



# Full wwPDB X-ray Structure Validation Report

Jul 18, 2014 – 04:56 AM EDT

PDB ID : 4TNI  
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 Å resolution  
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.  
Deposited on : 2014-06-04  
Resolution : 4.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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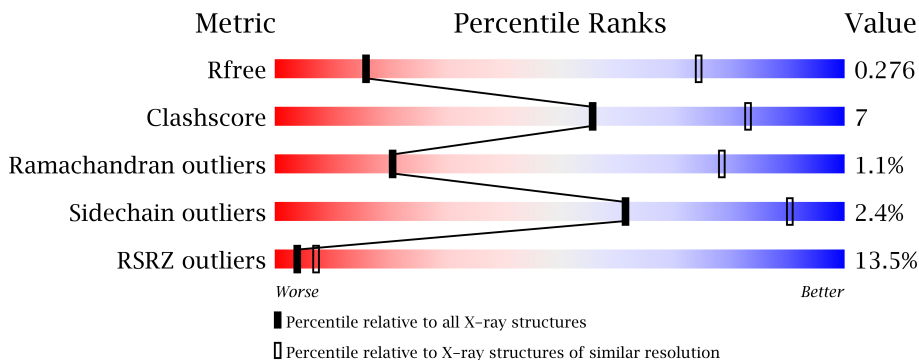
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 4.60 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))
$R_{free}$	66092	1032 (5.70-3.50)
Clashscore	79885	1304 (5.70-3.50)
Ramachandran outliers	78287	1225 (5.70-3.50)
Sidechain outliers	78261	1206 (5.70-3.50)
RSRZ outliers	66119	1031 (5.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	

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Mol	Chain	Length	Quality of chain
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
22	CLA	A	405	-	X
22	CLA	B	601	-	X
22	CLA	B	603	-	X
22	CLA	B	604	-	X
22	CLA	B	605	-	X
22	CLA	B	608	-	X
22	CLA	B	614	-	X
22	CLA	B	615	-	X
22	CLA	C	501	-	X
22	CLA	C	502	-	X
22	CLA	C	506	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
22	CLA	C	508	-	X
22	CLA	C	510	-	X
22	CLA	C	511	-	X
22	CLA	C	512	-	X
22	CLA	D	406	-	X
22	CLA	a	404	-	X
22	CLA	a	405	-	X
22	CLA	a	407	-	X
22	CLA	b	605	-	X
22	CLA	b	606	-	X
22	CLA	b	607	-	X
22	CLA	b	609	-	X
22	CLA	b	612	-	X
22	CLA	b	613	-	X
22	CLA	b	618	-	X
22	CLA	b	619	-	X
22	CLA	c	501	-	X
22	CLA	c	502	-	X
22	CLA	c	503	-	X
22	CLA	c	505	-	X
22	CLA	c	506	-	X
22	CLA	c	511	-	X
22	CLA	c	512	-	X
22	CLA	d	406	-	X
23	PL9	J	101	-	X
23	PL9	d	407	-	X
23	PL9	j	101	-	X
24	BCR	A	407	-	X
24	BCR	B	619	-	X
24	BCR	C	513	-	X
24	BCR	C	514	-	X
24	BCR	H	102	-	X
24	BCR	J	102	-	X
24	BCR	K	102	-	X
24	BCR	a	409	-	X
24	BCR	b	623	-	X
24	BCR	c	513	-	X
24	BCR	c	514	-	X
24	BCR	c	521	-	X
24	BCR	g	101	-	X
24	BCR	x	101	-	X
24	BCR	y	101	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
25	DGD	B	625	-	X
25	DGD	D	410	-	X
25	DGD	b	601	-	X
25	DGD	d	410	-	X
27	LMG	C	518	-	X
27	LMG	E	101	-	X
27	LMG	I	101	-	X
27	LMG	M	101	-	X
27	LMG	c	518	-	X
27	LMG	i	101	-	X
29	SQD	B	622	-	X
29	SQD	B	626	-	X
29	SQD	F	103	-	X
29	SQD	a	401	-	X
29	SQD	d	403	-	X
29	SQD	f	103	-	X
30	LMT	B	623	-	X
30	LMT	B	624	-	X
30	LMT	B	627	-	X
30	LMT	D	411	-	X
30	LMT	I	102	-	X
30	LMT	b	603	-	X
30	LMT	b	626	-	X
30	LMT	b	627	-	X
30	LMT	d	411	-	X
30	LMT	i	102	-	X
34	HEM	v	201	-	X
35	CA	K	101	-	X
35	CA	O	301	-	X
35	CA	o	301	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	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
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	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
			293	204	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	x	37	Total	C	N	O		0	0	0
			270	182	41	47				

- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	G	28	Total	C	N	O		0	0	0
			140	84	28	28				

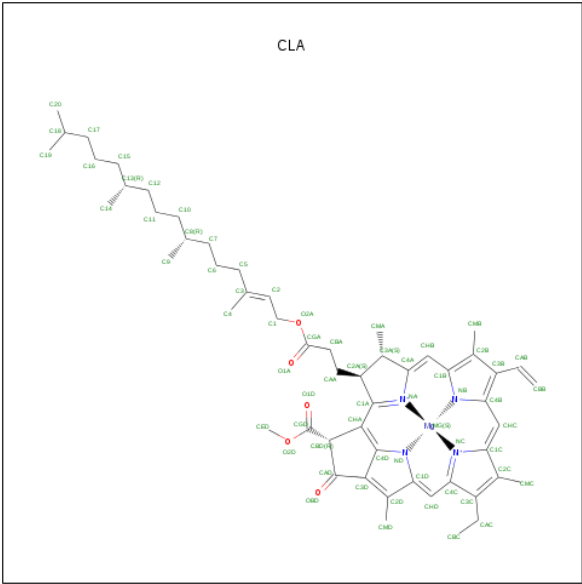
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- 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>).



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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 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
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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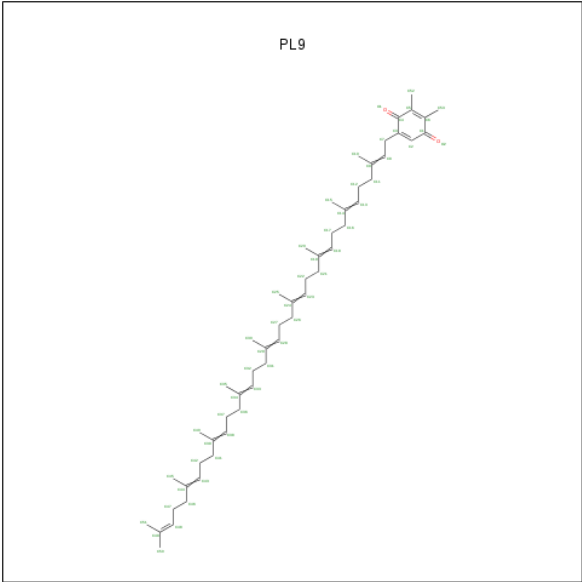
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	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 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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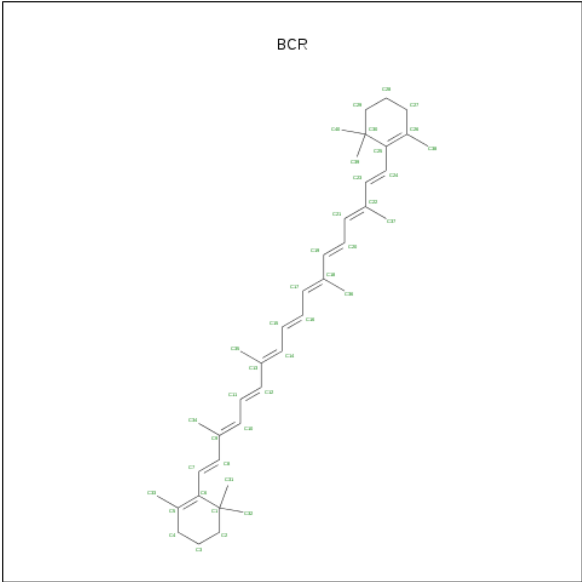
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	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	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		
22	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 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<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	a	1	Total	C	O	0	0
			45	43	2		
23	d	1	Total	C	O	0	0
			55	53	2		
23	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



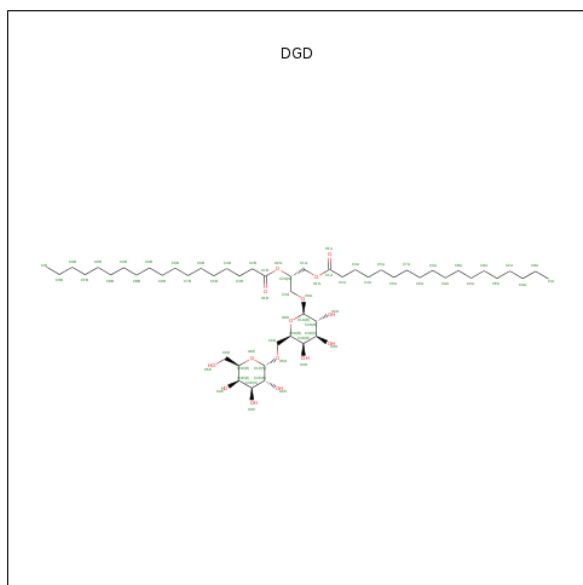
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	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	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



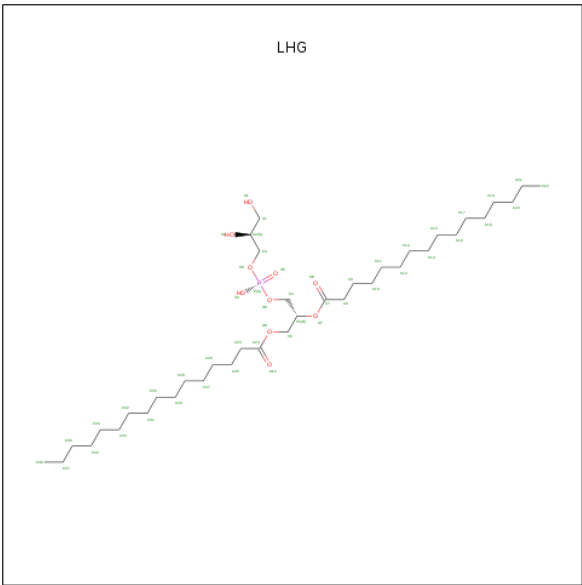
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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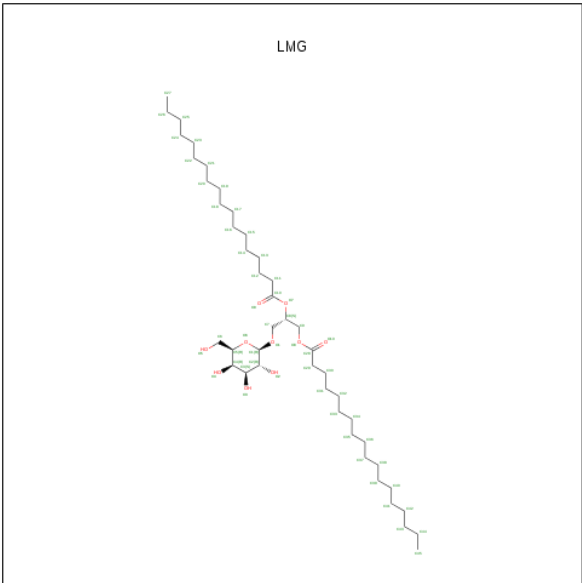
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total	C	O	0	0
			52	37	15		
25	b	1	Total	C	O	0	0
			58	43	15		
25	c	1	Total	C	O	0	0
			53	38	15		
25	c	1	Total	C	O	0	0
			62	47	15		
25	c	1	Total	C	O	0	0
			66	51	15		
25	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



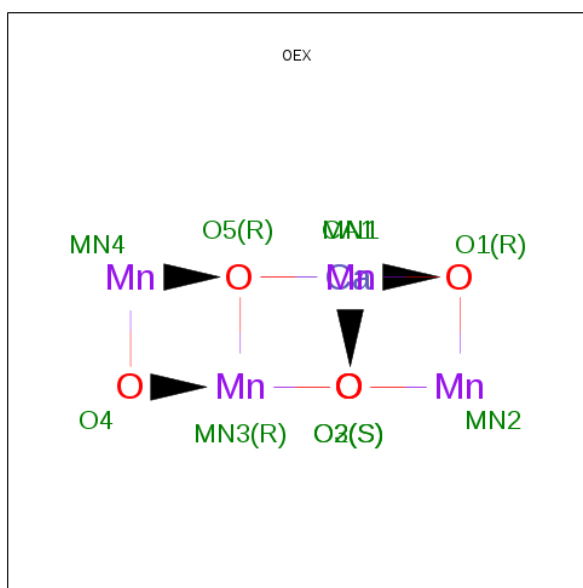
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



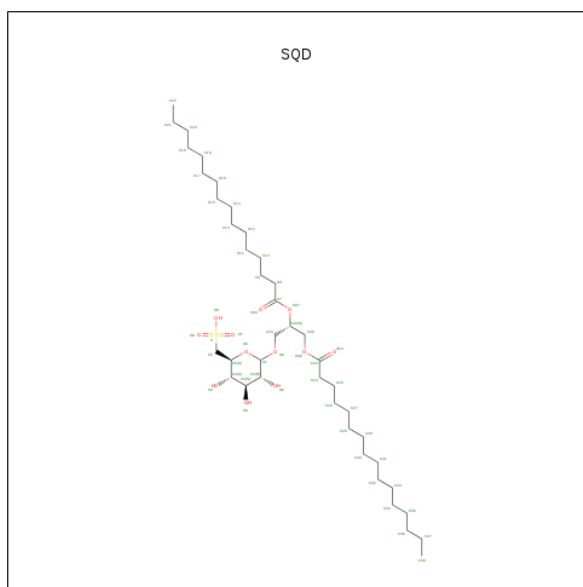
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	E	1	Total	C	O	0	0
			44	34	10		
27	I	1	Total	C	O	0	0
			43	33	10		
27	M	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			49	39	10		
27	c	1	Total	C	O	0	0
			45	35	10		
27	c	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			49	39	10		
27	d	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			46	36	10		
27	e	1	Total	C	O	0	0
			44	34	10		
27	i	1	Total	C	O	0	0
			43	33	10		
27	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



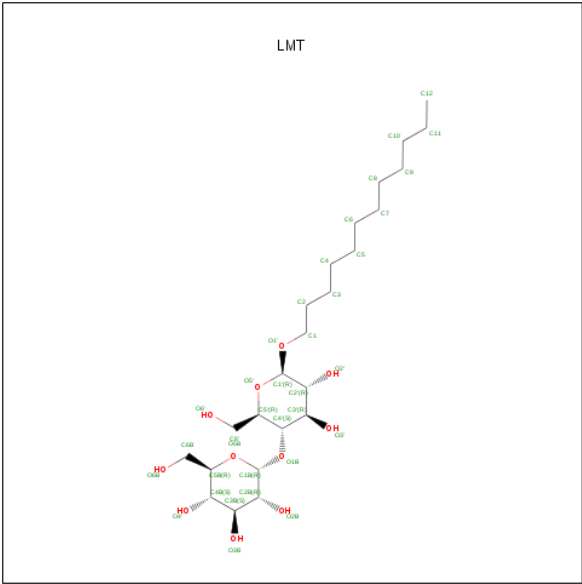
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			51	38	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			43	30	12	1		
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	F	1	Total	C	O	S	0	0
			45	32	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O	S	0	0
			51	38	12	1		
29	b	1	Total	C	O	S	0	0
			47	34	12	1		
29	d	1	Total	C	O	S	0	0
			43	30	12	1		
29	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



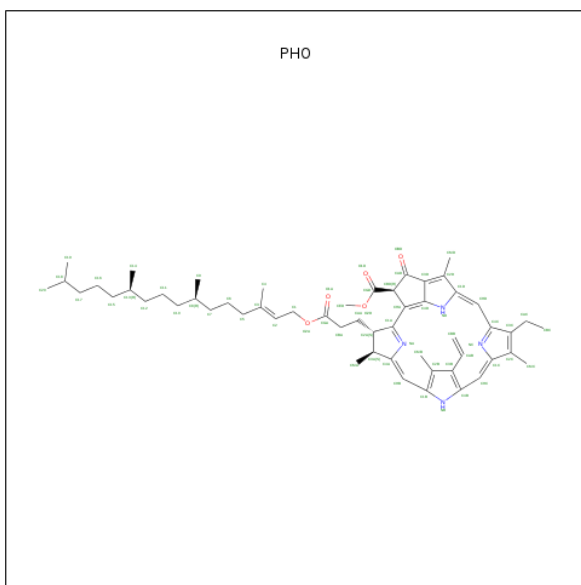
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	B	1	Total	C	O		0	0
			35	24	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	D	1	Total	C	O	0	0
			31	20	11		
30	I	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	d	1	Total	C	O	0	0
			31	20	11		
30	i	1	Total	C	O	0	0
			35	24	11		

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).

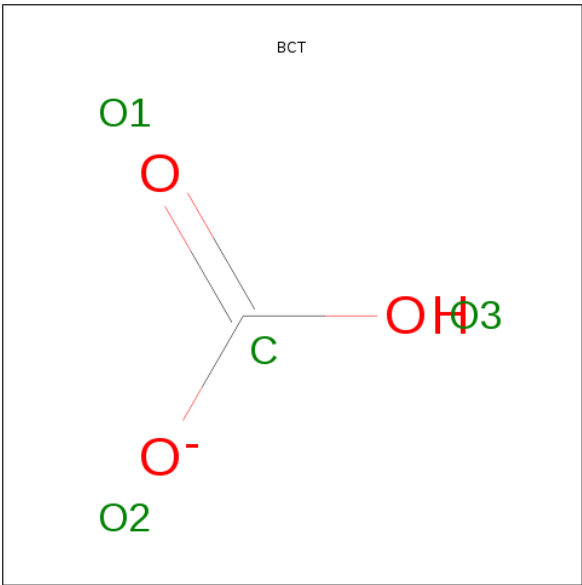


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

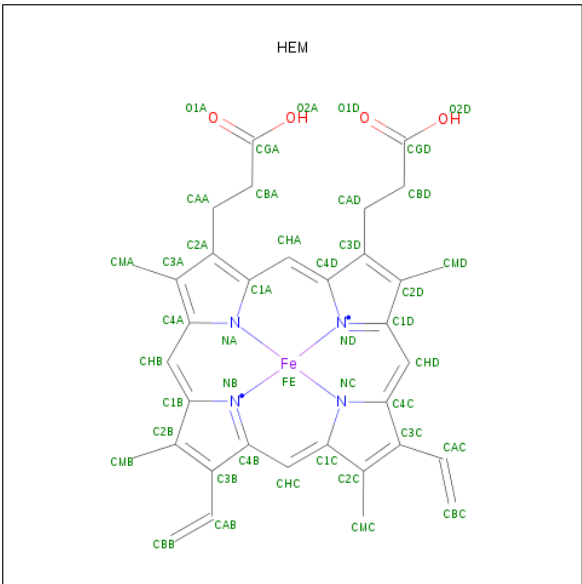
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	a	1	Total	Cl	0	0
			1	1		
32	D	1	Total	Cl	0	0
			1	1		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

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



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

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

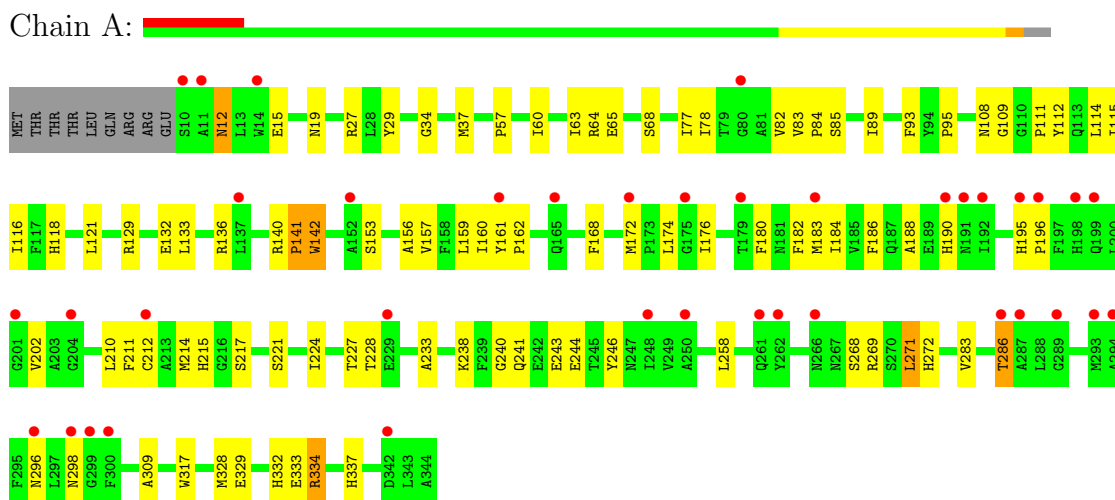
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total 1	Ca 1	0	0
35	O	1	Total 1	Ca 1	0	0
35	K	1	Total 1	Ca 1	0	0
35	k	1	Total 1	Ca 1	0	0

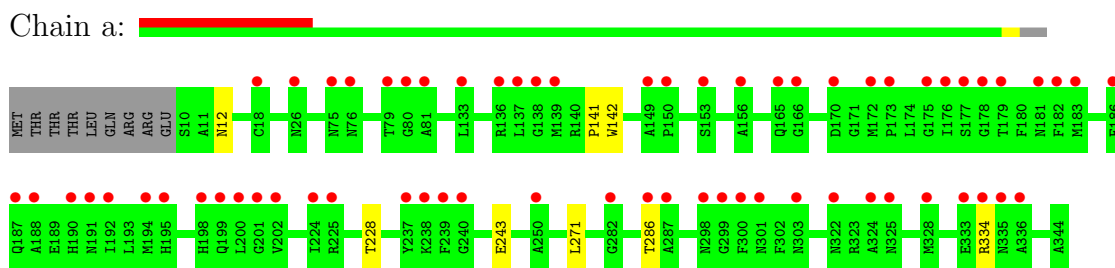
### 3 Residue-property plots

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

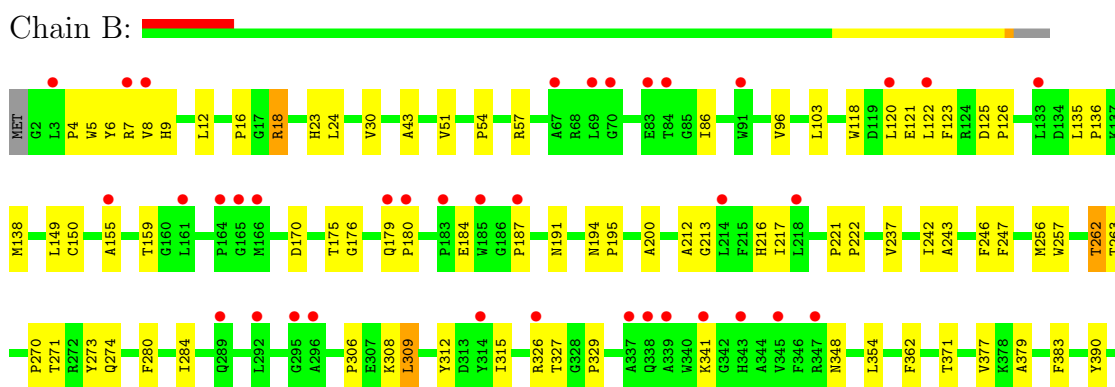
- Molecule 1: Photosystem Q(B) protein 1

