110,112	0
29	LMT	B	622	24/35	0.84	0.16	0.97	57,67,73,78	0
22	CLA	c	909	65/65	0.96	0.14	0.95	31,37,80,97	0
25	LMG	i	101	51/55	0.88	0.16	0.93	45,57,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LHG	D	409	49/49	0.91	0.19	0.90	38,56,85,97	0
31	DMS	d	411	4/4	0.98	0.13	0.89	60,62,64,64	0
31	DMS	O	314	4/4	0.89	0.26	0.88	78,80,86,91	0
35	DGD	c	917	62/66	0.96	0.14	0.84	26,42,81,94	0
25	LMG	c	920	51/55	0.85	0.18	0.84	37,61,87,91	0
34	HTG	B	623	19/19	0.95	0.11	0.83	41,47,64,66	0
25	LMG	j	101	47/55	0.94	0.11	0.83	33,43,69,74	0
22	CLA	C	510	65/65	0.95	0.16	0.82	31,36,59,64	0
30	UNL	x	101	15/-	0.89	0.13	0.80	43,50,56,58	0
27	LHG	D	410	49/49	0.97	0.12	0.79	29,36,51,61	0
22	CLA	c	910	65/65	0.96	0.16	0.79	28,38,58,64	0
30	UNL	X	101	16/-	0.89	0.13	0.78	35,53,62,64	0
28	SQD	a	414	54/54	0.91	0.14	0.77	36,69,81,87	0
35	DGD	c	919	62/66	0.96	0.12	0.76	29,40,73,79	0
22	CLA	C	514	65/65	0.92	0.15	0.75	44,55,83,86	0
25	LMG	C	520	51/55	0.87	0.19	0.75	34,60,90,92	0
31	DMS	c	928	4/4	0.94	0.17	0.75	73,74,74,80	0
31	DMS	V	210	4/4	0.90	0.13	0.74	70,73,78,88	0
27	LHG	C	522	30/49	0.82	0.16	0.73	55,79,127,134	0
28	SQD	C	501	54/54	0.94	0.13	0.73	32,64,83,89	0
37	RRX	H	101	41/41	0.85	0.16	0.71	32,42,58,62	0
22	CLA	B	606	65/65	0.97	0.14	0.70	24,30,42,46	0
24	BCR	d	404	40/40	0.95	0.10	0.67	27,38,63,66	0
27	LHG	l	102	49/49	0.89	0.18	0.65	38,61,91,95	0
24	BCR	A	409	40/40	0.97	0.12	0.65	25,30,37,38	0
31	DMS	v	206	4/4	0.97	0.20	0.63	69,72,72,77	0
22	CLA	c	913	65/65	0.92	0.14	0.63	42,54,96,98	0
35	DGD	H	102	62/66	0.90	0.19	0.61	28,37,46,50	0
22	CLA	C	511	65/65	0.97	0.20	0.58	31,36,41,46	0
22	CLA	B	616	65/65	0.97	0.11	0.56	30,36,50,57	0
22	CLA	C	502	65/65	0.95	0.13	0.55	33,39,52,62	0
35	DGD	h	102	62/66	0.86	0.20	0.54	28,42,53,58	0
22	CLA	a	409	61/65	0.97	0.15	0.53	25,29,80,87	0
23	PHO	D	402	64/64	0.97	0.14	0.53	25,29,35,39	0
23	PHO	A	407	64/64	0.97	0.13	0.52	20,25,30,32	0
22	CLA	a	412	65/65	0.96	0.10	0.52	27,32,102,116	0
22	CLA	b	604	65/65	0.97	0.16	0.51	26,32,45,50	0
37	RRX	h	101	41/41	0.78	0.21	0.49	40,49,75,82	0
22	CLA	A	406	55/65	0.98	0.12	0.48	21,27,49,60	0
31	DMS	c	933	4/4	0.96	0.10	0.47	57,64,66,70	0