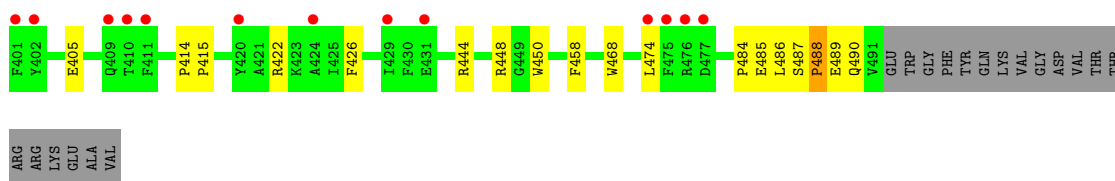


- Molecule 1: Photosystem Q(B) protein 1



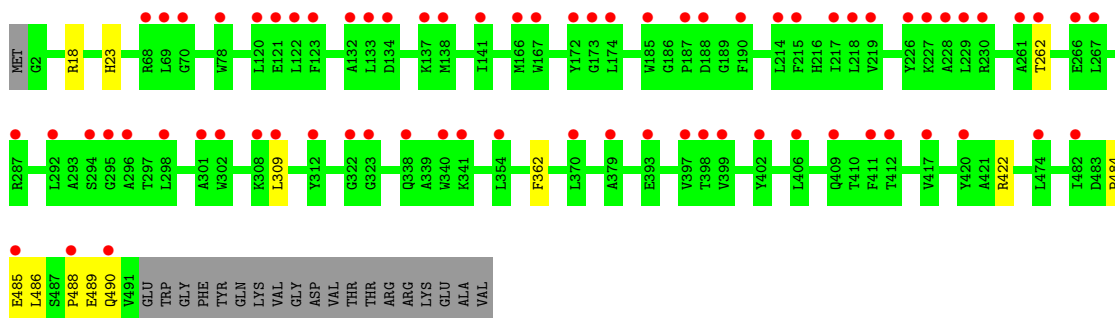
- Molecule 2: Photosystem II core light harvesting protein





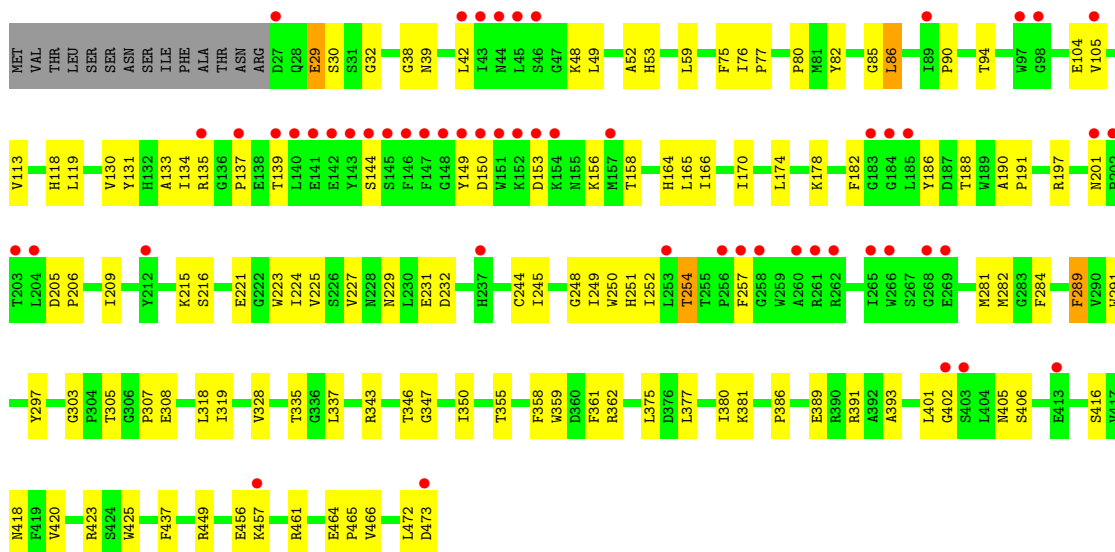
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



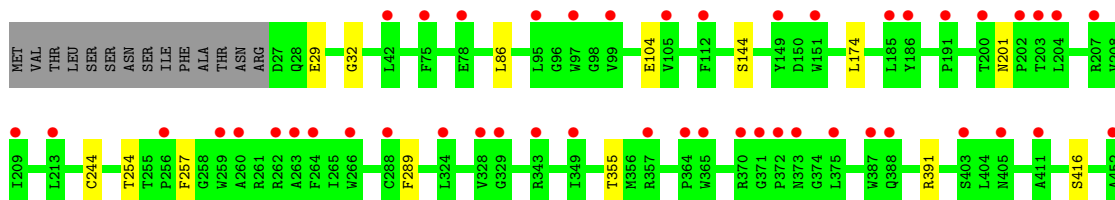
• Molecule 3: Photosystem II CP43 protein

Chain C:



• Molecule 3: Photosystem II CP43 protein

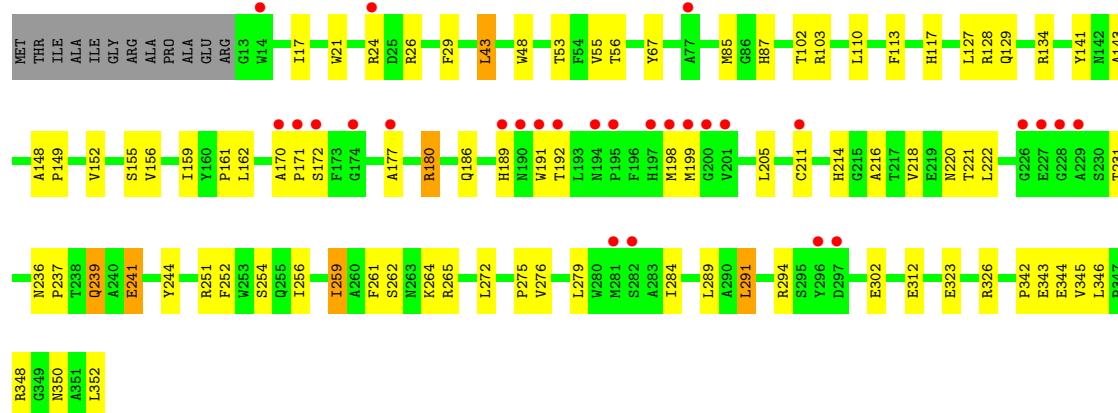
Chain c:





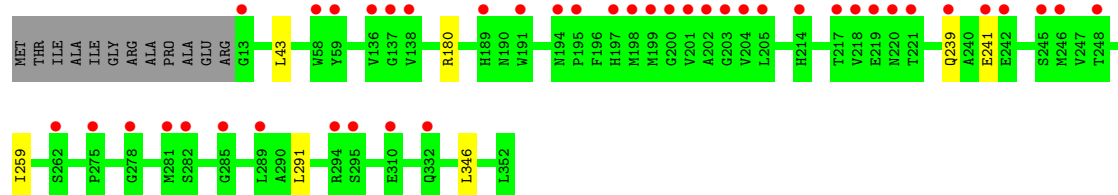
- Molecule 4: Photosystem II D2 protein

Chain D:



- Molecule 4: Photosystem II D2 protein

Chain d:



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:



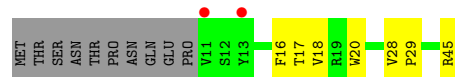
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:



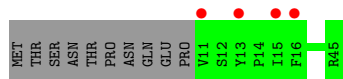
- Molecule 6: Cytochrome b559 subunit beta

Chain F:



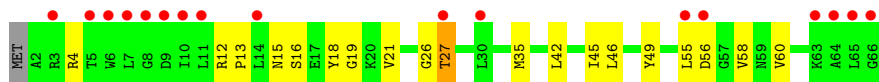
- Molecule 6: Cytochrome b559 subunit beta

Chain f:



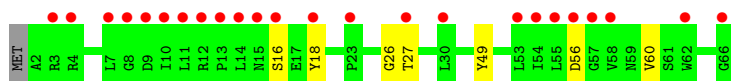
- Molecule 7: Photosystem II reaction center protein H

Chain H:



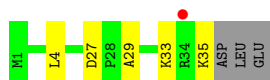
- Molecule 7: Photosystem II reaction center protein H

Chain h:



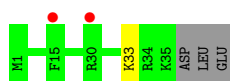
- Molecule 8: Photosystem II reaction center protein I

Chain I:



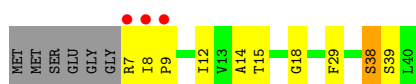
- Molecule 8: Photosystem II reaction center protein I

Chain i:



- Molecule 9: Photosystem II reaction center protein J

Chain J:



- Molecule 9: Photosystem II reaction center protein J

Chain j:



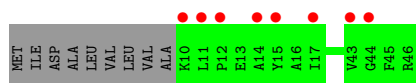
- Molecule 10: Photosystem II reaction center protein K

Chain K:



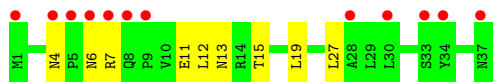
- Molecule 10: Photosystem II reaction center protein K

Chain k:



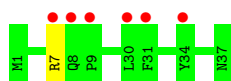
- Molecule 11: Photosystem II reaction center protein L

Chain L:



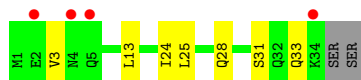
- Molecule 11: Photosystem II reaction center protein L

Chain l:



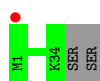
- Molecule 12: Photosystem II reaction center protein M

Chain M:



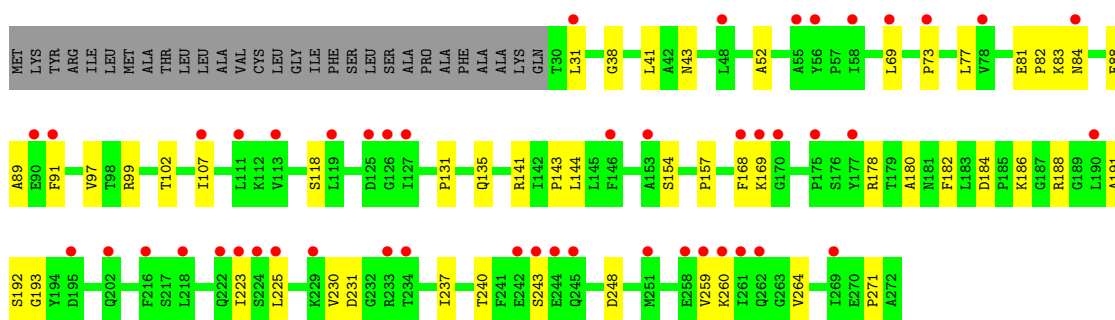
- Molecule 12: Photosystem II reaction center protein M

Chain m:



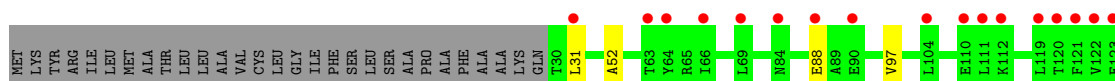
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

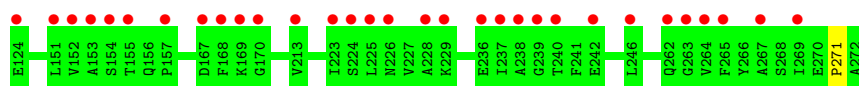
Chain O:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

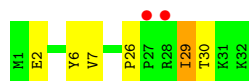
Chain o:





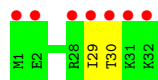
- Molecule 14: Photosystem II reaction center protein T

Chain T:



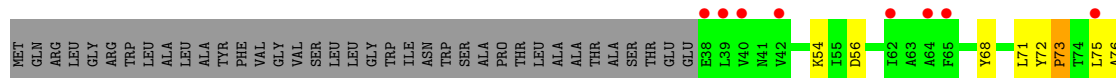
- Molecule 14: Photosystem II reaction center protein T

Chain t:



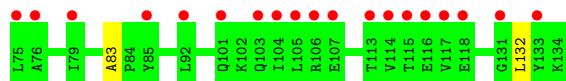
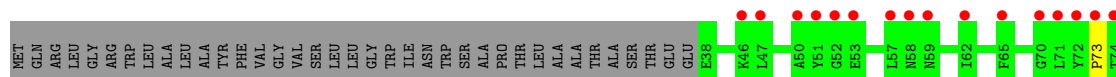
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



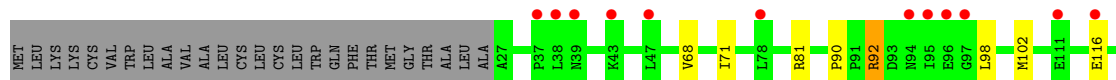
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



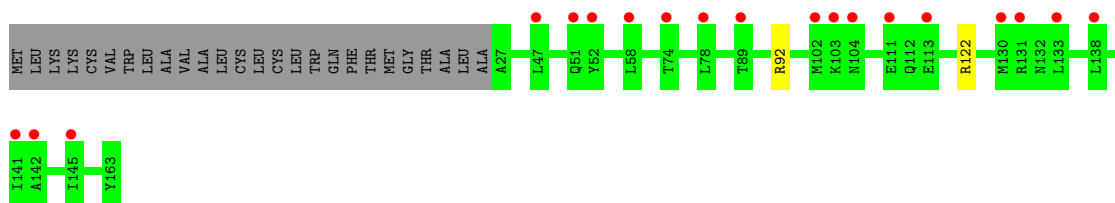
- Molecule 16: Cytochrome c-550

Chain V:



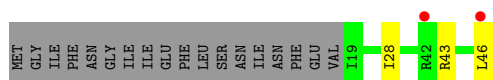
- Molecule 16: Cytochrome c-550

Chain v:



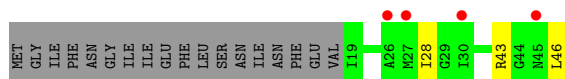
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



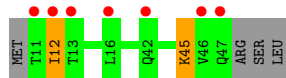
- Molecule 18: Photosystem II reaction center X protein

Chain X:



- Molecule 18: Photosystem II reaction center X protein

Chain x:



- Molecule 19: Photosystem II reaction center protein Y

Chain Y:

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

Chain G:

There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z

Chain Z:



- Molecule 20: 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, $\alpha$ , $\beta$ , $\gamma$	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.7 (72.96-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, $R_{free}$	0.278 , 0.284 0.273 , 0.276	Depositor DCC
$R_{free}$ test set	2524 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 119.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 51515 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, BCT, HEM, LMG, BCR, SQD

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	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.22	0/3556	0.41	0/4842
3	c	0.22	0/3556	0.41	0/4842
4	D	0.23	0/2801	0.40	0/3818
4	d	0.24	0/2801	0.40	0/3818
5	E	0.23	0/685	0.42	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.45	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.21	0/255	0.39	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.48	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.43	0/367
12	m	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.42	0/1064
15	u	0.22	0/785	0.43	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.40	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	g	0.21	0/202	0.45	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.25	0/273	0.43	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	78	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	83	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	74	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	17	0
7	h	507	0	521	0	0
8	I	286	0	308	3	0
8	i	286	0	308	0	0
9	J	249	0	262	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	249	0	262	0	0
10	K	293	0	305	8	0
10	k	293	0	305	0	0
11	L	304	0	316	7	0
11	l	304	0	316	0	0
12	M	267	0	289	7	0
12	m	267	0	289	0	0
13	O	1845	0	1801	31	0
13	o	1845	0	1801	0	0
14	T	275	0	288	5	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	44	0
22	B	975	0	1080	90	0
22	C	845	0	936	47	0
22	D	130	0	144	11	0
22	H	65	0	72	9	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	4	0
23	D	55	0	80	12	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	160	0	224	10	0
24	C	80	0	112	14	0
24	F	40	0	56	4	0
24	H	40	0	56	2	0
24	J	40	0	56	1	0
24	K	40	0	56	3	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	11	0
25	D	63	0	87	2	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	4	0
27	D	143	0	196	11	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	93	0	126	0	0
27	b	49	0	68	0	0
27	c	93	0	126	0	0
27	d	143	0	196	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	m	42	0	54	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	105	0	147	6	0
29	B	90	0	111	4	0
29	F	45	0	54	3	0
29	a	105	0	147	0	0
29	b	47	0	61	0	0
29	d	43	0	50	0	0
29	f	45	0	54	0	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	1	0
30	M	70	0	91	0	0
30	b	140	0	183	0	0
30	d	31	0	35	0	0
30	i	35	0	46	0	0
31	D	128	0	148	15	0
31	d	128	0	148	0	0
32	D	1	0	0	0	0
32	a	1	0	0	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51372	579	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (579) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.55	0.87
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.51	0.81
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.61	0.80
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.66	0.77
4:D:199:MET:HG2	23:D:407:PL9:H322	1.69	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.72	0.74
22:B:605:CLA:H72	24:B:619:BCR:H311	1.70	0.73
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.70	0.72
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.72	0.71
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.74	0.70
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.56	0.70
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.73	0.70
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.74	0.70
4:D:29:PHE:O	4:D:128:ARG:NH2	2.25	0.70
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.73	0.70
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.69
3:C:250:TRP:O	3:C:254:THR:OG1	2.10	0.69
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.68
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.28	0.68
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.67
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.76	0.67
4:D:259:ILE:HG12	27:D:409:LMG:H292	1.78	0.67
1:A:63:ILE:HB	3:C:335:THR:HG21	1.77	0.67
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.76	0.67
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.76	0.67
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.76	0.66
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.77	0.66
12:M:31:SER:HA	27:M:101:LMG:HC1	1.83	0.66
22:B:611:CLA:H42	4:D:127:LEU:HD11	29.95	0.66
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.66
22:C:506:CLA:H112	24:C:514:BCR:H362	1.77	0.66
4:D:236:ASN:ND2	4:D:239:GLN:O	2.30	0.66
1:A:15:GLU:O	1:A:19:ASN:ND2	2.27	0.66
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.69	0.65
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.65
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.79	0.65
1:A:174:LEU:HD22	31:D:401:PHO:H151	1.82	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.81	0.64
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.78	0.64
22:A:404:CLA:H142	22:D:405:CLA:H151	1.79	0.64
22:B:607:CLA:HBA2	29:B:622:SQD:H101	1.80	0.64
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.79	0.64
1:A:183:MET:HB3	22:A:404:CLA:HBC2	14.89	0.63
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.63
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.80	0.63
3:C:406:SER:O	3:C:418:ASN:ND2	2.32	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:D:402:PHO:H151	22:D:405:CLA:H172	1.89	0.63
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.80	0.63
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.63
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
27:D:409:LMG:HO4	27:D:409:LMG:HO5	1.52	0.62
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.87	0.62
1:A:183:MET:HA	22:A:404:CLA:HMD2	12.59	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.32	0.62
2:B:149:LEU:HG	22:B:606:CLA:HBC1	27.91	0.62
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.62
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.81	0.62
1:A:329:GLU:O	1:A:332:HIS:ND1	2.36	0.61
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.82	0.61
22:H:101:CLA:HBD	22:H:101:CLA:H2	1.87	0.61
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.61
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.82	0.61
22:A:404:CLA:H122	31:D:401:PHO:H3A	32.56	0.61
22:A:404:CLA:HHC	22:A:404:CLA:HBB1	3.83	0.61
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.82	0.61
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.85	0.61
29:A:412:SQD:H172	26:C:519:LHG:H172	1.84	0.60
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.60
22:A:404:CLA:H71	22:A:405:CLA:HAB	46.99	0.60
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.67	0.60
2:B:327:THR:HG21	27:B:621:LMG:H111	1.83	0.60
22:B:612:CLA:HMD1	7:H:27:THR:HB	39.61	0.60
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.84	0.59
4:D:216:ALA:O	4:D:220:ASN:ND2	2.34	0.59
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.67	0.59
2:B:262:THR:OG1	22:B:606:CLA:O1D	22.24	0.59
4:D:24:ARG:NH2	18:X:44:ASP:O	2.36	0.59
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.84	0.59
22:B:606:CLA:H193	7:H:42:LEU:HD12	33.90	0.59
2:B:12:LEU:HB2	22:B:615:CLA:HMC2	13.41	0.59
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.59
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.84	0.58
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.86	0.58
29:B:622:SQD:H171	29:B:622:SQD:H301	1.86	0.58
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.88	0.58
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.85	0.57
3:C:118:HIS:CE1	27:C:518:LMG:H192	2.39	0.57
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:D:409:LMG:O6	11:L:15:THR:HG21	2.05	0.57
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.88	0.57
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.78	0.57
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.87	0.57
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.86	0.57
13:O:83:LYS:HG2	13:O:84:ASN:H	1.69	0.57
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.34	0.57
1:A:268:SER:O	1:A:272:HIS:ND1	2.35	0.57
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.57
1:A:64:ARG:O	13:O:178:ARG:NH2	2.41	0.56
22:A:402:CLA:H122	31:D:401:PHO:H3A	1.87	0.56
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.56
22:A:404:CLA:H93	22:D:405:CLA:H152	1.87	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.23	0.56
1:A:217:SER:HA	4:D:272:LEU:HD12	1.91	0.56
27:D:412:LMG:H171	24:F:102:BCR:H383	1.95	0.56
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.45	0.56
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.88	0.56
22:C:501:CLA:HMB3	24:C:514:BCR:H403	1.88	0.56
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
4:D:214:HIS:ND1	23:D:407:PL9:O2	2.27	0.55
22:B:607:CLA:HBD	22:B:608:CLA:H43	4.18	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.88	0.55
22:A:403:CLA:H203	31:D:401:PHO:H71	1.87	0.55
22:B:606:CLA:C2D	22:B:608:CLA:H2	40.02	0.55
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.40	0.55
27:A:410:LMG:H231	23:D:407:PL9:H352	1.89	0.55
22:D:406:CLA:H43	18:X:23:LEU:HA	1.89	0.55
22:D:406:CLA:H42	18:X:26:GLY:HA3	1.92	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.88	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.55
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.41	0.55
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.39	0.55
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.88	0.55
1:A:29:TYR:O	1:A:129:ARG:NH1	2.55	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.55
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.55
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.92	0.55
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.25	0.55
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.55
22:B:611:CLA:H151	22:B:612:CLA:H203	19.95	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.35	0.54
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.37	0.54
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.54
2:B:458:PHE:HB3	22:B:607:CLA:HBC2	12.96	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.91	0.54
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.89	0.54
2:B:262:THR:HG22	2:B:263:THR:HG23	1.89	0.54
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.38	0.54
22:A:405:CLA:HED1	23:D:407:PL9:H372	28.93	0.54
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.90	0.54
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.90	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
24:A:407:BCR:H342	29:A:413:SQD:H311	1.90	0.54
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.85	0.54
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.89	0.54
25:B:625:DGD:O2D	25:B:625:DGD:O1B	2.25	0.54
26:C:519:LHG:H101	26:C:519:LHG:H271	1.90	0.54
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.54
13:O:73:PRO:HG2	13:O:102:THR:HB	1.90	0.54
22:A:403:CLA:HED1	23:D:407:PL9:H372	1.90	0.53
22:A:405:CLA:H203	31:D:401:PHO:H71	33.12	0.53
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.53
29:F:103:SQD:H131	18:X:36:VAL:HG11	1.96	0.53
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.94	0.53
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.90	0.53
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.91	0.53
2:B:474:LEU:O	4:D:134:ARG:NH1	2.50	0.53
29:B:626:SQD:H1	29:B:626:SQD:H462	1.90	0.53
22:B:607:CLA:H151	22:B:608:CLA:H203	1.90	0.53
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.47	0.53
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.91	0.53
2:B:103:LEU:HD21	22:B:608:CLA:HMC3	26.63	0.53
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.93	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.91	0.53
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.44	0.53
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.91	0.53
22:C:510:CLA:HMB2	24:C:513:BCR:H382	1.90	0.53
22:B:605:CLA:OBD	30:B:623:LMT:O6'	2.20	0.52
24:A:407:BCR:H321	29:A:413:SQD:H321	1.91	0.52
2:B:271:THR:HB	2:B:274:GLN:HG3	1.91	0.52
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.91	0.52
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
1:A:244:GLU:HG3	1:A:246:TYR:H	1.76	0.52
22:B:606:CLA:C3D	22:B:608:CLA:H2	40.25	0.52
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.74	0.52
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.93	0.52
1:A:211:PHE:HA	1:A:214:MET:HB2	1.91	0.52
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.91	0.52
1:A:153:SER:HB3	22:A:404:CLA:HED1	19.17	0.51
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.92	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.91	0.51
2:B:150:CYS:HB2	22:B:606:CLA:HMC3	24.92	0.51
2:B:212:ALA:HB2	22:B:612:CLA:HMC3	27.35	0.51
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.91	0.51
4:D:275:PRO:O	4:D:279:LEU:HD23	2.14	0.51
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.93	0.51
22:A:405:CLA:H42	23:D:407:PL9:H162	36.95	0.51
29:A:412:SQD:H311	22:C:507:CLA:H71	1.93	0.51
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.51
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.94	0.51
22:C:504:CLA:HBD	22:C:504:CLA:HBA1	1.94	0.51
3:C:85:GLY:N	25:C:516:DGD:HE4	2.26	0.51
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.54	0.51
1:A:132:GLU:O	1:A:136:ARG:HG2	2.11	0.51
2:B:135:LEU:HA	2:B:138:MET:HE3	2.02	0.51
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	2.05	0.50
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.94	0.50
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.79	0.50
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.94	0.50
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.92	0.50
22:B:608:CLA:H202	22:B:612:CLA:HBB2	21.88	0.50
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.97	0.50
22:A:403:CLA:HMA2	23:D:407:PL9:H411	1.93	0.50
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.50
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.42	0.50
2:B:150:CYS:HA	22:B:606:CLA:HBC2	29.83	0.50
4:D:85:MET:HA	5:E:69:ARG:HB3	2.03	0.50
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.44	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.50
29:A:412:SQD:H223	25:C:517:DGD:HAE1	1.93	0.50
4:D:279:LEU:HG	31:D:402:PHO:HBC3	1.96	0.50
25:D:410:DGD:O5E	25:D:410:DGD:O4E	2.25	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.83	0.50
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.27	0.49
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.93	0.49
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.94	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.49
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.51	0.49
4:D:348:ARG:NH2	4:D:352:LEU:O	2.39	0.49
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.49
2:B:327:THR:HG22	22:B:606:CLA:H12	1.94	0.49
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.77	0.49
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.00	0.49
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.75	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.49
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.42	0.49
27:D:409:LMG:H111	11:L:19:LEU:HD21	1.97	0.49
1:A:210:LEU:HG	31:D:402:PHO:NC	2.28	0.49
29:F:103:SQD:H162	18:X:33:THR:HA	1.94	0.49
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.94	0.49
22:B:611:CLA:H51	22:B:612:CLA:H101	18.01	0.49
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.95	0.49
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.49
2:B:222:PRO:HG3	7:H:27:THR:H	1.78	0.48
29:B:622:SQD:H111	29:B:622:SQD:H241	1.96	0.48
22:B:612:CLA:H51	27:D:408:LMG:H231	1.95	0.48
30:B:627:LMT:H62	8:I:4:LEU:HD22	82.08	0.48
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.95	0.48
1:A:78:ILE:O	1:A:176:ILE:HB	2.13	0.48
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.48	0.48
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.48
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.94	0.48
2:B:327:THR:HG22	22:B:610:CLA:H12	26.92	0.48
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.95	0.48
25:B:625:DGD:HD1	30:B:627:LMT:H32	1.95	0.48
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.94	0.48
27:A:414:LMG:H112	2:B:43:ALA:HA	42.29	0.48
4:D:102:THR:OG1	25:D:410:DGD:HD62	2.16	0.48
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.48
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.48
13:O:118:SER:HB3	13:O:157:PRO:HA	1.99	0.48
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.95	0.48
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.70	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
27:C:518:LMG:H292	27:C:518:LMG:H111	1.95	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
22:A:405:CLA:HMA2	23:D:407:PL9:H411	24.71	0.47
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.96	0.47
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.52	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	1.99	0.47
3:C:158:THR:O	3:C:251:HIS:HB3	2.14	0.47
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.47
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.63	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.80	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.97	0.47
22:B:615:CLA:H72	22:B:615:CLA:H12	1.97	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.98	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.47
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.97	0.47
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.97	0.47
22:C:501:CLA:H193	22:C:506:CLA:H111	2.04	0.47
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.47
4:D:262:SER:N	27:D:409:LMG:O3	2.46	0.47
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.47	0.47
22:A:405:CLA:H162	22:A:405:CLA:H141	1.71	0.46
22:B:607:CLA:H18	22:B:608:CLA:H192	1.97	0.46
27:I:101:LMG:H181	30:I:102:LMT:H42	2.04	0.46
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.98	0.46
1:A:202:VAL:HB	22:A:404:CLA:HMB3	12.99	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.01	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
4:D:48:TRP:CE2	31:D:402:PHO:H161	2.50	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.99	0.46
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.05	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.98	0.46
22:H:101:CLA:H62	22:H:101:CLA:H41	1.56	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.52	0.46
22:H:101:CLA:H162	22:H:101:CLA:H122	1.50	0.46
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.46
22:A:404:CLA:H161	23:A:406:PL9:H253	1.96	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
4:D:261:PHE:HB2	23:D:407:PL9:H522	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:170:ASP:OD1	2:B:175:THR:N	2.50	0.46
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.46
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.51	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.18	0.46
31:D:401:PHO:H41	31:D:401:PHO:H62	1.47	0.46
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.51	0.46
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.01	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.98	0.46
24:B:616:BCR:H20C	24:B:616:BCR:H361	1.76	0.46
22:C:510:CLA:H61	22:C:510:CLA:H93	1.81	0.46
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.79	0.46
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.46
27:D:409:LMG:HC1	27:D:409:LMG:O9	2.18	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.52	0.45
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.82	0.45
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.45
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.45
12:M:24:ILE:HG21	27:M:101:LMG:H322	9.39	0.45
22:B:607:CLA:H51	22:B:608:CLA:H101	1.98	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.48	0.45
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.99	0.45
22:B:603:CLA:HMD2	22:B:611:CLA:H193	1.99	0.45
24:B:618:BCR:H361	24:B:618:BCR:H20C	1.82	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.45
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.77	0.45
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.45
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.45
1:A:114:LEU:O	1:A:118:HIS:ND1	2.46	0.45
22:A:402:CLA:HBA1	22:A:402:CLA:H3A	1.53	0.45
2:B:212:ALA:O	2:B:216:HIS:ND1	2.52	0.45
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.19	0.45
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.45
22:B:614:CLA:H172	22:B:614:CLA:H111	1.99	0.45
24:C:514:BCR:H361	24:C:514:BCR:H20C	1.83	0.45
13:O:143:PRO:HG2	13:O:248:ASP:HB3	1.98	0.45
22:A:402:CLA:H51	31:D:401:PHO:C3B	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:B:611:CLA:H162	22:B:611:CLA:H122	1.76	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.18	0.45
30:B:628:LMT:H122	14:T:7:VAL:HG12	34.40	0.45
16:V:98:LEU:O	16:V:102:MET:HG3	2.22	0.45
1:A:224:ILE:O	4:D:265:ARG:NH2	2.49	0.45
22:A:405:CLA:H162	22:A:405:CLA:H202	3.78	0.45
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.45
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.17	0.45
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.45
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.04	0.45
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.31	0.45
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.03	0.45
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.57	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.27	0.44
22:B:605:CLA:HBA2	22:B:605:CLA:H3A	1.26	0.44
22:C:508:CLA:H11	22:C:508:CLA:H51	1.82	0.44
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.00	0.44
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.42	0.44
22:C:504:CLA:H11	24:C:514:BCR:H312	2.01	0.44
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.44
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.44
22:B:613:CLA:H51	24:B:616:BCR:H372	1.98	0.44
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.44
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.78	0.44
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.99	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.18	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.44
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.99	0.44
22:C:501:CLA:H141	22:C:501:CLA:H162	1.78	0.44
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.44
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.71	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.01	0.44
3:C:224:ILE:O	3:C:227:VAL:HG23	2.18	0.44
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.00	0.44
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.44
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.18	0.44
1:A:202:VAL:HB	22:A:402:CLA:HMB3	2.00	0.44
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:49:THR:HA	5:E:50:PRO:HD3	1.92	0.44
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.00	0.44
22:C:512:CLA:HBA2	22:C:512:CLA:H3A	1.72	0.43
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.43
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.81	0.43
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.06	0.43
3:C:245:ILE:O	3:C:249:ILE:HG12	2.17	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.43
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
22:B:605:CLA:C3D	30:B:623:LMT:H11	2.49	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
1:A:271:LEU:HD21	23:A:406:PL9:HC71	1.99	0.43
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.43
22:C:503:CLA:H201	22:C:503:CLA:HMD2	2.02	0.43
31:D:401:PHO:H13	31:D:401:PHO:H102	1.82	0.43
22:D:405:CLA:H62	22:D:405:CLA:H92	1.79	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.58	0.43
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.18	0.43
22:B:606:CLA:H2	22:B:608:CLA:H93	34.06	0.43
24:C:513:BCR:H24C	24:C:513:BCR:H371	1.78	0.43
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.54	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.43
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.43
22:A:404:CLA:H143	22:A:404:CLA:H161	1.86	0.43
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.06	0.43
30:B:628:LMT:H3'	30:B:628:LMT:H1B	1.53	0.43
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.58	0.43
11:L:4:ASN:OD1	11:L:6:ASN:ND2	2.49	0.43
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.06	0.43
2:B:468:TRP:HH2	27:D:408:LMG:HO2	1.63	0.43
22:B:615:CLA:H162	22:B:615:CLA:H122	5.18	0.43
3:C:29:GLU:HB2	3:C:30:SER:H	1.64	0.43
6:F:16:PHE:HB3	29:F:103:SQD:H241	2.07	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.03	0.43
22:B:611:CLA:H171	22:B:612:CLA:HBB2	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.84	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.35	0.43
26:A:409:LHG:H382	22:C:509:CLA:H93	2.01	0.43
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.01	0.43
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.01	0.43
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.76	0.43
22:D:405:CLA:H3A	22:D:405:CLA:HBA1	1.82	0.43
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.67	0.43
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.12	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.42
22:B:606:CLA:H41	22:B:606:CLA:H61	2.89	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.78	0.42
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
7:H:12:ARG:HD3	7:H:12:ARG:O	2.19	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.04	0.42
23:D:407:PL9:H421	23:D:407:PL9:H401	1.86	0.42
24:F:102:BCR:H15C	24:F:102:BCR:H351	1.91	0.42
15:U:72:TYR:O	15:U:76:ALA:HB3	2.19	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.74	0.42
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.88	0.42
25:B:620:DGD:HAW2	22:H:101:CLA:H152	2.02	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.01	0.42
22:C:511:CLA:H61	22:C:511:CLA:H13	2.05	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.53	0.42
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.32	0.42
1:A:140:ARG:HH22	26:A:409:LHG:P	2.41	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.42
22:A:404:CLA:H51	31:D:401:PHO:C3B	21.31	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.91	0.42
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.86	0.42
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.02	0.42
3:C:377:LEU:O	3:C:381:LYS:HB2	2.20	0.42
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.95	0.42
22:C:511:CLA:H143	22:C:512:CLA:H162	2.02	0.42
22:B:612:CLA:H171	27:D:408:LMG:H401	2.01	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.04	0.42
22:B:613:CLA:H12	22:B:613:CLA:H51	4.48	0.42
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.84	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:A:403:CLA:H42	23:D:407:PL9:H162	2.01	0.42
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.42
3:C:456:GLU:N	3:C:456:GLU:OE1	2.52	0.42
22:C:520:CLA:H112	22:C:520:CLA:H142	1.77	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.02	0.42
22:A:405:CLA:H11	22:A:405:CLA:H51	4.35	0.42
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.42
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.88	0.42
31:D:401:PHO:H202	31:D:401:PHO:H162	1.87	0.42
13:O:192:SER:OG	13:O:193:GLY:N	2.52	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.42
1:A:182:PHE:O	1:A:186:PHE:HB2	2.21	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.02	0.42
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.42
4:D:155:SER:HA	4:D:159:ILE:HB	2.05	0.42
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.63	0.41
22:D:406:CLA:H41	22:D:406:CLA:H61	1.86	0.41
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.83	0.41
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.50	0.41
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.02	0.41
4:D:252:PHE:O	4:D:256:ILE:HG22	2.21	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.48	0.41
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.02	0.41
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.41
22:A:403:CLA:H202	22:A:403:CLA:H162	1.76	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.03	0.41
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.41
22:B:611:CLA:H18	22:B:612:CLA:H192	22.27	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.41
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
1:A:238:LYS:O	1:A:241:GLN:HG3	2.21	0.41
22:A:403:CLA:H41	22:A:403:CLA:H62	1.76	0.41
22:A:403:CLA:HED2	4:D:198:MET:SD	2.60	0.41
22:B:602:CLA:H92	22:B:602:CLA:HBB2	2.03	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.79	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.84	0.41
24:F:102:BCR:H11C	24:F:102:BCR:H341	1.94	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:282:MET:HG2	22:C:501:CLA:H61	2.09	0.41
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.54	0.41
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.54	0.41
1:A:269:ARG:NH1	4:D:231:THR:HB	2.38	0.41
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.37	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.41
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.04	0.41
1:A:153:SER:HB2	22:A:404:CLA:H43	19.16	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.97	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.88	0.41
31:D:402:PHO:CHB	22:D:405:CLA:H101	2.51	0.41
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.41
1:A:258:LEU:O	4:D:128:ARG:NH1	2.54	0.41
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.10	0.41
24:A:407:BCR:H341	24:A:407:BCR:H11C	1.94	0.41
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.02	0.41
22:B:611:CLA:H161	22:B:611:CLA:H143	4.42	0.41
3:C:303:GLY:O	3:C:423:ARG:NE	2.41	0.41
3:C:119:LEU:HG	24:C:513:BCR:H10C	2.15	0.41
4:D:342:PRO:O	4:D:345:VAL:HG12	2.22	0.41
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.02	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.21	0.41
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.21	0.41
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.92	0.41
22:B:602:CLA:H162	22:B:602:CLA:H192	1.77	0.41
7:H:35:MET:HB2	7:H:35:MET:HE3	1.87	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.07	0.41
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.26	0.41
22:A:404:CLA:H62	22:A:404:CLA:H102	4.12	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.04	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.94	0.41
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.21	0.41
24:H:102:BCR:HC31	24:H:102:BCR:H323	1.89	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.40
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.40
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.40
22:B:605:CLA:H41	22:B:605:CLA:H62	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.03	0.40
2:B:179:GLN:HA	2:B:180:PRO:HD3	1.97	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.40
3:C:375:LEU:HB3	3:C:380:ILE:HD11	2.04	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
24:K:102:BCR:H361	24:K:102:BCR:H20C	1.81	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
22:B:602:CLA:H61	22:B:602:CLA:H41	1.67	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.90	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.04	0.40
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.08	0.40
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.61	0.40
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.04	0.40
1:A:180:PHE:O	1:A:184:ILE:HG13	2.26	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.40
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.52	0.40
22:B:606:CLA:H161	22:B:606:CLA:H141	2.05	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.51	0.40
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.86	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.96	0.40
11:L:11:GLU:HG2	11:L:12:LEU:N	2.35	0.40
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.59	0.40
29:A:413:SQD:H332	22:B:609:CLA:H203	66.25	0.40
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.40
2:B:6:TYR:OH	27:D:408:LMG:HC5	2.26	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	19 77
1	a	333/344 (97%)	309 (93%)	20 (6%)	4 (1%)	19 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	27	82
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	33	86
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	25	81
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	25	81
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	50	91
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	50	91
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	18	75
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	18	75
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	4	44
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	4	44
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	7	57
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	7	57
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	19	77
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	19	77
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	6	55
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	6	55
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	11	66
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	11	66
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	5	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	5	51
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	3	39
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	3	39
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	14	70
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	14	70
All	All	5138/5618 (92%)	4675 (91%)	408 (8%)	55 (1%)	21	78

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
7	H	26	GLY
9	J	38	SER
13	O	52	ALA
14	T	30	THR
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
2	B	489	GLU
4	D	239	GLN
13	O	88	GLU

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Mol	Chain	Res	Type
13	O	271	PRO
18	X	12	ILE
2	b	489	GLU
3	c	32	GLY
4	d	239	GLN
7	h	26	GLY
9	j	38	SER
13	o	88	GLU
1	A	142	TRP
3	C	32	GLY
5	E	82	GLN
1	a	142	TRP
1	a	334	ARG
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
7	H	16	SER
15	U	73	PRO
3	c	144	SER
7	h	16	SER
15	u	73	PRO
3	C	144	SER
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY

### 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	271/280 (97%)	267 (98%)	4 (2%)	76	94
1	a	271/280 (97%)	267 (98%)	4 (2%)	76	94
2	B	390/407 (96%)	381 (98%)	9 (2%)	63	91
2	b	390/407 (96%)	381 (98%)	9 (2%)	63	91
3	C	347/362 (96%)	336 (97%)	11 (3%)	51	87
3	c	347/362 (96%)	336 (97%)	11 (3%)	51	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	275/283 (97%)	269 (98%)	6 (2%)	64	91
4	d	275/283 (97%)	269 (98%)	6 (2%)	64	91
5	E	72/73 (99%)	70 (97%)	2 (3%)	56	89
5	e	72/73 (99%)	70 (97%)	2 (3%)	56	89
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	19	65
7	h	53/55 (96%)	49 (92%)	4 (8%)	19	65
8	I	32/35 (91%)	31 (97%)	1 (3%)	52	88
8	i	32/35 (91%)	31 (97%)	1 (3%)	52	88
9	J	24/28 (86%)	23 (96%)	1 (4%)	40	82
9	j	24/28 (86%)	23 (96%)	1 (4%)	40	82
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	55	88
11	l	35/35 (100%)	34 (97%)	1 (3%)	55	88
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	85	96
13	o	202/228 (89%)	200 (99%)	2 (1%)	85	96
14	T	29/29 (100%)	28 (97%)	1 (3%)	49	87
14	t	29/29 (100%)	28 (97%)	1 (3%)	49	87
15	U	84/112 (75%)	83 (99%)	1 (1%)	82	95
15	u	84/112 (75%)	83 (99%)	1 (1%)	82	95
16	V	116/138 (84%)	114 (98%)	2 (2%)	73	93
16	v	116/138 (84%)	114 (98%)	2 (2%)	73	93
17	g	20/37 (54%)	18 (90%)	2 (10%)	11	51
17	y	20/37 (54%)	18 (90%)	2 (10%)	11	51
18	X	30/34 (88%)	28 (93%)	2 (7%)	23	70
18	x	30/34 (88%)	28 (93%)	2 (7%)	23	70
20	Z	52/52 (100%)	50 (96%)	2 (4%)	44	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	z	52/52 (100%)	50 (96%)	2 (4%)	44 85
All	All	4244/4594 (92%)	4142 (98%)	102 (2%)	61 90

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	346	LEU
5	E	18	ARG
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL

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Mol	Chain	Res	Type
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU
16	V	92	ARG
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	45	LYS
20	Z	33	TRP
20	Z	62	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	472	LEU
4	d	43	LEU
4	d	180	ARG
4	d	241	GLU