22	CLA	B	604	65/65	0.95	0.15	0.46	26,30,40,47	0
22	CLA	D	404	65/65	0.95	0.11	0.46	30,37,94,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	C	505	65/65	0.96	0.17	0.45	28,34,58,60	0
22	CLA	B	613	65/65	0.96	0.15	0.43	24,30,37,40	0
22	CLA	c	911	65/65	0.97	0.20	0.41	29,38,46,52	0
22	CLA	B	609	65/65	0.97	0.17	0.41	25,30,38,39	0
24	BCR	b	620	40/40	0.95	0.12	0.41	33,39,48,49	0
22	CLA	b	613	65/65	0.96	0.14	0.40	26,32,37,40	0
22	CLA	c	905	65/65	0.96	0.18	0.39	30,35,62,66	0
35	DGD	c	918	62/66	0.94	0.15	0.39	34,42,98,113	0
31	DMS	v	209	4/4	0.97	0.25	0.39	72,74,76,81	0
22	CLA	C	509	65/65	0.96	0.14	0.37	29,35,81,102	0
22	CLA	c	914	65/65	0.93	0.16	0.35	47,60,95,108	0
22	CLA	B	608	65/65	0.95	0.12	0.33	24,29,64,79	0
22	CLA	C	503	65/65	0.96	0.17	0.33	28,32,47,56	0
28	SQD	f	101	14/54	0.88	0.22	0.33	77,89,96,96	0
22	CLA	c	902	65/65	0.96	0.11	0.32	34,39,50,51	0
24	BCR	a	413	40/40	0.96	0.09	0.30	26,31,38,39	0
35	DGD	C	517	62/66	0.95	0.13	0.28	24,35,80,88	0
27	LHG	a	423	45/49	0.90	0.15	0.28	39,58,72,74	0
22	CLA	A	405	65/65	0.97	0.11	0.28	18,23,36,54	0
22	CLA	A	408	65/65	0.97	0.11	0.27	19,29,99,110	0
22	CLA	a	407	65/65	0.98	0.13	0.24	23,26,45,61	0
31	DMS	B	633	4/4	0.98	0.16	0.23	65,71,71,73	0
24	BCR	C	516	40/40	0.95	0.10	0.23	32,39,47,54	0
22	CLA	a	408	65/65	0.98	0.10	0.22	20,26,35,41	0
22	CLA	B	610	65/65	0.93	0.12	0.22	30,37,42,46	0
31	DMS	B	641	4/4	0.95	0.10	0.22	46,49,61,66	0
22	CLA	D	401	65/65	0.98	0.09	0.21	19,23,31,36	0
27	LHG	d	407	49/49	0.96	0.11	0.21	28,36,56,63	0
24	BCR	y	101	40/40	0.91	0.12	0.20	32,41,51,53	0
22	CLA	c	907	65/65	0.95	0.12	0.20	39,47,102,108	0
24	BCR	B	620	40/40	0.95	0.10	0.17	30,37,49,50	0
22	CLA	b	607	65/65	0.93	0.11	0.17	29,37,58,65	0
24	BCR	C	515	40/40	0.94	0.10	0.17	37,50,58,59	0
22	CLA	B	603	65/65	0.93	0.14	0.16	27,36,43,47	0
22	CLA	C	506	65/65	0.96	0.14	0.16	30,37,50,54	0
22	CLA	b	605	65/65	0.97	0.17	0.13	23,29,63,65	0
22	CLA	b	611	65/65	0.96	0.11	0.10	28,35,40,43	0
22	CLA	B	605	65/65	0.97	0.18	0.09	24,28,60,66	0
27	LHG	L	101	40/49	0.94	0.12	0.09	37,53,63,66	0
22	CLA	c	906	65/65	0.95	0.10	0.08	30,40,50,54	0