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Mol	Chain	Res	Type
4	d	259	ILE
4	d	291	LEU
4	d	346	LEU
5	e	18	ARG
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	132	LEU
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	45	LYS
20	z	33	TRP
20	z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	118	HIS
4	D	117	HIS
4	d	117	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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$
22	CLA	A	402	-	73,73,73	1.63	10 (13%)	96,113,113	1.21	11 (11%)
22	CLA	A	403	-	73,73,73	1.60	10 (13%)	96,113,113	1.23	11 (11%)
22	CLA	A	404	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	A	405	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
23	PL9	A	406	-	45,45,55	1.11	3 (6%)	55,57,69	1.72	12 (21%)
24	BCR	A	407	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	6 (10%)
25	DGD	A	408	-	57,57,67	2.14	2 (3%)	71,71,81	1.56	9 (12%)
26	LHG	A	409	-	38,38,48	2.28	1 (2%)	44,44,54	1.40	6 (13%)
27	LMG	A	410	-	51,51,55	2.32	3 (5%)	59,59,63	1.44	8 (13%)
28	OEX	A	411	1,3	8,15,15	10.57	8 (100%)	0,32,32	0.00	-
29	SQD	A	412	-	51,51,54	1.54	4 (7%)	62,62,65	1.96	11 (17%)
29	SQD	A	413	-	54,54,54	0.92	3 (5%)	65,65,65	1.71	12 (18%)
27	LMG	A	414	-	42,42,55	2.46	2 (4%)	50,50,63	1.35	6 (12%)
22	CLA	B	601	-	73,73,73	1.62	10 (13%)	96,113,113	1.22	12 (12%)
22	CLA	B	602	-	73,73,73	1.58	10 (13%)	96,113,113	1.25	12 (12%)
22	CLA	B	603	-	73,73,73	1.60	10 (13%)	96,113,113	1.30	15 (15%)
22	CLA	B	604	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	11 (11%)
22	CLA	B	605	-	73,73,73	1.58	10 (13%)	96,113,113	1.24	14 (14%)
22	CLA	B	606	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	13 (13%)
22	CLA	B	607	-	73,73,73	1.59	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	B	608	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	14 (14%)
22	CLA	B	609	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	12 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	610	-	73,73,73	1.57	11 (15%)	96,113,113	1.39	12 (12%)
22	CLA	B	611	-	73,73,73	1.60	10 (13%)	96,113,113	1.26	14 (14%)
22	CLA	B	612	-	73,73,73	1.59	10 (13%)	96,113,113	1.29	14 (14%)
22	CLA	B	613	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	B	614	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	B	615	-	73,73,73	1.60	11 (15%)	96,113,113	1.22	12 (12%)
24	BCR	B	616	-	41,41,41	1.07	2 (4%)	56,56,56	1.20	7 (12%)
24	BCR	B	617	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	8 (14%)
24	BCR	B	618	-	41,41,41	1.06	2 (4%)	56,56,56	1.32	8 (14%)
24	BCR	B	619	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	8 (14%)
25	DGD	B	620	-	59,59,67	2.25	3 (5%)	73,73,81	1.45	7 (9%)
27	LMG	B	621	-	49,49,55	2.34	3 (6%)	57,57,63	1.41	9 (15%)
29	SQD	B	622	-	43,43,54	1.23	4 (9%)	54,54,65	1.96	13 (24%)
30	LMT	B	623	-	36,36,36	1.09	4 (11%)	47,47,47	0.99	2 (4%)
30	LMT	B	624	-	36,36,36	1.06	4 (11%)	47,47,47	1.04	3 (6%)
25	DGD	B	625	-	53,53,67	2.30	5 (9%)	67,67,81	1.46	9 (13%)
29	SQD	B	626	-	47,47,54	1.09	4 (8%)	58,58,65	1.96	10 (17%)
30	LMT	B	627	-	36,36,36	1.08	4 (11%)	47,47,47	0.98	1 (2%)
30	LMT	B	628	-	36,36,36	1.10	5 (13%)	47,47,47	1.06	1 (2%)
22	CLA	C	501	-	73,73,73	1.60	11 (15%)	96,113,113	1.20	13 (13%)
22	CLA	C	502	-	73,73,73	1.60	11 (15%)	96,113,113	1.25	13 (13%)
22	CLA	C	503	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
22	CLA	C	504	-	73,73,73	1.60	10 (13%)	96,113,113	1.25	14 (14%)
22	CLA	C	505	-	73,73,73	1.61	10 (13%)	96,113,113	1.28	13 (13%)
22	CLA	C	506	-	73,73,73	1.58	10 (13%)	96,113,113	1.28	13 (13%)
22	CLA	C	507	-	73,73,73	1.60	10 (13%)	96,113,113	1.29	13 (13%)
22	CLA	C	508	-	73,73,73	1.61	10 (13%)	96,113,113	1.21	11 (11%)
22	CLA	C	509	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	11 (11%)
22	CLA	C	510	3	73,73,73	1.60	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	C	511	-	73,73,73	1.61	10 (13%)	96,113,113	1.25	14 (14%)
22	CLA	C	512	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	13 (13%)
24	BCR	C	513	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
24	BCR	C	514	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	9 (16%)
25	DGD	C	515	-	54,54,67	2.39	4 (7%)	68,68,81	1.34	10 (14%)
25	DGD	C	516	-	63,63,67	1.48	2 (3%)	77,77,81	1.45	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	DGD	C	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.42	10 (12%)
27	LMG	C	518	-	45,45,55	2.56	2 (4%)	53,53,63	1.42	6 (11%)
26	LHG	C	519	-	36,36,48	2.36	3 (8%)	42,42,54	1.50	8 (19%)
22	CLA	C	520	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	12 (12%)
27	LMG	C	521	-	48,48,55	2.34	2 (4%)	56,56,63	1.42	9 (16%)
31	PHO	D	401	-	69,69,69	1.24	9 (13%)	92,99,99	1.18	10 (10%)
31	PHO	D	402	-	69,69,69	1.26	11 (15%)	92,99,99	1.17	9 (9%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	405	-	73,73,73	1.62	10 (13%)	96,113,113	1.21	11 (11%)
22	CLA	D	406	-	73,73,73	1.59	10 (13%)	96,113,113	1.26	14 (14%)
23	PL9	D	407	-	55,55,55	1.12	3 (5%)	69,69,69	1.66	15 (21%)
27	LMG	D	408	-	49,49,55	2.48	3 (6%)	57,57,63	1.40	8 (14%)
27	LMG	D	409	-	48,48,55	2.37	2 (4%)	56,56,63	1.49	7 (12%)
25	DGD	D	410	-	64,64,67	1.40	1 (1%)	78,78,81	1.33	9 (11%)
30	LMT	D	411	-	32,32,36	2.83	5 (15%)	43,43,47	1.07	2 (4%)
27	LMG	D	412	-	46,46,55	2.58	3 (6%)	54,54,63	1.41	7 (12%)
27	LMG	E	101	-	44,44,55	2.57	2 (4%)	52,52,63	1.40	7 (13%)
34	HEM	F	101	5,6	42,50,50	3.64	13 (30%)	27,82,82	1.20	2 (7%)
24	BCR	F	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	6 (10%)
29	SQD	F	103	-	45,45,54	1.39	5 (11%)	56,56,65	1.85	11 (19%)
22	CLA	H	101	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	13 (13%)
24	BCR	H	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	5 (8%)
27	LMG	I	101	-	43,43,55	2.30	2 (4%)	51,51,63	1.36	7 (13%)
30	LMT	I	102	-	36,36,36	1.07	4 (11%)	47,47,47	1.06	2 (4%)
23	PL9	J	101	-	35,35,55	1.13	1 (2%)	43,45,69	1.79	8 (18%)
24	BCR	J	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.59	12 (21%)
24	BCR	K	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	8 (14%)
27	LMG	M	101	-	42,42,55	2.44	3 (7%)	50,50,63	1.33	5 (10%)
30	LMT	M	102	-	36,36,36	1.11	4 (11%)	47,47,47	1.02	2 (4%)
30	LMT	M	103	-	36,36,36	1.11	5 (13%)	47,47,47	1.01	3 (6%)
34	HEM	V	201	16	42,50,50	3.68	13 (30%)	27,82,82	1.13	1 (3%)
29	SQD	a	401	-	54,54,54	0.92	3 (5%)	65,65,65	1.71	11 (16%)
27	LMG	a	402	-	42,42,55	2.49	2 (4%)	50,50,63	1.36	5 (10%)
22	CLA	a	404	-	73,73,73	1.63	10 (13%)	96,113,113	1.21	10 (10%)
22	CLA	a	405	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	11 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	a	406	-	73,73,73	1.60	10 (13%)	96,113,113	1.23	11 (11%)
22	CLA	a	407	-	73,73,73	1.59	10 (13%)	96,113,113	1.25	13 (13%)
23	PL9	a	408	-	45,45,55	1.16	3 (6%)	55,57,69	1.71	11 (20%)
24	BCR	a	409	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	7 (12%)
25	DGD	a	410	-	57,57,67	2.15	3 (5%)	71,71,81	1.54	9 (12%)
26	LHG	a	411	-	38,38,48	2.29	2 (5%)	44,44,54	1.41	6 (13%)
27	LMG	a	412	-	51,51,55	2.30	3 (5%)	59,59,63	1.42	9 (15%)
28	OEX	a	414	1,3	8,15,15	10.50	8 (100%)	0,32,32	0.00	-
29	SQD	a	415	-	51,51,54	1.55	4 (7%)	62,62,65	1.98	11 (17%)
25	DGD	b	601	-	53,53,67	2.26	6 (11%)	67,67,81	1.46	10 (14%)
29	SQD	b	602	-	47,47,54	1.09	5 (10%)	58,58,65	1.97	10 (17%)
30	LMT	b	603	-	36,36,36	1.09	4 (11%)	47,47,47	0.96	1 (2%)
30	LMT	b	604	-	36,36,36	1.09	4 (11%)	47,47,47	1.06	1 (2%)
22	CLA	b	605	-	73,73,73	1.62	10 (13%)	96,113,113	1.23	12 (12%)
22	CLA	b	606	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	11 (11%)
22	CLA	b	607	-	73,73,73	1.60	10 (13%)	96,113,113	1.29	14 (14%)
22	CLA	b	608	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
22	CLA	b	609	-	73,73,73	1.59	10 (13%)	96,113,113	1.25	13 (13%)
22	CLA	b	610	-	73,73,73	1.59	10 (13%)	96,113,113	1.22	11 (11%)
22	CLA	b	611	-	73,73,73	1.60	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	b	612	-	73,73,73	1.62	10 (13%)	96,113,113	1.21	13 (13%)
22	CLA	b	613	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	13 (13%)
22	CLA	b	614	-	73,73,73	1.58	11 (15%)	96,113,113	1.38	12 (12%)
22	CLA	b	615	-	73,73,73	1.60	11 (15%)	96,113,113	1.26	14 (14%)
22	CLA	b	616	-	73,73,73	1.59	10 (13%)	96,113,113	1.29	15 (15%)
22	CLA	b	617	-	73,73,73	1.59	10 (13%)	96,113,113	1.24	12 (12%)
22	CLA	b	618	-	73,73,73	1.61	10 (13%)	96,113,113	1.24	14 (14%)
22	CLA	b	619	-	73,73,73	1.61	11 (15%)	96,113,113	1.20	12 (12%)
24	BCR	b	620	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	5 (8%)
24	BCR	b	621	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	9 (16%)
24	BCR	b	622	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	9 (16%)
24	BCR	b	623	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	8 (14%)
25	DGD	b	624	-	59,59,67	2.23	3 (5%)	73,73,81	1.44	6 (8%)
27	LMG	b	625	-	49,49,55	2.35	3 (6%)	57,57,63	1.40	9 (15%)
30	LMT	b	626	-	36,36,36	1.09	4 (11%)	47,47,47	0.98	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	LMT	b	627	-	36,36,36	1.06	4 (11%)	47,47,47	1.01	3 (6%)
22	CLA	c	501	-	73,73,73	1.59	11 (15%)	96,113,113	1.21	13 (13%)
22	CLA	c	502	-	73,73,73	1.60	10 (13%)	96,113,113	1.25	13 (13%)
22	CLA	c	503	-	73,73,73	1.61	10 (13%)	96,113,113	1.23	13 (13%)
22	CLA	c	504	-	73,73,73	1.62	10 (13%)	96,113,113	1.23	14 (14%)
22	CLA	c	505	-	73,73,73	1.60	10 (13%)	96,113,113	1.27	13 (13%)
22	CLA	c	506	-	73,73,73	1.59	10 (13%)	96,113,113	1.28	14 (14%)
22	CLA	c	507	-	73,73,73	1.59	10 (13%)	96,113,113	1.31	14 (14%)
22	CLA	c	508	-	73,73,73	1.63	10 (13%)	96,113,113	1.20	11 (11%)
22	CLA	c	509	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	13 (13%)
22	CLA	c	510	3	73,73,73	1.61	10 (13%)	96,113,113	1.27	14 (14%)
22	CLA	c	511	-	73,73,73	1.61	10 (13%)	96,113,113	1.25	14 (14%)
22	CLA	c	512	-	73,73,73	1.60	10 (13%)	96,113,113	1.24	13 (13%)
24	BCR	c	513	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	8 (14%)
24	BCR	c	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	8 (14%)
25	DGD	c	515	-	54,54,67	2.43	3 (5%)	68,68,81	1.34	9 (13%)
25	DGD	c	516	-	63,63,67	1.47	2 (3%)	77,77,81	1.45	12 (15%)
25	DGD	c	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.41	8 (9%)
27	LMG	c	518	-	45,45,55	2.54	2 (4%)	53,53,63	1.42	7 (13%)
26	LHG	c	519	-	36,36,48	2.31	2 (5%)	42,42,54	1.51	8 (19%)
22	CLA	c	520	-	73,73,73	1.60	10 (13%)	96,113,113	1.22	12 (12%)
24	BCR	c	521	-	41,41,41	1.03	2 (4%)	56,56,56	1.21	7 (12%)
27	LMG	c	522	-	48,48,55	2.32	2 (4%)	56,56,63	1.41	8 (14%)
31	PHO	d	401	-	69,69,69	1.24	9 (13%)	92,99,99	1.18	10 (10%)
31	PHO	d	402	-	69,69,69	1.26	11 (15%)	92,99,99	1.15	10 (10%)
29	SQD	d	403	-	43,43,54	1.23	4 (9%)	54,54,65	1.97	12 (22%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	405	-	73,73,73	1.62	10 (13%)	96,113,113	1.19	12 (12%)
22	CLA	d	406	-	73,73,73	1.60	10 (13%)	96,113,113	1.26	14 (14%)
23	PL9	d	407	-	55,55,55	1.13	2 (3%)	69,69,69	1.66	15 (21%)
27	LMG	d	408	-	49,49,55	2.41	2 (4%)	57,57,63	1.40	7 (12%)
27	LMG	d	409	-	48,48,55	2.37	2 (4%)	56,56,63	1.49	6 (10%)
25	DGD	d	410	-	64,64,67	1.41	2 (3%)	78,78,81	1.35	8 (10%)
30	LMT	d	411	-	32,32,36	2.83	5 (15%)	43,43,47	1.04	2 (4%)
27	LMG	d	412	-	46,46,55	2.59	3 (6%)	54,54,63	1.41	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	e	101	-	44,44,55	2.61	2 (4%)	52,52,63	1.40	7 (13%)
34	HEM	f	101	5,6	42,50,50	3.64	13 (30%)	27,82,82	1.23	2 (7%)
24	BCR	f	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	5 (8%)
29	SQD	f	103	-	45,45,54	1.39	6 (13%)	56,56,65	1.85	11 (19%)
24	BCR	g	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.25	7 (12%)
22	CLA	h	101	-	73,73,73	1.61	10 (13%)	96,113,113	1.22	12 (12%)
27	LMG	i	101	-	43,43,55	2.35	2 (4%)	51,51,63	1.37	7 (13%)
30	LMT	i	102	-	36,36,36	1.06	4 (11%)	47,47,47	1.04	2 (4%)
23	PL9	j	101	-	35,35,55	1.11	1 (2%)	43,45,69	1.80	8 (18%)
24	BCR	j	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.57	12 (21%)
27	LMG	m	101	-	42,42,55	2.44	3 (7%)	50,50,63	1.33	5 (10%)
34	HEM	v	201	16	42,50,50	3.70	14 (33%)	27,82,82	1.13	1 (3%)
24	BCR	x	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	2 (3%)
24	BCR	y	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	6 (10%)

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
22	CLA	A	402	-	-	0/37/135/135	0/0/9/9
22	CLA	A	403	-	-	0/37/135/135	0/0/9/9
22	CLA	A	404	-	-	0/37/135/135	0/0/9/9
22	CLA	A	405	-	-	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	BCR	A	407	-	-	0/29/63/63	0/2/2/2
25	DGD	A	408	-	-	0/45/85/95	0/2/2/2
26	LHG	A	409	-	-	0/43/43/53	0/0/0/0
27	LMG	A	410	-	-	0/46/66/70	0/1/1/1
28	OEX	A	411	1,3	-	0/0/68/68	0/0/6/6
29	SQD	A	412	-	-	0/46/66/69	0/1/1/1
29	SQD	A	413	-	-	0/49/69/69	0/1/1/1
27	LMG	A	414	-	-	0/37/57/70	0/1/1/1
22	CLA	B	601	-	-	0/37/135/135	0/0/9/9
22	CLA	B	602	-	-	0/37/135/135	0/0/9/9
22	CLA	B	603	-	-	0/37/135/135	0/0/9/9
22	CLA	B	604	-	-	0/37/135/135	0/0/9/9
22	CLA	B	605	-	-	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	606	-	-	0/37/135/135	0/0/9/9
22	CLA	B	607	-	-	0/37/135/135	0/0/9/9
22	CLA	B	608	-	-	0/37/135/135	0/0/9/9
22	CLA	B	609	-	-	0/37/135/135	0/0/9/9
22	CLA	B	610	-	-	0/37/135/135	0/0/9/9
22	CLA	B	611	-	-	0/37/135/135	0/0/9/9
22	CLA	B	612	-	-	0/37/135/135	0/0/9/9
22	CLA	B	613	-	-	0/37/135/135	0/0/9/9
22	CLA	B	614	-	-	0/37/135/135	0/0/9/9
22	CLA	B	615	-	-	0/37/135/135	0/0/9/9
24	BCR	B	616	-	-	0/29/63/63	0/2/2/2
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	DGD	B	620	-	-	0/47/87/95	0/2/2/2
27	LMG	B	621	-	-	0/44/64/70	0/1/1/1
29	SQD	B	622	-	-	1/38/58/69	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
30	LMT	B	624	-	-	0/21/61/61	0/2/2/2
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
29	SQD	B	626	-	-	0/42/62/69	0/1/1/1
30	LMT	B	627	-	-	0/21/61/61	0/2/2/2
30	LMT	B	628	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	-	0/37/135/135	0/0/9/9
22	CLA	C	502	-	-	0/37/135/135	0/0/9/9
22	CLA	C	503	-	-	0/37/135/135	0/0/9/9
22	CLA	C	504	-	-	0/37/135/135	0/0/9/9
22	CLA	C	505	-	-	0/37/135/135	0/0/9/9
22	CLA	C	506	-	-	0/37/135/135	0/0/9/9
22	CLA	C	507	-	-	0/37/135/135	0/0/9/9
22	CLA	C	508	-	-	0/37/135/135	0/0/9/9
22	CLA	C	509	-	-	0/37/135/135	0/0/9/9
22	CLA	C	510	3	-	0/37/135/135	0/0/9/9
22	CLA	C	511	-	-	0/37/135/135	0/0/9/9
22	CLA	C	512	-	-	0/37/135/135	0/0/9/9
24	BCR	C	513	-	-	0/29/63/63	0/2/2/2
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	DGD	C	515	-	-	0/42/82/95	0/2/2/2
25	DGD	C	516	-	-	1/51/91/95	0/2/2/2
25	DGD	C	517	-	-	0/55/95/95	0/2/2/2
27	LMG	C	518	-	-	0/40/60/70	0/1/1/1
26	LHG	C	519	-	-	0/41/41/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	520	-	-	0/37/135/135	0/0/9/9
27	LMG	C	521	-	-	0/43/63/70	0/1/1/1
31	PHO	D	401	-	-	0/49/103/103	0/1/6/6
31	PHO	D	402	-	-	0/49/103/103	0/1/6/6
33	BCT	D	404	21	-	0/0/0/0	0/0/0/0
22	CLA	D	405	-	-	0/37/135/135	0/0/9/9
22	CLA	D	406	-	-	0/37/135/135	0/0/9/9
23	PL9	D	407	-	-	0/53/73/73	0/1/1/1
27	LMG	D	408	-	-	0/44/64/70	0/1/1/1
27	LMG	D	409	-	-	0/43/63/70	0/1/1/1
25	DGD	D	410	-	-	0/52/92/95	0/2/2/2
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
27	LMG	D	412	-	-	0/41/61/70	0/1/1/1
27	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/14/114/114	0/0/8/8
24	BCR	F	102	-	-	0/29/63/63	0/2/2/2
29	SQD	F	103	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	-	0/37/135/135	0/0/9/9
24	BCR	H	102	-	-	0/29/63/63	0/2/2/2
27	LMG	I	101	-	-	0/38/58/70	0/1/1/1
30	LMT	I	102	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
24	BCR	J	102	-	-	0/29/63/63	0/2/2/2
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	-	0/37/57/70	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/14/114/114	0/0/8/8
29	SQD	a	401	-	-	0/49/69/69	0/1/1/1
27	LMG	a	402	-	-	0/37/57/70	0/1/1/1
22	CLA	a	404	-	-	0/37/135/135	0/0/9/9
22	CLA	a	405	-	-	0/37/135/135	0/0/9/9
22	CLA	a	406	-	-	0/37/135/135	0/0/9/9
22	CLA	a	407	-	-	0/37/135/135	0/0/9/9
23	PL9	a	408	-	-	0/41/61/73	0/1/1/1
24	BCR	a	409	-	-	0/29/63/63	0/2/2/2
25	DGD	a	410	-	-	0/45/85/95	0/2/2/2
26	LHG	a	411	-	-	0/43/43/53	0/0/0/0
27	LMG	a	412	-	-	0/46/66/70	0/1/1/1
28	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
29	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	b	602	-	-	0/42/62/69	0/1/1/1
30	LMT	b	603	-	-	0/21/61/61	0/2/2/2
30	LMT	b	604	-	-	0/21/61/61	0/2/2/2
22	CLA	b	605	-	-	0/37/135/135	0/0/9/9
22	CLA	b	606	-	-	0/37/135/135	0/0/9/9
22	CLA	b	607	-	-	0/37/135/135	0/0/9/9
22	CLA	b	608	-	-	0/37/135/135	0/0/9/9
22	CLA	b	609	-	-	0/37/135/135	0/0/9/9
22	CLA	b	610	-	-	0/37/135/135	0/0/9/9
22	CLA	b	611	-	-	0/37/135/135	0/0/9/9
22	CLA	b	612	-	-	0/37/135/135	0/0/9/9
22	CLA	b	613	-	-	0/37/135/135	0/0/9/9
22	CLA	b	614	-	-	0/37/135/135	0/0/9/9
22	CLA	b	615	-	-	0/37/135/135	0/0/9/9
22	CLA	b	616	-	-	0/37/135/135	0/0/9/9
22	CLA	b	617	-	-	0/37/135/135	0/0/9/9
22	CLA	b	618	-	-	0/37/135/135	0/0/9/9
22	CLA	b	619	-	-	0/37/135/135	0/0/9/9
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	DGD	b	624	-	-	0/47/87/95	0/2/2/2
27	LMG	b	625	-	-	0/44/64/70	0/1/1/1
30	LMT	b	626	-	-	0/21/61/61	0/2/2/2
30	LMT	b	627	-	-	0/21/61/61	0/2/2/2
22	CLA	c	501	-	-	0/37/135/135	0/0/9/9
22	CLA	c	502	-	-	0/37/135/135	0/0/9/9
22	CLA	c	503	-	-	0/37/135/135	0/0/9/9
22	CLA	c	504	-	-	0/37/135/135	0/0/9/9
22	CLA	c	505	-	-	0/37/135/135	0/0/9/9
22	CLA	c	506	-	-	0/37/135/135	0/0/9/9
22	CLA	c	507	-	-	0/37/135/135	0/0/9/9
22	CLA	c	508	-	-	0/37/135/135	0/0/9/9
22	CLA	c	509	-	-	0/37/135/135	0/0/9/9
22	CLA	c	510	3	-	0/37/135/135	0/0/9/9
22	CLA	c	511	-	-	0/37/135/135	0/0/9/9
22	CLA	c	512	-	-	0/37/135/135	0/0/9/9
24	BCR	c	513	-	-	0/29/63/63	0/2/2/2
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	DGD	c	515	-	-	0/42/82/95	0/2/2/2
25	DGD	c	516	-	-	1/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	c	517	-	-	0/55/95/95	0/2/2/2
27	LMG	c	518	-	-	0/40/60/70	0/1/1/1
26	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	-	0/37/135/135	0/0/9/9
24	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	LMG	c	522	-	-	0/43/63/70	0/1/1/1
31	PHO	d	401	-	-	0/49/103/103	0/1/6/6
31	PHO	d	402	-	-	0/49/103/103	0/1/6/6
29	SQD	d	403	-	-	1/38/58/69	0/1/1/1
33	BCT	d	404	21	-	0/0/0/0	0/0/0/0
22	CLA	d	405	-	-	0/37/135/135	0/0/9/9
22	CLA	d	406	-	-	0/37/135/135	0/0/9/9
23	PL9	d	407	-	-	0/53/73/73	0/1/1/1
27	LMG	d	408	-	-	0/44/64/70	0/1/1/1
27	LMG	d	409	-	-	0/43/63/70	0/1/1/1
25	DGD	d	410	-	-	0/52/92/95	0/2/2/2
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
27	LMG	d	412	-	-	0/41/61/70	0/1/1/1
27	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/14/114/114	0/0/8/8
24	BCR	f	102	-	-	0/29/63/63	0/2/2/2
29	SQD	f	103	-	-	0/40/60/69	0/1/1/1
24	BCR	g	101	-	-	0/29/63/63	0/2/2/2
22	CLA	h	101	-	-	0/37/135/135	0/0/9/9
27	LMG	i	101	-	-	0/38/58/70	0/1/1/1
30	LMT	i	102	-	-	0/21/61/61	0/2/2/2
23	PL9	j	101	-	-	0/29/49/73	0/1/1/1
24	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/14/114/114	0/0/8/8
24	BCR	x	101	-	-	0/29/63/63	0/2/2/2
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

All (1083) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	411	OEX	O3-MN1	-15.24	1.87	2.02
28	a	414	OEX	O3-MN1	-15.06	1.87	2.02
30	D	411	LMT	C8-C7	-14.66	1.49	1.55
30	d	411	LMT	C8-C7	-14.62	1.49	1.55
34	v	201	HEM	C3C-C2C	-14.56	1.34	1.45
34	V	201	HEM	C3C-C2C	-14.51	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	411	OEX	O1-MN1	-14.24	1.88	2.02
28	a	414	OEX	O1-MN1	-14.07	1.88	2.02
25	c	515	DGD	C9B-C8B	-13.66	1.49	1.55
26	a	411	LHG	C12-C11	-13.52	1.49	1.55
26	A	409	LHG	C12-C11	-13.41	1.49	1.55
25	C	515	DGD	C9B-C8B	-13.35	1.49	1.55
25	B	625	DGD	CDB-CCB	-13.15	1.49	1.55
25	B	620	DGD	CDB-CCB	-13.09	1.49	1.55
25	A	408	DGD	CDB-CCB	-13.05	1.50	1.55
25	a	410	DGD	CDB-CCB	-13.03	1.50	1.55
34	F	101	HEM	C3C-C2C	-13.01	1.35	1.45
34	f	101	HEM	C3C-C2C	-12.93	1.35	1.45
25	b	624	DGD	CDB-CCB	-12.85	1.50	1.55
25	b	601	DGD	CDB-CCB	-12.65	1.50	1.55
34	f	101	HEM	C3B-C2B	-12.33	1.33	1.45
34	F	101	HEM	C3B-C2B	-12.31	1.33	1.45
27	a	402	LMG	C22-C21	-11.96	1.50	1.55
27	D	412	LMG	C22-C21	-11.94	1.50	1.55
27	d	412	LMG	C22-C21	-11.94	1.50	1.55
27	d	412	LMG	C41-C40	-11.81	1.50	1.55
27	D	408	LMG	C41-C40	-11.79	1.50	1.55
27	C	518	LMG	C22-C21	-11.78	1.50	1.55
27	e	101	LMG	C22-C21	-11.77	1.50	1.55
27	c	518	LMG	C22-C21	-11.73	1.50	1.55
27	A	414	LMG	C22-C21	-11.73	1.50	1.55
27	D	412	LMG	C41-C40	-11.72	1.50	1.55
27	i	101	LMG	C23-C22	-11.72	1.50	1.55
27	e	101	LMG	C39-C38	-11.68	1.50	1.55
27	d	408	LMG	C41-C40	-11.67	1.50	1.55
27	E	101	LMG	C22-C21	-11.65	1.50	1.55
28	A	411	OEX	O1-MN2	-11.63	1.91	2.02
28	a	414	OEX	O1-MN2	-11.63	1.91	2.02
27	D	408	LMG	C25-C24	-11.59	1.50	1.55
27	M	101	LMG	C22-C21	-11.52	1.50	1.55
27	m	101	LMG	C22-C21	-11.46	1.50	1.55
27	C	521	LMG	C23-C22	-11.44	1.50	1.55
27	C	518	LMG	C40-C39	-11.38	1.50	1.55
27	E	101	LMG	C39-C38	-11.36	1.50	1.55
27	D	409	LMG	C40-C39	-11.29	1.50	1.55
27	c	518	LMG	C40-C39	-11.23	1.50	1.55
27	I	101	LMG	C23-C22	-11.21	1.50	1.55
27	B	621	LMG	C23-C22	-11.21	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	410	LMG	C43-C42	-11.20	1.50	1.55
27	b	625	LMG	C23-C22	-11.18	1.50	1.55
27	d	409	LMG	C40-C39	-11.16	1.50	1.55
27	a	412	LMG	C43-C42	-11.16	1.50	1.55
27	c	522	LMG	C23-C22	-11.16	1.50	1.55
27	A	410	LMG	C25-C24	-11.03	1.50	1.55
27	d	408	LMG	C25-C24	-10.97	1.50	1.55
27	b	625	LMG	C43-C42	-10.83	1.50	1.55
27	d	409	LMG	C25-C24	-10.80	1.50	1.55
27	a	412	LMG	C25-C24	-10.75	1.50	1.55
34	v	201	HEM	C3B-C2B	-10.72	1.35	1.45
34	V	201	HEM	C3B-C2B	-10.71	1.35	1.45
27	B	621	LMG	C43-C42	-10.65	1.50	1.55
27	D	409	LMG	C25-C24	-10.64	1.50	1.55
27	c	522	LMG	C42-C41	-10.31	1.51	1.55
27	C	521	LMG	C42-C41	-10.23	1.51	1.55
28	A	411	OEX	O2-MN3	-9.92	1.89	2.06
28	a	414	OEX	O2-MN3	-9.92	1.89	2.06
28	A	411	OEX	O3-MN3	-9.85	1.90	2.06
28	a	414	OEX	O3-MN3	-9.76	1.90	2.06
26	c	519	LHG	C18-C17	-9.64	1.51	1.55
26	C	519	LHG	C18-C17	-9.64	1.51	1.55
26	C	519	LHG	C30-C29	-9.52	1.51	1.55
27	a	402	LMG	C37-C36	-9.49	1.51	1.55
27	m	101	LMG	C37-C36	-9.44	1.51	1.55
27	A	414	LMG	C37-C36	-9.39	1.51	1.55
25	C	516	DGD	CEA-CDA	-9.38	1.51	1.55
25	c	516	DGD	CEA-CDA	-9.35	1.51	1.55
27	M	101	LMG	C37-C36	-9.34	1.51	1.55
25	c	515	DGD	CEA-CDA	-9.17	1.51	1.55
25	C	515	DGD	CEA-CDA	-9.08	1.51	1.55
26	c	519	LHG	C30-C29	-9.01	1.51	1.55
25	B	620	DGD	CFA-CEA	-8.99	1.51	1.55
25	b	624	DGD	CFA-CEA	-8.95	1.51	1.55
29	a	415	SQD	C35-C34	-8.83	1.51	1.55
29	A	412	SQD	C35-C34	-8.77	1.51	1.55
25	d	410	DGD	CFA-CEA	-8.72	1.51	1.55
27	I	101	LMG	C37-C36	-8.67	1.51	1.55
27	i	101	LMG	C37-C36	-8.56	1.51	1.55
25	D	410	DGD	CFA-CEA	-8.53	1.51	1.55
28	a	414	OEX	O3-MN2	-7.74	1.94	2.02
22	A	402	CLA	C3B-C4B	7.64	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	411	OEX	O3-MN2	-7.63	1.95	2.02
22	a	404	CLA	C3B-C4B	7.62	1.50	1.41
25	b	601	DGD	C9A-C8A	-7.41	1.52	1.55
22	c	508	CLA	C3B-C4B	7.20	1.49	1.41
22	a	405	CLA	C3B-C4B	7.19	1.49	1.41
22	C	508	CLA	C3B-C4B	7.14	1.49	1.41
22	A	403	CLA	C3B-C4B	7.13	1.49	1.41
22	b	605	CLA	C3B-C4B	7.06	1.49	1.41
22	C	505	CLA	C3B-C4B	7.05	1.49	1.41
22	c	520	CLA	C3B-C4B	7.04	1.49	1.41
25	B	625	DGD	C9A-C8A	-7.03	1.52	1.55
22	C	520	CLA	C3B-C4B	7.01	1.49	1.41
22	B	613	CLA	C3B-C4B	7.01	1.49	1.41
22	c	505	CLA	C3B-C4B	7.00	1.49	1.41
22	B	601	CLA	C3B-C4B	6.99	1.49	1.41
22	b	606	CLA	C3B-C4B	6.98	1.49	1.41
22	b	611	CLA	C3B-C4B	6.98	1.49	1.41
22	c	511	CLA	C3B-C4B	6.98	1.49	1.41
22	b	612	CLA	C3B-C4B	6.98	1.49	1.41
22	c	510	CLA	C3B-C4B	6.97	1.49	1.41
22	c	509	CLA	C3B-C4B	6.96	1.49	1.41
22	d	406	CLA	C3B-C4B	6.96	1.49	1.41
22	h	101	CLA	C3B-C4B	6.95	1.49	1.41
22	b	615	CLA	C3B-C4B	6.94	1.49	1.41
22	C	511	CLA	C3B-C4B	6.94	1.49	1.41
22	B	608	CLA	C3B-C4B	6.93	1.49	1.41
22	H	101	CLA	C3B-C4B	6.92	1.49	1.41
22	C	507	CLA	C3B-C4B	6.92	1.49	1.41
22	a	406	CLA	C3B-C4B	6.90	1.49	1.41
22	D	405	CLA	C3B-C4B	6.90	1.49	1.41
22	b	618	CLA	C3B-C4B	6.90	1.49	1.41
22	C	509	CLA	C3B-C4B	6.90	1.49	1.41
22	B	614	CLA	C3B-C4B	6.89	1.49	1.41
22	c	507	CLA	C3B-C4B	6.89	1.49	1.41
22	B	612	CLA	C3B-C4B	6.89	1.49	1.41
22	c	512	CLA	C3B-C4B	6.88	1.49	1.41
22	b	619	CLA	C3B-C4B	6.88	1.49	1.41
22	B	607	CLA	C3B-C4B	6.87	1.49	1.41
22	C	510	CLA	C3B-C4B	6.87	1.49	1.41
22	B	615	CLA	C3B-C4B	6.87	1.49	1.41
22	B	611	CLA	C3B-C4B	6.87	1.49	1.41
25	a	410	DGD	CDA-CCA	-6.85	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	406	CLA	C3B-C4B	6.85	1.49	1.41
22	A	404	CLA	C3B-C4B	6.85	1.49	1.41
22	b	617	CLA	C3B-C4B	6.84	1.49	1.41
22	a	407	CLA	C3B-C4B	6.83	1.49	1.41
22	b	616	CLA	C3B-C4B	6.83	1.49	1.41
22	B	609	CLA	C3B-C4B	6.83	1.49	1.41
22	C	512	CLA	C3B-C4B	6.81	1.49	1.41
22	B	604	CLA	C3B-C4B	6.80	1.49	1.41
22	B	602	CLA	C3B-C4B	6.80	1.49	1.41
22	C	502	CLA	C3B-C4B	6.80	1.49	1.41
22	c	503	CLA	C3B-C4B	6.79	1.49	1.41
22	B	606	CLA	C3B-C4B	6.79	1.49	1.41
22	b	613	CLA	C3B-C4B	6.79	1.49	1.41
22	b	608	CLA	C3B-C4B	6.77	1.49	1.41
22	c	502	CLA	C3B-C4B	6.75	1.49	1.41
22	B	605	CLA	C3B-C4B	6.75	1.49	1.41
22	C	506	CLA	C3B-C4B	6.74	1.49	1.41
22	d	405	CLA	C3B-C4B	6.74	1.49	1.41
22	b	610	CLA	C3B-C4B	6.74	1.49	1.41
22	c	506	CLA	C3B-C4B	6.73	1.49	1.41
22	A	405	CLA	C3B-C4B	6.72	1.49	1.41
22	c	504	CLA	C3B-C4B	6.71	1.49	1.41
22	b	609	CLA	C3B-C4B	6.70	1.49	1.41
22	C	503	CLA	C3B-C4B	6.69	1.49	1.41
22	B	603	CLA	C3B-C4B	6.68	1.49	1.41
22	C	504	CLA	C3B-C4B	6.65	1.49	1.41
22	b	607	CLA	C3B-C4B	6.64	1.49	1.41
22	C	501	CLA	C3B-C4B	6.64	1.49	1.41
25	A	408	DGD	CDA-CCA	-6.62	1.52	1.55
22	c	501	CLA	C3B-C4B	6.53	1.49	1.41
28	A	411	OEX	O5-MN3	-6.21	1.85	2.11
28	a	414	OEX	O5-MN3	-6.17	1.86	2.11
22	B	610	CLA	C3B-C4B	6.07	1.48	1.41
22	b	614	CLA	C3B-C4B	6.05	1.48	1.41
34	f	101	HEM	CMC-C2C	5.92	1.55	1.45
34	F	101	HEM	CMC-C2C	5.89	1.55	1.45
34	V	201	HEM	CMB-C2B	5.88	1.55	1.45
34	v	201	HEM	CMD-C2D	5.85	1.55	1.45
34	v	201	HEM	CMB-C2B	5.84	1.55	1.45
34	V	201	HEM	CMD-C2D	5.83	1.55	1.45
34	F	101	HEM	CMD-C2D	5.74	1.54	1.45
34	v	201	HEM	CMC-C2C	5.73	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	CMD-C2D	5.73	1.54	1.45
34	V	201	HEM	CMC-C2C	5.72	1.54	1.45
34	f	101	HEM	CMB-C2B	5.71	1.54	1.45
34	F	101	HEM	CMB-C2B	5.68	1.54	1.45
28	A	411	OEX	O2-MN2	-5.57	1.97	2.02
28	a	414	OEX	O2-MN2	-5.49	1.97	2.02
29	F	103	SQD	C19-C18	-5.45	1.53	1.55
29	f	103	SQD	C19-C18	-5.44	1.53	1.55
23	d	407	PL9	C7-C3	-4.91	1.47	1.51
22	A	402	CLA	C4B-NB	4.78	1.42	1.34
22	c	508	CLA	C4B-NB	4.78	1.42	1.34
22	C	509	CLA	C4B-NB	4.75	1.42	1.34
22	B	601	CLA	C4B-NB	4.74	1.42	1.34
22	b	605	CLA	C4B-NB	4.74	1.42	1.34
22	a	404	CLA	C4B-NB	4.74	1.42	1.34
22	C	508	CLA	C4B-NB	4.73	1.42	1.34
22	b	619	CLA	C4B-NB	4.71	1.42	1.34
22	c	509	CLA	C4B-NB	4.70	1.42	1.34
34	V	201	HEM	C3B-CAB	4.70	1.55	1.40
22	C	505	CLA	C4B-NB	4.70	1.42	1.34
22	b	614	CLA	C4B-NB	4.70	1.42	1.34
34	v	201	HEM	C3B-CAB	4.69	1.55	1.40
34	f	101	HEM	C3C-CAC	4.68	1.55	1.40
22	B	610	CLA	C4B-NB	4.67	1.42	1.34
22	c	505	CLA	C4B-NB	4.67	1.42	1.34
22	B	615	CLA	C4B-NB	4.67	1.42	1.34
22	c	511	CLA	C4B-NB	4.67	1.42	1.34
22	C	507	CLA	C4B-NB	4.66	1.42	1.34
34	F	101	HEM	C3C-CAC	4.66	1.55	1.40
22	c	504	CLA	C4B-NB	4.65	1.42	1.34
22	b	612	CLA	C4B-NB	4.65	1.42	1.34
22	c	520	CLA	C4B-NB	4.64	1.42	1.34
22	B	614	CLA	C4B-NB	4.64	1.42	1.34
22	b	615	CLA	C4B-NB	4.64	1.42	1.34
22	c	503	CLA	C4B-NB	4.64	1.42	1.34
22	D	405	CLA	C4B-NB	4.63	1.42	1.34
22	d	406	CLA	C4B-NB	4.63	1.42	1.34
22	b	610	CLA	C4B-NB	4.63	1.42	1.34
22	a	405	CLA	C4B-NB	4.63	1.42	1.34
22	b	618	CLA	C4B-NB	4.63	1.42	1.34
22	B	611	CLA	C4B-NB	4.63	1.42	1.34
22	B	606	CLA	C4B-NB	4.62	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3C-CAC	4.62	1.55	1.40
22	B	608	CLA	C4B-NB	4.61	1.41	1.34
22	B	609	CLA	C4B-NB	4.61	1.41	1.34
34	V	201	HEM	C3C-CAC	4.61	1.55	1.40
22	c	510	CLA	C4B-NB	4.61	1.41	1.34
22	a	406	CLA	C4B-NB	4.60	1.41	1.34
22	d	405	CLA	C4B-NB	4.60	1.41	1.34
22	c	512	CLA	C4B-NB	4.60	1.41	1.34
22	C	511	CLA	C4B-NB	4.60	1.41	1.34
22	c	507	CLA	C4B-NB	4.60	1.41	1.34
22	H	101	CLA	C4B-NB	4.59	1.41	1.34
22	B	604	CLA	C4B-NB	4.59	1.41	1.34
22	A	403	CLA	C4B-NB	4.59	1.41	1.34
22	b	608	CLA	C4B-NB	4.59	1.41	1.34
22	A	405	CLA	C4B-NB	4.58	1.41	1.34
22	C	512	CLA	C4B-NB	4.58	1.41	1.34
22	D	406	CLA	C4B-NB	4.57	1.41	1.34
22	h	101	CLA	C4B-NB	4.57	1.41	1.34
22	C	510	CLA	C4B-NB	4.57	1.41	1.34
22	a	407	CLA	C4B-NB	4.56	1.41	1.34
22	b	609	CLA	C4B-NB	4.56	1.41	1.34
22	b	611	CLA	C4B-NB	4.56	1.41	1.34
22	C	502	CLA	C4B-NB	4.55	1.41	1.34
22	b	616	CLA	C4B-NB	4.54	1.41	1.34
34	F	101	HEM	C3B-CAB	4.54	1.55	1.40
22	B	607	CLA	C4B-NB	4.54	1.41	1.34
22	A	404	CLA	C4B-NB	4.54	1.41	1.34
22	C	503	CLA	C4B-NB	4.53	1.41	1.34
23	D	407	PL9	C7-C3	-4.53	1.47	1.51
22	C	504	CLA	C4B-NB	4.53	1.41	1.34
22	B	605	CLA	C4B-NB	4.53	1.41	1.34
22	B	613	CLA	C4B-NB	4.53	1.41	1.34
22	C	520	CLA	C4B-NB	4.52	1.41	1.34
22	c	501	CLA	C4B-NB	4.52	1.41	1.34
34	f	101	HEM	C3B-CAB	4.52	1.55	1.40
22	b	617	CLA	C4B-NB	4.51	1.41	1.34
22	C	501	CLA	C4B-NB	4.51	1.41	1.34
22	b	613	CLA	C4B-NB	4.51	1.41	1.34
22	b	607	CLA	C4B-NB	4.50	1.41	1.34
22	c	506	CLA	C4B-NB	4.50	1.41	1.34
22	c	502	CLA	C4B-NB	4.50	1.41	1.34
22	B	612	CLA	C4B-NB	4.50	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	C4B-NB	4.49	1.41	1.34
22	C	506	CLA	C4B-NB	4.48	1.41	1.34
22	B	603	CLA	C4B-NB	4.47	1.41	1.34
22	B	602	CLA	C4B-NB	4.46	1.41	1.34
23	a	408	PL9	C7-C3	-4.45	1.47	1.51
22	d	405	CLA	CHB-C4A	4.33	1.39	1.33
22	c	504	CLA	CHB-C4A	4.27	1.39	1.33
22	D	405	CLA	CHB-C4A	4.20	1.39	1.33
22	c	503	CLA	CHB-C4A	4.19	1.39	1.33
34	V	201	HEM	C3D-C2D	4.18	1.54	1.43
34	v	201	HEM	C3D-C2D	4.17	1.54	1.43
34	F	101	HEM	FE-ND	4.17	2.12	1.95
22	b	607	CLA	CHB-C4A	4.16	1.39	1.33
22	B	611	CLA	CHB-C4A	4.16	1.39	1.33
22	C	504	CLA	CHB-C4A	4.15	1.39	1.33
22	B	603	CLA	CHB-C4A	4.15	1.39	1.33
22	b	609	CLA	CHB-C4A	4.13	1.39	1.33
22	C	501	CLA	CHB-C4A	4.12	1.38	1.33
22	B	613	CLA	CHB-C4A	4.12	1.38	1.33
22	b	617	CLA	CHB-C4A	4.10	1.38	1.33
22	b	619	CLA	CHB-C4A	4.10	1.38	1.33
22	C	502	CLA	CHB-C4A	4.10	1.38	1.33
22	H	101	CLA	CHB-C4A	4.08	1.38	1.33
22	B	614	CLA	CHB-C4A	4.08	1.38	1.33
22	C	510	CLA	CHB-C4A	4.08	1.38	1.33
22	c	502	CLA	CHB-C4A	4.08	1.38	1.33
22	c	510	CLA	CHB-C4A	4.08	1.38	1.33
22	C	511	CLA	CHB-C4A	4.07	1.38	1.33
22	b	616	CLA	CHB-C4A	4.06	1.38	1.33
22	c	511	CLA	CHB-C4A	4.06	1.38	1.33
22	b	618	CLA	CHB-C4A	4.06	1.38	1.33
22	c	501	CLA	CHB-C4A	4.06	1.38	1.33
22	C	503	CLA	CHB-C4A	4.05	1.38	1.33
22	c	504	CLA	C1A-NA	4.05	1.41	1.32
22	B	604	CLA	CHB-C4A	4.05	1.38	1.33
22	b	605	CLA	CHB-C4A	4.04	1.38	1.33
22	C	507	CLA	CHB-C4A	4.04	1.38	1.33
22	C	512	CLA	CHB-C4A	4.04	1.38	1.33
22	B	601	CLA	CHB-C4A	4.04	1.38	1.33
22	b	615	CLA	CHB-C4A	4.04	1.38	1.33
22	B	615	CLA	CHB-C4A	4.04	1.38	1.33
22	c	510	CLA	C1A-NA	4.04	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	C1A-NA	4.03	1.41	1.32
22	C	504	CLA	C1A-NA	4.02	1.41	1.32
22	c	503	CLA	C1A-NA	4.02	1.41	1.32
22	c	512	CLA	CHB-C4A	4.02	1.38	1.33
22	d	405	CLA	C1A-NA	4.01	1.41	1.32
23	J	101	PL9	C7-C3	-4.01	1.48	1.51
22	b	612	CLA	CHB-C4A	4.01	1.38	1.33
22	B	603	CLA	C1A-NA	4.01	1.41	1.32
22	h	101	CLA	CHB-C4A	4.00	1.38	1.33
22	C	511	CLA	C1A-NA	4.00	1.41	1.32
22	B	605	CLA	CHB-C4A	4.00	1.38	1.33
22	B	606	CLA	CHB-C4A	4.00	1.38	1.33
22	C	510	CLA	C1A-NA	4.00	1.41	1.32
22	c	504	CLA	C1B-C2B	4.00	1.50	1.43
23	A	406	PL9	C7-C3	-4.00	1.48	1.51
22	b	607	CLA	C1A-NA	4.00	1.41	1.32
22	c	506	CLA	C1A-NA	3.99	1.41	1.32
22	C	509	CLA	CHB-C4A	3.99	1.38	1.33
22	a	406	CLA	CHB-C4A	3.99	1.38	1.33
22	B	608	CLA	CHB-C4A	3.99	1.38	1.33
22	b	618	CLA	C1A-NA	3.98	1.41	1.32
22	c	520	CLA	CHB-C4A	3.97	1.38	1.33
22	b	608	CLA	CHB-C4A	3.97	1.38	1.33
22	c	508	CLA	CHB-C4A	3.97	1.38	1.33
22	C	506	CLA	C1A-NA	3.97	1.41	1.32
22	D	405	CLA	C1B-C2B	3.97	1.49	1.43
22	B	612	CLA	CHB-C4A	3.97	1.38	1.33
22	B	607	CLA	CHB-C4A	3.97	1.38	1.33
22	c	508	CLA	C1A-NA	3.96	1.41	1.32
22	b	613	CLA	CHB-C4A	3.96	1.38	1.33
22	C	502	CLA	C1A-NA	3.96	1.41	1.32
34	F	101	HEM	C3D-C2D	3.96	1.53	1.43
22	d	406	CLA	CHB-C4A	3.95	1.38	1.33
22	C	501	CLA	C1B-C2B	3.95	1.49	1.43
22	B	609	CLA	CHB-C4A	3.95	1.38	1.33
22	D	405	CLA	C1A-NA	3.95	1.40	1.32
22	B	610	CLA	C1A-NA	3.94	1.40	1.32
22	A	404	CLA	CHB-C4A	3.94	1.38	1.33
22	b	612	CLA	C1A-NA	3.94	1.40	1.32
22	b	610	CLA	CHB-C4A	3.94	1.38	1.33
22	c	506	CLA	CHB-C4A	3.94	1.38	1.33
22	B	614	CLA	C1A-NA	3.94	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	C1A-NA	3.94	1.40	1.32
22	b	616	CLA	C1A-NA	3.93	1.40	1.32
34	f	101	HEM	C3D-C2D	3.93	1.53	1.43
22	B	608	CLA	C1A-NA	3.93	1.40	1.32
22	A	405	CLA	CHB-C4A	3.93	1.38	1.33
22	b	614	CLA	C1A-NA	3.92	1.40	1.32
22	b	619	CLA	C1B-C2B	3.92	1.49	1.43
22	b	609	CLA	C1A-NA	3.92	1.40	1.32
22	C	507	CLA	C1A-NA	3.92	1.40	1.32
22	B	602	CLA	CHB-C4A	3.92	1.38	1.33
22	C	512	CLA	C1A-NA	3.91	1.40	1.32
22	d	405	CLA	C1B-C2B	3.91	1.49	1.43
22	H	101	CLA	C1A-NA	3.91	1.40	1.32
22	c	509	CLA	CHB-C4A	3.91	1.38	1.33
22	b	605	CLA	C1A-NA	3.91	1.40	1.32
22	b	611	CLA	CHB-C4A	3.91	1.38	1.33
22	B	611	CLA	C1B-C2B	3.91	1.49	1.43
22	C	501	CLA	C1A-NA	3.90	1.40	1.32