22	CLA	C	504	65/65	0.96	0.13	0.02	29,37,42,51	0
31	DMS	D	416	4/4	0.98	0.19	0.01	55,59,60,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	HTG	v	203	16/19	0.84	0.16	-0.02	52,69,81,97	0
22	CLA	b	603	65/65	0.94	0.14	-0.04	29,36,46,49	0
22	CLA	D	403	65/65	0.97	0.12	-0.05	18,24,45,52	0
38	MG	j	102	1/1	0.99	0.11	-0.08	40,40,40,40	0
22	CLA	d	403	65/65	0.95	0.11	-0.11	35,40,85,90	0
24	BCR	c	915	40/40	0.93	0.12	-0.12	43,59,68,69	0
22	CLA	b	612	65/65	0.96	0.12	-0.13	27,31,72,83	0
31	DMS	V	208	4/4	0.97	0.10	-0.13	73,74,77,78	0
23	PHO	a	411	64/64	0.96	0.14	-0.14	26,33,40,48	0
22	CLA	C	507	65/65	0.94	0.12	-0.14	37,45,85,88	0
38	MG	J	102	1/1	0.99	0.07	-0.15	30,30,30,30	0
22	CLA	b	614	59/65	0.97	0.14	-0.16	26,32,76,82	0
22	CLA	d	402	65/65	0.98	0.13	-0.17	21,27,42,50	0
22	CLA	B	607	65/65	0.94	0.10	-0.18	28,34,56,65	0
22	CLA	c	908	65/65	0.95	0.10	-0.18	34,39,53,61	0
22	CLA	B	612	65/65	0.96	0.13	-0.18	23,29,55,60	0
24	BCR	K	101	40/40	0.96	0.10	-0.19	31,39,43,43	0
36	HEM	V	202	43/43	0.98	0.09	-0.19	23,29,36,40	0
19	OEX	A	401	10/10	0.99	0.12	-0.19	25,27,31,32	0
36	HEM	e	101	43/43	0.98	0.17	-0.20	43,55,85,93	0
22	CLA	B	614	61/65	0.97	0.14	-0.21	25,31,70,83	0
31	DMS	V	206	4/4	0.96	0.09	-0.22	45,48,51,62	0
22	CLA	c	912	65/65	0.93	0.10	-0.24	35,45,50,53	0
22	CLA	b	616	65/65	0.94	0.10	-0.27	30,37,53,57	0
22	CLA	b	608	65/65	0.95	0.10	-0.28	27,31,73,74	0
22	CLA	B	615	53/65	0.93	0.11	-0.29	31,36,71,84	0
22	CLA	b	609	65/65	0.96	0.14	-0.30	27,34,42,45	0
22	CLA	b	610	65/65	0.94	0.10	-0.30	32,41,45,54	0
24	BCR	k	101	40/40	0.93	0.11	-0.31	36,45,51,52	0
34	HTG	l	106	19/19	0.83	0.18	-0.33	63,97,108,109	0
22	CLA	b	615	52/65	0.95	0.10	-0.34	36,42,71,76	0
24	BCR	Y	101	39/40	0.96	0.09	-0.37	34,40,48,50	0
36	HEM	E	102	43/43	0.96	0.14	-0.41	48,56,62,65	0
24	BCR	c	916	40/40	0.96	0.10	-0.42	33,42,48,49	0
22	CLA	C	513	56/65	0.95	0.10	-0.45	37,48,62,65	0
22	CLA	C	512	65/65	0.95	0.09	-0.46	31,39,48,51	0
32	BCT	A	421[A]	4/4	0.98	0.08	-0.46	34,36,39,39	4
32	BCT	A	421[B]	4/4	0.98	0.08	-0.47	27,29,30,34	4
22	CLA	C	508	65/65	0.96	0.10	-0.47	32,42,55,59	0
31	DMS	v	208	4/4	0.94	0.13	-0.48	88,90,91,94	0