22	C	508	CLA	CHB-C4A	3.90	1.38	1.33
22	a	406	CLA	C1A-NA	3.90	1.40	1.32
22	B	601	CLA	C1A-NA	3.90	1.40	1.32
22	c	501	CLA	C1B-C2B	3.90	1.49	1.43
22	B	609	CLA	C1A-NA	3.90	1.40	1.32
22	D	406	CLA	CHB-C4A	3.90	1.38	1.33
22	C	506	CLA	CHB-C4A	3.90	1.38	1.33
22	C	503	CLA	C1A-NA	3.90	1.40	1.32
22	a	407	CLA	CHB-C4A	3.89	1.38	1.33
22	c	512	CLA	C1A-NA	3.89	1.40	1.32
22	A	403	CLA	C1A-NA	3.89	1.40	1.32
34	f	101	HEM	FE-ND	3.89	2.11	1.95
22	c	520	CLA	C1A-NA	3.89	1.40	1.32
22	B	612	CLA	C1A-NA	3.89	1.40	1.32
22	c	501	CLA	C1A-NA	3.89	1.40	1.32
22	c	505	CLA	C1A-NA	3.88	1.40	1.32
22	C	504	CLA	C1B-C2B	3.88	1.49	1.43
22	C	509	CLA	C1A-NA	3.88	1.40	1.32
22	C	520	CLA	CHB-C4A	3.88	1.38	1.33
22	A	405	CLA	C1A-NA	3.88	1.40	1.32
23	j	101	PL9	C7-C3	-3.87	1.48	1.51
22	b	613	CLA	C1A-NA	3.87	1.40	1.32
22	C	520	CLA	C1A-NA	3.87	1.40	1.32
22	b	606	CLA	CHB-C4A	3.87	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C1A-NA	3.87	1.40	1.32
22	B	611	CLA	C1A-NA	3.87	1.40	1.32
22	h	101	CLA	C1A-NA	3.87	1.40	1.32
22	B	607	CLA	C1A-NA	3.87	1.40	1.32
22	h	101	CLA	C1B-C2B	3.87	1.49	1.43
22	b	611	CLA	C1A-NA	3.86	1.40	1.32
22	a	405	CLA	CHB-C4A	3.86	1.38	1.33
22	b	606	CLA	C1A-NA	3.86	1.40	1.32
22	B	602	CLA	C1A-NA	3.86	1.40	1.32
22	B	605	CLA	C1A-NA	3.86	1.40	1.32
22	C	505	CLA	C1A-NA	3.86	1.40	1.32
22	B	615	CLA	C1B-C2B	3.86	1.49	1.43
22	A	403	CLA	CHB-C4A	3.86	1.38	1.33
22	a	405	CLA	C1A-NA	3.86	1.40	1.32
22	d	406	CLA	C1A-NA	3.86	1.40	1.32
22	B	603	CLA	C1B-C2B	3.86	1.49	1.43
22	c	509	CLA	C1A-NA	3.85	1.40	1.32
22	B	604	CLA	C1A-NA	3.85	1.40	1.32
22	c	503	CLA	C1B-C2B	3.85	1.49	1.43
22	H	101	CLA	C1B-C2B	3.85	1.49	1.43
22	c	511	CLA	C1B-C2B	3.85	1.49	1.43
22	B	613	CLA	C1B-C2B	3.85	1.49	1.43
22	b	615	CLA	C1B-C2B	3.85	1.49	1.43
22	C	505	CLA	CHB-C4A	3.85	1.38	1.33
22	A	402	CLA	CHB-C4A	3.85	1.38	1.33
22	a	407	CLA	C1A-NA	3.85	1.40	1.32
22	B	613	CLA	C1A-NA	3.84	1.40	1.32
22	B	601	CLA	C1B-C2B	3.84	1.49	1.43
22	c	507	CLA	CHB-C4A	3.84	1.38	1.33
22	b	607	CLA	C1B-C2B	3.84	1.49	1.43
22	b	618	CLA	C1B-C2B	3.84	1.49	1.43
22	c	505	CLA	CHB-C4A	3.84	1.38	1.33
22	b	615	CLA	C1A-NA	3.84	1.40	1.32
22	A	404	CLA	C1A-NA	3.84	1.40	1.32
22	b	619	CLA	C1A-NA	3.84	1.40	1.32
22	B	614	CLA	C1B-C2B	3.83	1.49	1.43
22	c	507	CLA	C1A-NA	3.83	1.40	1.32
22	b	617	CLA	C1A-NA	3.83	1.40	1.32
22	b	609	CLA	C1B-C2B	3.83	1.49	1.43
22	B	615	CLA	C1A-NA	3.83	1.40	1.32
22	a	404	CLA	CHB-C4A	3.83	1.38	1.33
22	b	617	CLA	C1B-C2B	3.82	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C1A-NA	3.82	1.40	1.32
22	C	511	CLA	C1B-C2B	3.82	1.49	1.43
22	b	608	CLA	C1A-NA	3.82	1.40	1.32
22	b	614	CLA	CHB-C4A	3.82	1.38	1.33
22	c	510	CLA	C1B-C2B	3.81	1.49	1.43
22	b	616	CLA	C1B-C2B	3.81	1.49	1.43
34	v	201	HEM	FE-NB	3.81	2.09	1.95
22	b	612	CLA	C1B-C2B	3.80	1.49	1.43
22	a	406	CLA	C1B-C2B	3.79	1.49	1.43
22	C	502	CLA	C1B-C2B	3.79	1.49	1.43
22	c	502	CLA	C1B-C2B	3.79	1.49	1.43
22	D	406	CLA	C1A-NA	3.79	1.40	1.32
22	B	610	CLA	CHB-C4A	3.79	1.38	1.33
22	C	503	CLA	C1B-C2B	3.79	1.49	1.43
22	B	606	CLA	C1B-C2B	3.79	1.49	1.43
22	b	605	CLA	C1B-C2B	3.78	1.49	1.43
22	B	608	CLA	C1B-C2B	3.78	1.49	1.43
22	C	510	CLA	C1B-C2B	3.77	1.49	1.43
22	b	610	CLA	C1A-NA	3.77	1.40	1.32
22	b	608	CLA	C1B-C2B	3.77	1.49	1.43
22	B	612	CLA	C1B-C2B	3.77	1.49	1.43
22	B	604	CLA	C1B-C2B	3.76	1.49	1.43
34	f	101	HEM	FE-NB	3.75	2.09	1.95
22	B	605	CLA	C1B-C2B	3.75	1.49	1.43
22	d	406	CLA	C1B-C2B	3.75	1.49	1.43
22	C	512	CLA	C1B-C2B	3.75	1.49	1.43
22	c	520	CLA	C1B-C2B	3.75	1.49	1.43
22	A	404	CLA	C1B-C2B	3.74	1.49	1.43
22	b	606	CLA	C1B-C2B	3.74	1.49	1.43
22	b	610	CLA	C1B-C2B	3.74	1.49	1.43
22	c	506	CLA	C1B-C2B	3.73	1.49	1.43
22	c	512	CLA	C1B-C2B	3.73	1.49	1.43
22	A	402	CLA	C1A-NA	3.73	1.40	1.32
22	c	508	CLA	C1B-C2B	3.72	1.49	1.43
22	B	602	CLA	C1B-C2B	3.72	1.49	1.43
34	v	201	HEM	FE-ND	3.72	2.10	1.95
22	a	404	CLA	C1A-NA	3.71	1.40	1.32
22	D	406	CLA	C1B-C2B	3.71	1.49	1.43
22	b	614	CLA	CMB-C2B	-3.70	1.44	1.51
22	C	509	CLA	C1B-C2B	3.70	1.49	1.43
34	V	201	HEM	FE-ND	3.69	2.10	1.95
22	C	505	CLA	C1B-C2B	3.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C1B-C2B	3.69	1.49	1.43
22	c	505	CLA	C1B-C2B	3.68	1.49	1.43
22	C	506	CLA	C1B-C2B	3.68	1.49	1.43
22	c	509	CLA	C1B-C2B	3.68	1.49	1.43
22	C	508	CLA	C1B-C2B	3.68	1.49	1.43
22	B	607	CLA	C1B-C2B	3.67	1.49	1.43
22	b	613	CLA	C1B-C2B	3.66	1.49	1.43
22	B	609	CLA	C1B-C2B	3.65	1.49	1.43
22	a	405	CLA	C1B-C2B	3.65	1.49	1.43
22	C	520	CLA	C1B-C2B	3.64	1.49	1.43
22	C	507	CLA	C1B-C2B	3.64	1.49	1.43
22	a	407	CLA	C1B-C2B	3.64	1.49	1.43
22	b	611	CLA	C1B-C2B	3.61	1.49	1.43
22	B	610	CLA	CMB-C2B	-3.60	1.44	1.51
24	y	101	BCR	C1-C6	-3.60	1.48	1.53
22	A	403	CLA	C1B-C2B	3.59	1.49	1.43
29	f	103	SQD	C32-C31	-3.57	1.53	1.55
34	V	201	HEM	FE-NB	3.55	2.08	1.95
24	H	102	BCR	C1-C6	-3.54	1.48	1.53
22	A	402	CLA	C1B-C2B	3.52	1.49	1.43
24	g	101	BCR	C1-C6	-3.52	1.48	1.53
29	F	103	SQD	C32-C31	-3.50	1.53	1.55
24	F	102	BCR	C1-C6	-3.49	1.48	1.53
22	c	507	CLA	C1B-C2B	3.48	1.49	1.43
29	d	403	SQD	C18-C17	-3.46	1.53	1.55
24	f	102	BCR	C1-C6	-3.44	1.48	1.53
24	x	101	BCR	C1-C6	-3.44	1.48	1.53
22	a	404	CLA	C1B-C2B	3.44	1.49	1.43
29	B	622	SQD	C18-C17	-3.41	1.53	1.55
31	d	402	PHO	C1D-ND	3.34	1.41	1.36
31	D	402	PHO	C1D-ND	3.32	1.41	1.36
31	D	401	PHO	C1D-ND	3.32	1.41	1.36
34	F	101	HEM	FE-NB	3.29	2.07	1.95
31	d	401	PHO	C1D-ND	3.28	1.41	1.36
31	D	402	PHO	C4B-C3B	3.28	1.50	1.42
31	d	402	PHO	C4B-C3B	3.27	1.50	1.42
24	B	616	BCR	C1-C6	-3.23	1.49	1.53
24	C	514	BCR	C1-C6	-3.23	1.49	1.53
24	c	514	BCR	C1-C6	-3.21	1.49	1.53
29	B	626	SQD	C31-C30	-3.21	1.53	1.55
24	b	620	BCR	C1-C6	-3.19	1.49	1.53
31	D	401	PHO	C4B-C3B	3.17	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	BCR	C1-C6	-3.16	1.49	1.53
24	y	101	BCR	C30-C25	-3.14	1.49	1.53
29	b	602	SQD	C31-C30	-3.13	1.53	1.55
24	b	622	BCR	C30-C25	-3.13	1.49	1.53
31	d	401	PHO	C4B-C3B	3.09	1.49	1.42
24	B	617	BCR	C1-C6	-3.09	1.49	1.53
29	B	622	SQD	C31-C30	-3.09	1.53	1.55
24	J	102	BCR	C30-C25	-3.09	1.49	1.53
24	g	101	BCR	C30-C25	-3.09	1.49	1.53
24	C	513	BCR	C1-C6	-3.09	1.49	1.53
24	j	102	BCR	C30-C25	-3.07	1.49	1.53
29	a	401	SQD	O48-C23	3.06	1.42	1.33
29	d	403	SQD	C31-C30	-3.05	1.53	1.55
24	c	513	BCR	C1-C6	-3.05	1.49	1.53
29	b	602	SQD	O48-C23	3.04	1.42	1.33
24	B	618	BCR	C30-C25	-3.04	1.49	1.53
31	D	402	PHO	C1B-C2B	3.03	1.50	1.42
24	K	102	BCR	C30-C25	-3.03	1.49	1.53
29	d	403	SQD	O48-C23	3.03	1.42	1.33
29	f	103	SQD	O48-C23	3.03	1.42	1.33
29	F	103	SQD	O48-C23	3.02	1.42	1.33
24	F	102	BCR	C30-C25	-3.00	1.49	1.53
29	A	413	SQD	O48-C23	3.00	1.42	1.33
29	B	622	SQD	O48-C23	3.00	1.42	1.33
31	d	401	PHO	C1B-C2B	2.99	1.50	1.42
29	B	626	SQD	O48-C23	2.99	1.42	1.33
24	c	521	BCR	C30-C25	-2.98	1.49	1.53
29	a	415	SQD	O48-C23	2.98	1.42	1.33
24	A	407	BCR	C30-C25	-2.97	1.49	1.53
24	B	618	BCR	C1-C6	-2.96	1.49	1.53
24	a	409	BCR	C30-C25	-2.95	1.49	1.53
24	f	102	BCR	C30-C25	-2.95	1.49	1.53
31	d	402	PHO	C1B-C2B	2.95	1.50	1.42
24	B	619	BCR	C30-C25	-2.95	1.49	1.53
24	b	623	BCR	C1-C6	-2.94	1.49	1.53
31	D	401	PHO	C1B-C2B	2.94	1.50	1.42
24	B	616	BCR	C30-C25	-2.94	1.49	1.53
24	b	620	BCR	C30-C25	-2.94	1.49	1.53
29	A	412	SQD	O48-C23	2.93	1.42	1.33
24	b	623	BCR	C30-C25	-2.92	1.49	1.53
31	d	402	PHO	C3D-C4D	2.92	1.44	1.40
24	b	622	BCR	C1-C6	-2.92	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	619	BCR	C1-C6	-2.92	1.49	1.53
24	A	407	BCR	C1-C6	-2.92	1.49	1.53
24	a	409	BCR	C1-C6	-2.91	1.49	1.53
31	d	401	PHO	C3D-C4D	2.89	1.44	1.40
31	D	402	PHO	C3D-C4D	2.88	1.44	1.40
31	D	401	PHO	C3D-C4D	2.87	1.44	1.40
24	C	514	BCR	C30-C25	-2.87	1.49	1.53
24	K	102	BCR	C1-C6	-2.87	1.49	1.53
25	b	601	DGD	C1E-C2E	2.84	1.61	1.52
24	C	513	BCR	C30-C25	-2.84	1.49	1.53
24	c	514	BCR	C30-C25	-2.84	1.49	1.53
22	b	614	CLA	C1B-C2B	2.82	1.48	1.43
22	B	610	CLA	C1B-C2B	2.80	1.48	1.43
24	x	101	BCR	C30-C25	-2.79	1.49	1.53
34	v	201	HEM	FE-NC	2.78	2.06	1.95
24	c	521	BCR	C1-C6	-2.77	1.49	1.53
25	B	625	DGD	C1E-C2E	2.77	1.60	1.52
29	d	403	SQD	O47-C7	2.75	1.42	1.34
24	H	102	BCR	C30-C25	-2.75	1.49	1.53
29	B	622	SQD	O47-C7	2.73	1.42	1.34
29	a	415	SQD	O47-C7	2.72	1.42	1.34
29	a	401	SQD	O47-C7	2.72	1.42	1.34
29	A	413	SQD	O47-C7	2.71	1.42	1.34
29	A	412	SQD	O47-C7	2.70	1.42	1.34
31	d	402	PHO	CHD-C4C	2.69	1.37	1.35
29	F	103	SQD	O47-C7	2.69	1.42	1.34
24	J	102	BCR	C1-C6	-2.68	1.50	1.53
24	j	102	BCR	C1-C6	-2.67	1.50	1.53
24	c	513	BCR	C30-C25	-2.66	1.50	1.53
31	D	402	PHO	CHD-C4C	2.65	1.37	1.35
29	b	602	SQD	O47-C7	2.65	1.42	1.34
29	B	626	SQD	O47-C7	2.64	1.42	1.34
29	f	103	SQD	O47-C7	2.64	1.42	1.34
22	C	507	CLA	CMB-C2B	-2.63	1.46	1.51
22	c	507	CLA	CMB-C2B	-2.62	1.46	1.51
24	b	621	BCR	C30-C25	-2.62	1.50	1.53
24	B	617	BCR	C30-C25	-2.60	1.50	1.53
30	d	411	LMT	O3'-C3'	-2.55	1.36	1.43
30	b	627	LMT	O3'-C3'	-2.55	1.36	1.43
22	B	611	CLA	CMD-C2D	-2.55	1.46	1.51
30	D	411	LMT	O3'-C3'	-2.53	1.36	1.43
30	M	102	LMT	O3'-C3'	-2.53	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	I	102	LMT	O3'-C3'	-2.53	1.36	1.43
30	M	103	LMT	O3'-C3'	-2.53	1.36	1.43
23	a	408	PL9	C3-C4	-2.53	1.45	1.49
22	a	404	CLA	CMB-C2B	-2.52	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.51	1.46	1.51
30	b	626	LMT	O3'-C3'	-2.51	1.36	1.43
22	c	509	CLA	CMB-C2B	-2.51	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	511	CLA	C4D-C3D	2.50	1.48	1.42
22	A	403	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	615	CLA	CMD-C2D	-2.49	1.46	1.51
30	b	604	LMT	O3'-C3'	-2.49	1.36	1.43
30	b	603	LMT	O3'-C3'	-2.49	1.36	1.43
22	B	609	CLA	CMB-C2B	-2.49	1.46	1.51
25	C	515	DGD	O2G-C2G	-2.49	1.40	1.46
22	B	603	CLA	CMB-C2B	-2.49	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.49	1.46	1.51
22	c	512	CLA	C1D-C2D	2.49	1.48	1.42
30	B	627	LMT	O3'-C3'	-2.49	1.37	1.43
23	D	407	PL9	C3-C4	-2.48	1.45	1.49
22	C	501	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	511	CLA	C4D-C3D	2.48	1.48	1.42
30	B	624	LMT	O3'-C3'	-2.48	1.37	1.43
22	A	404	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.48	1.46	1.51
22	a	407	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	510	CLA	C4D-C3D	2.47	1.48	1.42
22	C	505	CLA	CMB-C2B	-2.47	1.46	1.51
22	b	614	CLA	C3B-C2B	-2.47	1.37	1.40
22	d	405	CLA	CMB-C2B	-2.47	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.47	1.46	1.51
30	i	102	LMT	O3'-C3'	-2.47	1.37	1.43
22	a	406	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	512	CLA	C1D-C2D	2.46	1.48	1.42
30	B	623	LMT	O3'-C3'	-2.46	1.37	1.43
22	c	505	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	610	CLA	C1D-C2D	2.46	1.48	1.42
22	C	508	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	512	CLA	C4D-C3D	2.46	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C1D-C2D	2.46	1.48	1.42
22	c	508	CLA	C1D-C2D	2.45	1.48	1.42
22	B	606	CLA	CMB-C2B	-2.46	1.46	1.51
22	c	520	CLA	C1D-C2D	2.45	1.48	1.42
22	B	605	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	510	CLA	C4D-C3D	2.45	1.48	1.42
22	C	501	CLA	C1D-C2D	2.45	1.48	1.42
22	b	605	CLA	CMB-C2B	-2.45	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.45	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.45	1.46	1.51
23	d	407	PL9	C3-C4	-2.44	1.45	1.49
22	c	508	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.44	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	613	CLA	C1D-C2D	2.44	1.48	1.42
22	c	504	CLA	CMD-C2D	-2.44	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.44	1.46	1.51
34	v	201	HEM	C4D-ND	2.44	1.39	1.33
22	b	608	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.43	1.46	1.51
22	a	404	CLA	C1D-C2D	2.44	1.48	1.42
34	V	201	HEM	C4D-ND	2.43	1.39	1.33
22	a	406	CLA	C1D-C2D	2.43	1.48	1.42
22	h	101	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	606	CLA	C1D-C2D	2.43	1.48	1.42
22	c	501	CLA	C1D-C2D	2.43	1.48	1.42
22	a	405	CLA	C1D-C2D	2.43	1.48	1.42
22	C	503	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	512	CLA	C4D-C3D	2.43	1.48	1.42
22	B	608	CLA	CHC-C1C	2.43	1.43	1.35
22	A	403	CLA	C1D-C2D	2.43	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	406	CLA	CMB-C2B	-2.43	1.46	1.51
22	d	406	CLA	C1D-C2D	2.42	1.48	1.42
22	C	506	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	613	CLA	CHC-C1C	2.42	1.43	1.35
22	b	618	CLA	C4D-C3D	2.42	1.48	1.42
34	v	201	HEM	C1D-ND	2.42	1.39	1.33
31	d	401	PHO	CMD-C2D	-2.42	1.46	1.51
22	C	504	CLA	CMD-C2D	-2.42	1.46	1.51
22	D	406	CLA	C1D-C2D	2.42	1.48	1.42
22	B	604	CLA	C1D-C2D	2.41	1.48	1.42
22	B	614	CLA	CMB-C2B	-2.42	1.46	1.51
22	d	406	CLA	CMB-C2B	-2.42	1.46	1.51
22	c	503	CLA	C4D-C3D	2.42	1.48	1.42
22	c	504	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	508	CLA	C4D-C3D	2.41	1.48	1.42
22	c	506	CLA	C4D-C3D	2.41	1.48	1.42
22	C	509	CLA	C1D-C2D	2.41	1.48	1.42
31	D	402	PHO	CMD-C2D	-2.41	1.46	1.51
30	B	628	LMT	O3'-C3'	-2.41	1.37	1.43
22	b	616	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	601	CLA	C4D-C3D	2.41	1.48	1.42
22	C	511	CLA	CMB-C2B	-2.41	1.46	1.51
22	d	406	CLA	C4D-C3D	2.41	1.48	1.42
22	C	505	CLA	C1D-C2D	2.41	1.48	1.42
22	b	619	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	501	CLA	C4D-C3D	2.40	1.48	1.42
22	B	614	CLA	C1D-C2D	2.40	1.48	1.42
22	B	610	CLA	C3B-C2B	-2.40	1.37	1.40
22	c	509	CLA	CMD-C2D	-2.40	1.46	1.51
22	b	613	CLA	C4D-C3D	2.40	1.48	1.42
31	D	401	PHO	CMD-C2D	-2.40	1.46	1.51
22	C	520	CLA	C1D-C2D	2.40	1.48	1.42
22	c	505	CLA	C4D-C3D	2.40	1.48	1.42
22	B	602	CLA	CMB-C2B	-2.40	1.46	1.51
22	D	406	CLA	C4D-C3D	2.40	1.48	1.42
22	c	506	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	618	CLA	C1D-C2D	2.40	1.48	1.42
22	c	507	CLA	C4D-C3D	2.40	1.48	1.42
22	h	101	CLA	CHC-C1C	2.40	1.43	1.35
22	b	609	CLA	C1D-C2D	2.40	1.48	1.42
22	C	506	CLA	C4D-C3D	2.40	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	CLA	C1D-C2D	2.40	1.48	1.42
22	a	407	CLA	C4D-C3D	2.40	1.48	1.42
22	A	402	CLA	C1D-C2D	2.40	1.48	1.42
22	b	617	CLA	CMB-C2B	-2.40	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	603	CLA	C4D-C3D	2.40	1.48	1.42
22	b	616	CLA	C1D-C2D	2.40	1.48	1.42