31	DMS	v	204	4/4	0.94	0.13	-0.49	87,88,90,91	0
31	DMS	v	201	4/4	0.97	0.13	-0.54	42,48,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	b	617	60/65	0.94	0.11	-0.62	32,41,75,80	0
22	CLA	B	617	55/65	0.96	0.08	-0.64	28,35,72,76	0
21	CL	a	406	1/1	0.99	0.13	-0.64	32,32,32,32	0
36	HEM	v	202	43/43	0.98	0.08	-0.67	33,37,42,46	0
21	CL	A	403	1/1	0.99	0.09	-0.67	29,29,29,29	0
31	DMS	C	526	4/4	0.99	0.08	-0.70	48,48,50,51	0
32	BCT	a	422	4/4	0.96	0.07	-0.77	51,52,56,57	0
20	FE2	A	402	1/1	1.00	0.07	-0.98	39,39,39,39	0
20	FE2	a	404	1/1	0.99	0.07	-1.11	42,42,42,42	0
19	OEX	a	403	10/10	1.00	0.09	-1.40	29,31,32,33	0
31	DMS	C	525	4/4	0.99	0.06	-1.47	34,35,38,40	0
21	CL	A	404	1/1	0.99	0.12	-1.47	28,28,28,28	0
21	CL	a	405	1/1	0.99	0.07	-1.83	31,31,31,31	0
33	CA	O	302	1/1	0.96	0.04	-3.41	59,59,59,59	0
33	CA	c	901	1/1	0.99	0.03	-3.99	48,48,48,48	0
33	CA	o	301	1/1	0.99	0.03	-4.18	55,55,55,55	0
31	DMS	b	634	4/4	0.93	0.25	-	68,76,79,86	0
31	DMS	V	207	4/4	0.91	0.15	-	64,71,71,76	0
31	DMS	O	308	4/4	0.90	0.20	-	64,72,73,80	0
31	DMS	l	104	4/4	0.89	0.16	-	79,80,86,87	0
31	DMS	b	636	4/4	0.79	0.25	-	88,95,109,113	0
30	UNL	b	628	11/-	0.84	0.32	-	58,63,78,79	0
34	HTG	c	922	19/19	0.76	0.29	-	70,93,109,112	0
31	DMS	A	419	4/4	0.97	0.21	-	58,60,70,72	0
30	UNL	i	105	10/-	0.59	0.33	-	67,78,86,87	0
31	DMS	A	418	4/4	0.99	0.10	-	29,30,31,31	0
31	DMS	C	537	4/4	0.68	0.37	-	88,103,104,113	0
31	DMS	b	637	4/4	0.80	0.18	-	90,97,101,112	0
30	UNL	B	625	16/-	0.95	0.09	-	40,47,59,59	0
31	DMS	t	103	4/4	0.95	0.13	-	89,102,103,103	0
31	DMS	B	637	4/4	0.93	0.30	-	69,76,80,88	0
30	UNL	b	625	16/-	0.88	0.13	-	43,52,64,67	0
31	DMS	d	414	4/4	0.64	0.38	-	102,112,113,120	0
31	DMS	c	936	4/4	0.70	0.26	-	106,116,116,124	0
31	DMS	B	639	4/4	0.74	0.41	-	72,87,90,102	0
31	DMS	c	923	4/4	0.99	0.15	-	37,40,42,43	0
31	DMS	C	534	4/4	0.76	0.33	-	105,111,112,121	0
31	DMS	D	418	4/4	0.99	0.11	-	35,39,42,43	0
31	DMS	C	524	4/4	0.99	0.07	-	38,42,43,43	0
30	UNL	I	105	16/-	0.56	0.37	-	70,82,88,90	0
31	DMS	v	205	4/4	0.90	0.26	-	70,72,78,80	0
31	DMS	c	938	4/4	0.87	0.32	-	86,91,98,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	V	205	4/4	0.95	0.16	-	64,66,67,71	0