31	d	402	PHO	CMD-C2D	-2.40	1.46	1.51
22	c	510	CLA	C1D-C2D	2.40	1.48	1.42
22	b	618	CLA	CMB-C2B	-2.40	1.46	1.51
22	A	405	CLA	C4D-C3D	2.39	1.48	1.42
22	b	605	CLA	C1D-C2D	2.39	1.48	1.42
22	b	607	CLA	C4D-C3D	2.39	1.48	1.42
22	c	501	CLA	C4D-C3D	2.39	1.48	1.42
22	A	405	CLA	C1D-C2D	2.39	1.48	1.42
22	B	612	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	507	CLA	C1D-C2D	2.39	1.48	1.42
22	D	405	CLA	CMD-C2D	-2.39	1.46	1.51
22	C	503	CLA	C4D-C3D	2.39	1.48	1.42
22	B	615	CLA	C1D-C2D	2.39	1.48	1.42
22	c	503	CLA	C1D-C2D	2.39	1.48	1.42
22	H	101	CLA	CHC-C1C	2.39	1.43	1.35
22	B	608	CLA	C4D-C3D	2.39	1.48	1.42
22	b	619	CLA	C1D-C2D	2.39	1.48	1.42
22	C	520	CLA	C4D-C3D	2.39	1.48	1.42
22	b	612	CLA	CHC-C1C	2.39	1.43	1.35
22	B	612	CLA	C4D-C3D	2.38	1.48	1.42
22	c	505	CLA	C1D-C2D	2.38	1.48	1.42
22	b	611	CLA	CHC-C1C	2.38	1.43	1.35
22	c	502	CLA	C4D-C3D	2.38	1.48	1.42
22	d	405	CLA	C4D-C3D	2.38	1.48	1.42
22	b	614	CLA	C4D-C3D	2.38	1.48	1.42
22	C	507	CLA	C4D-C3D	2.38	1.48	1.42
22	b	616	CLA	C4D-C3D	2.38	1.48	1.42
22	b	608	CLA	C1D-C2D	2.38	1.48	1.42
22	b	605	CLA	C4D-C3D	2.38	1.48	1.42
22	B	602	CLA	C4D-C3D	2.38	1.48	1.42
22	C	502	CLA	C4D-C3D	2.38	1.48	1.42
22	c	520	CLA	C4D-C3D	2.38	1.48	1.42
22	B	613	CLA	C1D-C2D	2.37	1.48	1.42
22	B	601	CLA	C1D-C2D	2.37	1.48	1.42
22	C	508	CLA	C1D-C2D	2.37	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	C1D-C2D	2.37	1.48	1.42
22	B	612	CLA	C1D-C2D	2.37	1.48	1.42
22	C	503	CLA	C1D-C2D	2.37	1.48	1.42
22	c	511	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	605	CLA	C1D-C2D	2.37	1.48	1.42
34	V	201	HEM	C1D-ND	2.37	1.39	1.33
22	b	606	CLA	C4D-C3D	2.37	1.48	1.42
34	F	101	HEM	FE-NC	2.37	2.05	1.95
22	B	607	CLA	C4D-C3D	2.37	1.48	1.42
22	b	606	CLA	CHC-C1C	2.37	1.43	1.35
22	C	505	CLA	C4D-C3D	2.37	1.48	1.42
22	b	615	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	610	CLA	C1D-C2D	2.37	1.48	1.42
22	h	101	CLA	C4D-C3D	2.37	1.48	1.42
34	V	201	HEM	FE-NC	2.36	2.05	1.95
22	B	614	CLA	C4D-C3D	2.36	1.48	1.42
22	B	609	CLA	C4D-C3D	2.36	1.48	1.42
22	C	504	CLA	C4D-C3D	2.36	1.48	1.42
22	b	617	CLA	CHC-C1C	2.36	1.43	1.35
22	c	504	CLA	C4D-C3D	2.36	1.48	1.42
22	C	509	CLA	CMD-C2D	-2.36	1.46	1.51
22	c	506	CLA	C1D-C2D	2.36	1.48	1.42
22	C	510	CLA	C1D-C2D	2.36	1.48	1.42
23	A	406	PL9	C3-C4	-2.36	1.45	1.49
22	B	606	CLA	C4D-C3D	2.36	1.48	1.42
22	b	612	CLA	C4D-C3D	2.36	1.48	1.42
22	b	611	CLA	CMD-C2D	-2.36	1.46	1.51
22	b	611	CLA	C4D-C3D	2.36	1.48	1.42
25	B	625	DGD	C3G-C2G	2.35	1.57	1.50
22	H	101	CLA	C4D-C3D	2.35	1.48	1.42
22	B	607	CLA	CHC-C1C	2.35	1.43	1.35
22	C	508	CLA	C4D-C3D	2.35	1.48	1.42
22	a	404	CLA	CHC-C1C	2.35	1.43	1.35
22	b	608	CLA	C4D-C3D	2.35	1.48	1.42
22	d	406	CLA	CHC-C1C	2.35	1.43	1.35
34	F	101	HEM	C1D-ND	2.35	1.39	1.33
22	c	502	CLA	CHC-C1C	2.35	1.43	1.35
22	B	613	CLA	CMB-C2B	-2.35	1.46	1.51
22	H	101	CLA	C1D-C2D	2.35	1.48	1.42
22	B	603	CLA	CMD-C2D	-2.35	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	C4D-C3D	2.35	1.48	1.42
25	B	625	DGD	C4D-C5D	2.35	1.58	1.53
22	a	407	CLA	C1D-C2D	2.35	1.48	1.42
22	C	505	CLA	CHC-C1C	2.35	1.43	1.35
22	c	509	CLA	C1D-C2D	2.35	1.48	1.42
31	d	401	PHO	CHD-C4C	2.35	1.36	1.35
34	f	101	HEM	C1D-ND	2.34	1.39	1.33
34	f	101	HEM	FE-NC	2.34	2.05	1.95
22	B	610	CLA	C4D-C3D	2.34	1.48	1.42
22	A	403	CLA	C4D-C3D	2.34	1.48	1.42
22	b	609	CLA	C4D-C3D	2.34	1.48	1.42
22	D	405	CLA	CMB-C2B	-2.34	1.46	1.51
22	c	511	CLA	CHC-C1C	2.34	1.43	1.35
22	c	507	CLA	CHC-C1C	2.34	1.43	1.35
22	C	512	CLA	CHC-C1C	2.34	1.43	1.35
22	C	502	CLA	C1D-C2D	2.34	1.48	1.42
22	c	512	CLA	CHC-C1C	2.34	1.43	1.35
22	C	511	CLA	CHC-C1C	2.34	1.43	1.35
34	F	101	HEM	C4D-ND	2.34	1.39	1.33
22	C	509	CLA	C4D-C3D	2.33	1.48	1.42
22	c	509	CLA	CHC-C1C	2.34	1.43	1.35
22	B	604	CLA	C4D-C3D	2.33	1.48	1.42
22	d	405	CLA	CHC-C1C	2.33	1.43	1.35
22	A	402	CLA	CMD-C2D	-2.33	1.46	1.51
22	C	506	CLA	C1D-C2D	2.33	1.48	1.42
22	C	502	CLA	CHC-C1C	2.33	1.43	1.35
22	B	607	CLA	CMD-C2D	-2.33	1.46	1.51
22	c	509	CLA	C4D-C3D	2.33	1.48	1.42
22	c	504	CLA	CHC-C1C	2.33	1.43	1.35
22	a	406	CLA	CHC-C1C	2.33	1.43	1.35
22	c	505	CLA	CHC-C1C	2.33	1.43	1.35
22	C	509	CLA	CHC-C1C	2.33	1.43	1.35
22	B	613	CLA	C4D-C3D	2.33	1.48	1.42
34	f	101	HEM	C4D-ND	2.33	1.39	1.33
22	B	609	CLA	CHC-C1C	2.32	1.43	1.35
22	D	405	CLA	CHC-C1C	2.33	1.43	1.35
22	b	615	CLA	C4D-C3D	2.32	1.48	1.42
22	B	608	CLA	C1D-C2D	2.32	1.48	1.42
22	b	619	CLA	C4D-C3D	2.33	1.48	1.42
22	a	407	CLA	CHC-C1C	2.33	1.43	1.35
22	b	616	CLA	CHC-C1C	2.32	1.43	1.35
22	b	617	CLA	C1D-C2D	2.32	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	C1D-C2D	2.32	1.48	1.42
22	B	603	CLA	CHC-C1C	2.32	1.43	1.35
22	b	611	CLA	C1D-C2D	2.32	1.48	1.42
22	b	614	CLA	C1D-C2D	2.32	1.48	1.42
22	b	610	CLA	C4D-C3D	2.32	1.48	1.42
22	h	101	CLA	C1D-C2D	2.32	1.48	1.42
22	B	602	CLA	C1D-C2D	2.32	1.48	1.42
22	A	404	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	607	CLA	CHC-C1C	2.32	1.43	1.35
22	B	604	CLA	CHC-C1C	2.32	1.43	1.35
22	B	614	CLA	CHC-C1C	2.32	1.43	1.35
22	C	504	CLA	CHC-C1C	2.32	1.43	1.35
22	B	602	CLA	CHC-C1C	2.32	1.43	1.35
25	b	601	DGD	C3G-C2G	2.32	1.57	1.50
22	a	406	CLA	CMD-C2D	-2.32	1.46	1.51
22	a	406	CLA	C4D-C3D	2.32	1.48	1.42
22	b	618	CLA	CHC-C1C	2.32	1.43	1.35
22	c	507	CLA	C1D-C2D	2.32	1.48	1.42
22	c	508	CLA	CHC-C1C	2.31	1.43	1.35
22	a	404	CLA	CMD-C2D	-2.32	1.46	1.51
22	C	508	CLA	CHC-C1C	2.31	1.43	1.35
22	b	617	CLA	C4D-C3D	2.31	1.48	1.42
22	B	615	CLA	C4D-C3D	2.31	1.48	1.42
22	D	405	CLA	C4D-C3D	2.31	1.48	1.42
22	c	510	CLA	CHC-C1C	2.31	1.43	1.35
22	A	404	CLA	C4D-C3D	2.31	1.48	1.42
22	a	405	CLA	C4D-C3D	2.31	1.48	1.42
22	A	404	CLA	CHC-C1C	2.31	1.43	1.35
22	C	520	CLA	CHC-C1C	2.30	1.43	1.35
22	b	607	CLA	CMD-C2D	-2.30	1.46	1.51
22	C	511	CLA	C1D-C2D	2.30	1.48	1.42
22	b	613	CLA	CHC-C1C	2.30	1.43	1.35
22	b	619	CLA	CMD-C2D	-2.30	1.46	1.51
22	A	403	CLA	CHC-C1C	2.30	1.43	1.35
22	B	605	CLA	CHC-C1C	2.30	1.43	1.35
22	B	615	CLA	CMD-C2D	-2.30	1.46	1.51
22	b	607	CLA	C1D-C2D	2.30	1.48	1.42
22	b	608	CLA	CHC-C1C	2.29	1.42	1.35
22	B	606	CLA	CHC-C1C	2.29	1.42	1.35
22	C	510	CLA	CHC-C1C	2.29	1.42	1.35
22	A	402	CLA	CHC-C1C	2.29	1.42	1.35
22	c	503	CLA	CHC-C1C	2.29	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	C1D-C2D	2.29	1.48	1.42
30	I	102	LMT	O2'-C2'	-2.29	1.37	1.43
22	a	404	CLA	C4D-C3D	2.29	1.48	1.42
22	b	612	CLA	C1D-C2D	2.29	1.48	1.42
22	B	612	CLA	CHC-C1C	2.29	1.42	1.35
22	c	502	CLA	C1D-C2D	2.29	1.48	1.42
22	B	611	CLA	C4D-C3D	2.29	1.48	1.42
22	d	405	CLA	CMD-C2D	-2.29	1.46	1.51
22	b	610	CLA	CHC-C1C	2.29	1.42	1.35
22	a	405	CLA	CMD-C2D	-2.29	1.46	1.51
31	d	402	PHO	C4C-C3C	2.29	1.49	1.45
22	c	520	CLA	CHC-C1C	2.29	1.42	1.35
22	C	506	CLA	CHC-C1C	2.29	1.42	1.35
22	A	403	CLA	CMD-C2D	-2.29	1.46	1.51
22	d	405	CLA	C1D-C2D	2.28	1.48	1.42
22	B	602	CLA	CMD-C2D	-2.28	1.46	1.51
23	a	408	PL9	C53-C6	-2.28	1.46	1.50
22	B	601	CLA	CHC-C1C	2.28	1.42	1.35
22	b	605	CLA	CHC-C1C	2.28	1.42	1.35
22	b	609	CLA	CHC-C1C	2.28	1.42	1.35
22	C	508	CLA	CMD-C2D	-2.28	1.46	1.51
25	b	601	DGD	C1G-C2G	2.27	1.57	1.50
22	C	507	CLA	CHC-C1C	2.27	1.42	1.35
30	I	102	LMT	O2B-C2B	-2.28	1.37	1.43
22	B	604	CLA	CMD-C2D	-2.27	1.46	1.51
22	b	615	CLA	CHC-C1C	2.27	1.42	1.35
22	b	608	CLA	CMD-C2D	-2.27	1.46	1.51
22	H	101	CLA	CMD-C2D	-2.27	1.46	1.51
22	c	506	CLA	CHC-C1C	2.27	1.42	1.35
22	C	501	CLA	CHC-C1C	2.27	1.42	1.35
22	C	502	CLA	CMD-C2D	-2.26	1.46	1.51
22	C	503	CLA	CHC-C1C	2.26	1.42	1.35
22	A	402	CLA	C4D-C3D	2.26	1.48	1.42
31	D	401	PHO	C4C-C3C	2.26	1.49	1.45
22	C	505	CLA	CMD-C2D	-2.26	1.46	1.51
30	i	102	LMT	O2B-C2B	-2.26	1.37	1.43
30	i	102	LMT	O2'-C2'	-2.26	1.37	1.43
22	D	406	CLA	CHC-C1C	2.26	1.42	1.35
22	c	508	CLA	CMD-C2D	-2.26	1.46	1.51
30	b	626	LMT	O2'-C2'	-2.26	1.37	1.43
22	A	405	CLA	CHC-C1C	2.26	1.42	1.35
22	b	619	CLA	CHC-C1C	2.26	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	CHC-C1C	2.26	1.42	1.35
22	h	101	CLA	CMD-C2D	-2.26	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.25	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.25	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.26	1.46	1.51
22	C	507	CLA	CMD-C2D	-2.25	1.46	1.51
22	c	520	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	614	CLA	CMD-C2D	-2.25	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.25	1.46	1.51
31	D	401	PHO	CHD-C4C	2.25	1.36	1.35
22	b	610	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	615	CLA	CHC-C1C	2.25	1.42	1.35
22	b	606	CLA	CMD-C2D	-2.25	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	609	CLA	CMD-C2D	-2.24	1.46	1.51
22	C	511	CLA	CMD-C2D	-2.24	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.24	1.46	1.51
22	C	503	CLA	CMD-C2D	-2.25	1.46	1.51
22	c	507	CLA	CMD-C2D	-2.24	1.46	1.51
22	b	616	CLA	CMD-C2D	-2.24	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.24	1.46	1.51
22	c	501	CLA	CHC-C1C	2.24	1.42	1.35
22	c	503	CLA	CMD-C2D	-2.24	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.24	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.24	1.46	1.51
22	c	505	CLA	CMD-C2D	-2.24	1.46	1.51
22	B	601	CLA	CMD-C2D	-2.24	1.46	1.51
31	D	402	PHO	C4C-C3C	2.24	1.49	1.45
31	D	402	PHO	C1A-NA	2.24	1.42	1.37
22	a	405	CLA	CHC-C1C	2.23	1.42	1.35
22	b	618	CLA	CMD-C2D	-2.24	1.46	1.51
31	d	401	PHO	C4C-C3C	2.23	1.49	1.45
23	A	406	PL9	C53-C6	-2.23	1.46	1.50
22	c	511	CLA	CMD-C2D	-2.23	1.46	1.51
22	C	520	CLA	CMD-C2D	-2.23	1.46	1.51
31	d	401	PHO	C1A-NA	2.23	1.42	1.37
22	B	603	CLA	C1D-C2D	2.23	1.48	1.42
25	C	517	DGD	C1G-C2G	2.23	1.57	1.50
22	B	605	CLA	CMD-C2D	-2.22	1.46	1.51
25	c	517	DGD	C1G-C2G	2.22	1.56	1.50
22	c	510	CLA	CMD-C2D	-2.22	1.46	1.51
22	a	407	CLA	CMD-C2D	-2.22	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	406	CLA	CMD-C2D	-2.22	1.46	1.51
31	d	401	PHO	CMB-C2B	-2.21	1.46	1.51
22	c	506	CLA	CMD-C2D	-2.21	1.46	1.51
30	M	103	LMT	O2'-C2'	-2.21	1.37	1.43
22	B	612	CLA	CMD-C2D	-2.21	1.46	1.51
27	a	412	LMG	C7-C8	2.21	1.56	1.50
30	B	623	LMT	O2'-C2'	-2.21	1.37	1.43
22	c	501	CLA	CMD-C2D	-2.21	1.46	1.51
27	M	101	LMG	C7-C8	2.21	1.56	1.50
22	C	506	CLA	CMD-C2D	-2.21	1.46	1.51
22	b	613	CLA	CMD-C2D	-2.21	1.46	1.51
31	D	401	PHO	CMB-C2B	-2.21	1.46	1.51
22	C	510	CLA	CMD-C2D	-2.20	1.46	1.51
22	b	615	CLA	C1D-C2D	2.20	1.48	1.42
30	M	103	LMT	O3B-C3B	-2.20	1.37	1.43
22	c	504	CLA	C1D-C2D	2.20	1.48	1.42
30	b	627	LMT	O2'-C2'	-2.20	1.37	1.43
22	D	406	CLA	CMD-C2D	-2.20	1.46	1.51
25	c	515	DGD	O2G-C2G	-2.20	1.41	1.46
30	B	627	LMT	O2'-C2'	-2.20	1.37	1.43
31	D	401	PHO	C1A-NA	2.19	1.42	1.37
30	B	628	LMT	O3B-C3B	-2.19	1.37	1.43
30	M	102	LMT	O3B-C3B	-2.19	1.37	1.43
30	b	627	LMT	O3B-C3B	-2.19	1.37	1.43
30	M	102	LMT	O2'-C2'	-2.19	1.37	1.43
30	M	103	LMT	O2B-C2B	-2.19	1.37	1.43
22	B	610	CLA	CMD-C2D	-2.19	1.46	1.51
22	D	405	CLA	C1D-C2D	2.19	1.48	1.42
27	m	101	LMG	C7-C8	2.18	1.56	1.50
30	b	603	LMT	O2B-C2B	-2.18	1.37	1.43
30	D	411	LMT	O3B-C3B	-2.18	1.37	1.43
30	b	603	LMT	O3B-C3B	-2.18	1.37	1.43
22	c	512	CLA	CMD-C2D	-2.18	1.46	1.51
22	C	501	CLA	CMD-C2D	-2.18	1.46	1.51
31	d	402	PHO	C1A-NA	2.18	1.42	1.37
22	B	611	CLA	C1D-C2D	2.18	1.48	1.42
30	B	623	LMT	O3B-C3B	-2.18	1.37	1.43
30	M	102	LMT	O2B-C2B	-2.17	1.37	1.43
30	b	626	LMT	O2B-C2B	-2.17	1.37	1.43
31	d	402	PHO	CMB-C2B	-2.17	1.46	1.51
30	b	604	LMT	O3B-C3B	-2.17	1.37	1.43
30	B	624	LMT	O3B-C3B	-2.16	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	CMD-C2D	-2.16	1.46	1.51
30	I	102	LMT	O3B-C3B	-2.16	1.37	1.43
27	B	621	LMG	C4-C5	2.16	1.57	1.53
31	D	402	PHO	CMB-C2B	-2.16	1.46	1.51
27	A	410	LMG	C7-C8	2.16	1.56	1.50
30	D	411	LMT	O2'-C2'	-2.15	1.37	1.43
30	B	627	LMT	O2B-C2B	-2.15	1.37	1.43
22	C	512	CLA	CMD-C2D	-2.15	1.46	1.51
29	b	602	SQD	O2-C2	-2.15	1.37	1.43
30	d	411	LMT	O3B-C3B	-2.15	1.37	1.43
25	C	515	DGD	O1G-C1G	-2.15	1.40	1.45
22	C	504	CLA	C1D-C2D	2.15	1.48	1.42
30	b	603	LMT	O2'-C2'	-2.15	1.37	1.43
24	g	101	BCR	C33-C5	-2.15	1.47	1.51
25	c	516	DGD	O2G-C2G	-2.14	1.41	1.46
30	b	604	LMT	O2B-C2B	-2.14	1.37	1.43
30	d	411	LMT	O2'-C2'	-2.14	1.37	1.43
30	D	411	LMT	O2B-C2B	-2.14	1.37	1.43
30	b	626	LMT	O3B-C3B	-2.14	1.37	1.43
30	B	624	LMT	O2'-C2'	-2.14	1.37	1.43
30	i	102	LMT	O3B-C3B	-2.14	1.37	1.43
25	C	517	DGD	C3G-C2G	2.14	1.56	1.50
30	B	627	LMT	O3B-C3B	-2.13	1.37	1.43
30	B	628	LMT	O2'-C2'	-2.13	1.37	1.43
30	B	628	LMT	O2B-C2B	-2.13	1.37	1.43
26	a	411	LHG	O7-C5	-2.13	1.41	1.46
29	B	626	SQD	O2-C2	-2.13	1.37	1.43
30	B	623	LMT	O2B-C2B	-2.12	1.37	1.43
30	d	411	LMT	O2B-C2B	-2.12	1.37	1.43
25	C	516	DGD	O2G-C2G	-2.11	1.41	1.46
30	b	604	LMT	O2'-C2'	-2.10	1.37	1.43
22	B	610	CLA	CHC-C1C	2.09	1.42	1.35
27	D	412	LMG	O7-C8	-2.09	1.41	1.46
25	c	517	DGD	C3G-C2G	2.09	1.56	1.50
27	b	625	LMG	C4-C5	2.09	1.57	1.53
25	B	620	DGD	O2G-C2G	-2.09	1.41	1.46
22	b	614	CLA	CHC-C1C	2.09	1.42	1.35
27	d	412	LMG	O7-C8	-2.07	1.41	1.46
24	y	101	BCR	C33-C5	-2.07	1.47	1.51
22	b	619	CLA	CMC-C2C	-2.07	1.46	1.50
31	d	402	PHO	C4C-NC	2.06	1.42	1.38
29	A	413	SQD	O3-C3	-2.06	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	CMC-C2C	-2.05	1.46	1.50
30	b	627	LMT	O2B-C2B	-2.05	1.38	1.43
30	B	624	LMT	O2B-C2B	-2.05	1.38	1.43
31	D	402	PHO	CMC-C2C	-2.05	1.46	1.50
27	D	408	LMG	O7-C8	-2.04	1.41	1.46
25	d	410	DGD	C1D-C2D	2.04	1.58	1.52
25	b	601	DGD	C4D-C5D	2.04	1.57	1.53
29	a	401	SQD	O3-C3	-2.04	1.38	1.43
30	M	103	LMT	O4'-C4B	-2.04	1.38	1.43
25	a	410	DGD	O1G-C1G	-2.03	1.40	1.45
23	D	407	PL9	C53-C6	-2.03	1.46	1.50
29	f	103	SQD	O3-C3	-2.03	1.38	1.43
31	D	402	PHO	C4C-NC	2.03	1.42	1.38
34	v	201	HEM	C4C-NC	2.02	1.38	1.33
25	b	624	DGD	O2G-C2G	-2.02	1.41	1.46
29	A	412	SQD	O2-C2	-2.02	1.38	1.43
22	C	502	CLA	CMC-C2C	-2.02	1.46	1.50
22	c	501	CLA	C3B-C2B	-2.02	1.37	1.40
29	a	415	SQD	O2-C2	-2.01	1.38	1.43
31	d	402	PHO	CMC-C2C	-2.01	1.46	1.50
29	b	602	SQD	O3-C3	-2.01	1.38	1.43
22	C	501	CLA	C3B-C2B	-2.01	1.37	1.40
26	C	519	LHG	O7-C5	-2.01	1.41	1.46
29	f	103	SQD	O2-C2	-2.00	1.38	1.43
30	B	628	LMT	O4'-C4B	-2.00	1.38	1.43
29	F	103	SQD	O3-C3	-2.00	1.38	1.43
22	b	615	CLA	CMC-C2C	-2.00	1.46	1.50