31	DMS	c	940	4/4	0.93	0.30	-	74,74,75,80	0
31	DMS	o	308	4/4	0.91	0.26	-	76,77,82,91	0
38	MG	k	102	1/1	0.97	0.05	-	48,48,48,48	0
31	DMS	c	937	4/4	0.72	0.17	-	80,90,91,100	0
33	CA	b	601	1/1	0.99	0.04	-	59,59,59,59	0
30	UNL	c	932	10/-	0.79	0.23	-	56,74,80,83	0
31	DMS	l	105	4/4	0.80	0.19	-	100,103,110,115	0
31	DMS	H	103	4/4	0.83	0.26	-	63,67,69,74	0
31	DMS	A	417	4/4	0.96	0.14	-	76,82,83,85	0
38	MG	K	102	1/1	0.97	0.05	-	51,51,51,51	0
30	UNL	I	103	13/-	0.73	0.23	-	53,57,77,82	0
31	DMS	I	101	4/4	0.93	0.23	-	64,69,74,76	0
31	DMS	l	103	4/4	0.87	0.21	-	91,95,97,99	0
31	DMS	C	538	4/4	0.94	0.36	-	79,86,86,87	0
34	HTG	B	627	19/19	0.59	0.32	-	51,104,113,116	0
31	DMS	c	944	4/4	0.92	0.20	-	79,82,89,92	0
31	DMS	B	642	4/4	0.94	0.20	-	65,66,75,82	0
31	DMS	a	401	4/4	0.66	0.28	-	75,84,85,104	0
31	DMS	C	533	4/4	0.91	0.22	-	79,84,85,89	0
31	DMS	O	305	4/4	0.54	0.23	-	68,70,79,99	0
31	DMS	B	636	4/4	0.94	0.23	-	60,62,67,69	0
31	DMS	B	632	4/4	0.86	0.20	-	49,57,67,69	0
31	DMS	u	204	4/4	0.88	0.34	-	50,68,69,75	0
30	UNL	i	102	16/-	0.92	0.13	-	41,51,80,81	0
31	DMS	B	634	4/4	0.74	0.25	-	57,68,73,95	0
31	DMS	t	105	4/4	0.86	0.18	-	89,93,101,108	0
31	DMS	b	635	4/4	0.90	0.17	-	62,69,76,86	0
31	DMS	u	203	4/4	0.89	0.17	-	56,68,72,84	0
31	DMS	B	635	4/4	0.95	0.18	-	61,63,66,73	0
33	CA	B	601	1/1	0.95	0.04	-	64,64,64,64	0
31	DMS	O	309	4/4	0.95	0.25	-	61,70,70,74	0
31	DMS	c	941	4/4	0.96	0.23	-	73,79,87,88	0
31	DMS	c	942	4/4	0.56	0.23	-	101,103,111,117	0
34	HTG	C	521	19/19	0.88	0.22	-	55,80,93,96	0
34	HTG	C	532	19/19	0.69	0.27	-	69,98,111,112	0
31	DMS	B	638	4/4	0.94	0.16	-	81,82,86,93	0
31	DMS	t	104	4/4	0.87	0.15	-	101,101,104,111	0
30	UNL	i	103	16/-	0.82	0.20	-	53,64,79,82	0
31	DMS	a	402	4/4	0.99	0.10	-	30,32,34,34	0
34	HTG	b	627	19/19	0.59	0.25	-	50,92,108,109	0
31	DMS	C	529	4/4	0.89	0.32	-	72,78,78,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	c	943	4/4	0.91	0.15	-	77,82,87,92	0
30	UNL	Z	102	9/-	0.75	0.30	-	57,71,79,81	0
31	DMS	v	207	4/4	0.82	0.17	-	84,93,97,117	0
31	DMS	a	421	4/4	0.90	0.26	-	85,87,87,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.