All (1633) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	415	SQD	O6-C1-C2	7.00	117.13	108.15
29	A	412	SQD	O9-S-C6	6.90	112.92	106.83
29	A	412	SQD	O6-C1-C2	6.83	116.91	108.15
29	a	415	SQD	O9-S-C6	6.76	112.81	106.83
29	b	602	SQD	O6-C1-C2	6.70	116.74	108.15
29	B	626	SQD	O6-C1-C2	6.54	116.53	108.15
23	j	101	PL9	C7-C3-C2	-5.93	118.36	123.75
23	J	101	PL9	C7-C3-C2	-5.86	118.42	123.75
29	f	103	SQD	O7-S-C6	5.84	111.99	106.83
29	F	103	SQD	O7-S-C6	5.80	111.95	106.83
23	j	101	PL9	C7-C3-C4	5.72	121.50	116.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	C7-C3-C2	-5.71	118.55	123.75
29	a	401	SQD	O7-S-C6	5.63	111.81	106.83
23	J	101	PL9	C7-C3-C4	5.63	121.42	116.92
29	A	413	SQD	O7-S-C6	5.60	111.78	106.83
23	D	407	PL9	C7-C3-C2	-5.59	118.66	123.75
23	A	406	PL9	C7-C3-C2	-5.59	118.66	123.75
29	b	602	SQD	O9-S-C6	5.57	111.76	106.83
29	B	626	SQD	O9-S-C6	5.57	111.75	106.83
23	A	406	PL9	C7-C3-C4	5.47	121.30	116.92
23	a	408	PL9	C7-C3-C2	-5.46	118.78	123.75
29	b	602	SQD	O7-S-C6	5.36	111.56	106.83
23	d	407	PL9	C7-C3-C4	5.30	121.16	116.92
23	D	407	PL9	C7-C3-C4	5.25	121.12	116.92
31	D	401	PHO	C4D-CHA-C1A	-5.22	123.35	129.57
29	A	412	SQD	O7-S-C6	5.21	111.44	106.83
23	a	408	PL9	C7-C3-C4	5.20	121.08	116.92
29	B	622	SQD	O7-S-C6	5.20	111.42	106.83
31	d	401	PHO	C4D-CHA-C1A	-5.20	123.38	129.57
29	d	403	SQD	O6-C1-C2	5.19	114.81	108.15
29	B	622	SQD	O6-C1-C2	5.18	114.79	108.15
29	B	626	SQD	O7-S-C6	5.16	111.39	106.83
22	B	610	CLA	CMB-C2B-C1B	-5.16	120.54	128.46
29	d	403	SQD	O9-S-C6	5.12	111.36	106.83
29	a	415	SQD	O7-S-C6	5.11	111.35	106.83
22	b	614	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
31	D	402	PHO	C4D-CHA-C1A	-5.05	123.55	129.57
25	A	408	DGD	O3G-C3G-C2G	-4.95	99.22	110.99
29	B	622	SQD	O9-S-C6	4.93	111.19	106.83
31	d	402	PHO	C4D-CHA-C1A	-4.92	123.71	129.57
29	d	403	SQD	O7-S-C6	4.91	111.17	106.83
25	a	410	DGD	O3G-C3G-C2G	-4.85	99.46	110.99
25	A	408	DGD	CDB-CCB-CBB	-4.77	99.31	112.94
25	a	410	DGD	CDB-CCB-CBB	-4.76	99.32	112.94
29	f	103	SQD	O9-S-C6	4.74	111.02	106.83
29	a	401	SQD	O9-S-C6	4.70	110.98	106.83
29	A	413	SQD	O9-S-C6	4.67	110.96	106.83
29	F	103	SQD	O9-S-C6	4.59	110.89	106.83
25	B	620	DGD	CDB-CCB-CBB	-4.58	99.84	112.94
25	C	517	DGD	O3G-C3G-C2G	-4.56	100.13	110.99
25	b	624	DGD	CDB-CCB-CBB	-4.56	99.91	112.94
25	B	625	DGD	CDB-CCB-CBB	-4.54	99.96	112.94
29	F	103	SQD	O8-S-C6	4.52	111.27	105.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	DGD	CDB-CCB-CBB	-4.46	100.20	112.94
29	d	403	SQD	O5-C5-C4	4.41	117.94	109.73
25	c	517	DGD	O3G-C3G-C2G	-4.36	100.61	110.99
29	f	103	SQD	O8-S-C6	4.36	111.08	105.89
29	B	622	SQD	O5-C5-C4	4.33	117.79	109.73
29	d	403	SQD	O8-S-C6	4.26	110.96	105.89
22	c	507	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
29	F	103	SQD	O6-C1-C2	4.16	113.48	108.15
27	D	409	LMG	C1-C2-C3	-4.15	101.95	109.99
22	C	507	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
27	d	409	LMG	C1-C2-C3	-4.12	102.01	109.99
22	b	616	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
22	B	612	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
29	B	622	SQD	O8-S-C6	4.08	110.74	105.89
25	c	516	DGD	O5D-C6D-C5D	-3.95	102.11	108.96
29	f	103	SQD	O6-C1-C2	3.92	113.17	108.15
22	b	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
27	d	409	LMG	C40-C39-C38	-3.87	101.88	112.94
24	J	102	BCR	C11-C10-C9	-3.86	121.71	127.29
27	C	518	LMG	C40-C39-C38	-3.86	101.91	112.94
27	D	409	LMG	C40-C39-C38	-3.84	101.98	112.94
27	c	518	LMG	C40-C39-C38	-3.83	101.99	112.94
29	a	401	SQD	O8-S-C6	3.81	110.43	105.89
29	A	413	SQD	O5-C5-C4	3.81	116.81	109.73
29	B	626	SQD	O8-S-C6	3.81	110.42	105.89
22	B	607	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
25	C	516	DGD	O5D-C6D-C5D	-3.78	102.40	108.96
26	c	519	LHG	O4-P-O5	3.78	133.05	112.14
26	C	519	LHG	O4-P-O5	3.78	133.04	112.14
26	a	411	LHG	O4-P-O5	3.77	133.03	112.14
29	B	626	SQD	O5-C5-C4	3.76	116.72	109.73
29	a	415	SQD	O47-C7-C8	3.75	119.53	111.54
29	a	401	SQD	O5-C5-C4	3.75	116.70	109.73
26	A	409	LHG	O4-P-O5	3.75	132.89	112.14
22	c	510	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
26	A	409	LHG	O6-P-O3	-3.72	94.08	104.68
29	A	413	SQD	O8-S-C6	3.71	110.31	105.89
24	C	513	BCR	C2-C1-C6	3.71	116.29	110.37
25	B	625	DGD	O5D-C1E-C2E	3.70	112.90	108.15
22	b	615	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
29	b	602	SQD	O5-C5-C4	3.70	116.61	109.73
29	b	602	SQD	O8-S-C6	3.69	110.28	105.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	617	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
24	c	513	BCR	C2-C1-C6	3.69	116.25	110.37
22	B	602	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
24	j	102	BCR	C11-C10-C9	-3.68	121.97	127.29
22	c	512	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	C	505	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	B	613	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
29	F	103	SQD	O9-S-O7	-3.66	100.74	113.45
29	A	412	SQD	O47-C7-C8	3.66	119.33	111.54
22	B	611	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	a	411	LHG	O6-P-O3	-3.65	94.26	104.68
22	b	613	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
29	f	103	SQD	O9-S-O7	-3.64	100.78	113.45
22	C	506	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
22	c	503	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
22	A	405	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	C	510	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	B	609	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	c	506	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	C	516	DGD	O3G-C3G-C2G	-3.62	102.37	110.99
29	b	602	SQD	O47-C7-C8	3.62	119.24	111.54
25	c	516	DGD	O3G-C3G-C2G	-3.62	102.39	110.99
29	B	626	SQD	O47-C7-C8	3.61	119.24	111.54
24	J	102	BCR	C2-C1-C6	3.61	116.13	110.37
29	A	412	SQD	O9-S-O7	-3.61	100.90	113.45
24	j	102	BCR	C2-C1-C6	3.61	116.12	110.37
29	a	415	SQD	O9-S-O7	-3.60	100.93	113.45
22	a	404	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
30	I	102	LMT	O1'-C1'-C2'	3.59	112.76	108.15
22	C	512	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
29	a	415	SQD	O5-C5-C4	3.59	116.41	109.73
29	d	403	SQD	O9-S-O7	-3.59	100.97	113.45
22	c	511	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	a	407	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	C	502	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
29	B	622	SQD	O9-S-O7	-3.56	101.06	113.45
29	a	401	SQD	O9-S-O7	-3.56	101.07	113.45
29	B	626	SQD	O9-S-O7	-3.56	101.08	113.45
22	A	402	CLA	CMB-C2B-C1B	-3.56	122.99	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	410	DGD	O6D-C1D-O3G	-3.56	101.46	109.93
22	c	502	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
29	a	415	SQD	O8-S-C6	3.55	110.12	105.89
29	f	103	SQD	O5-C5-C4	3.55	116.33	109.73
29	b	602	SQD	O9-S-O7	-3.55	101.12	113.45
29	A	413	SQD	O9-S-O7	-3.54	101.13	113.45
30	i	102	LMT	O1'-C1'-C2'	3.54	112.68	108.15
25	D	410	DGD	O6D-C1D-O3G	-3.53	101.51	109.93
22	D	405	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	b	601	DGD	O5D-C1E-C2E	3.53	112.67	108.15
29	F	103	SQD	O5-C5-C4	3.51	116.27	109.73
22	D	406	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	B	614	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
29	A	412	SQD	O8-S-C6	3.50	110.06	105.89
22	C	509	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
29	A	412	SQD	O5-C5-C4	3.49	116.23	109.73
22	b	605	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
27	C	521	LMG	C42-C41-C40	-3.48	102.99	112.94
29	d	403	SQD	O47-C7-C8	3.48	118.96	111.54
29	B	622	SQD	O47-C7-C8	3.48	118.96	111.54
22	d	405	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
22	c	520	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	a	405	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	c	509	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
27	c	522	LMG	C42-C41-C40	-3.46	103.06	112.94
22	B	601	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
25	B	620	DGD	O3G-C3G-C2G	-3.45	102.78	110.99
22	B	605	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
22	C	520	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
29	F	103	SQD	O47-C7-C8	3.44	118.88	111.54
22	b	618	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	d	406	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	A	403	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	b	607	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	C	515	DGD	O3G-C3G-C2G	-3.40	102.89	110.99
22	C	508	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
25	c	515	DGD	O3G-C3G-C2G	-3.39	102.93	110.99
22	A	404	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
22	b	608	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.38	123.27	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	401	SQD	C44-O6-C1	3.37	120.57	113.80
25	b	624	DGD	O3G-C3G-C2G	-3.37	102.98	110.99
22	H	101	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
29	f	103	SQD	O47-C7-C8	3.36	118.71	111.54
29	A	413	SQD	O47-C7-C8	3.36	118.70	111.54
22	b	609	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	h	101	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	b	610	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	B	603	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
22	b	619	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
22	a	406	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
26	c	519	LHG	O6-P-O3	-3.27	95.36	104.68
25	d	410	DGD	O3G-C3G-C2G	-3.24	103.28	110.99
24	A	407	BCR	C2-C1-C6	3.23	115.53	110.37
24	b	622	BCR	C24-C23-C22	-3.23	121.38	126.22
24	j	102	BCR	C24-C23-C22	-3.23	121.38	126.22
29	a	401	SQD	O47-C7-C8	3.23	118.42	111.54
26	C	519	LHG	O6-P-O3	-3.21	95.52	104.68
24	J	102	BCR	C3-C4-C5	-3.21	108.53	113.81
22	B	606	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
24	J	102	BCR	C24-C23-C22	-3.19	121.44	126.22
34	f	101	HEM	CBD-CAD-C3D	-3.19	107.60	114.51
22	b	612	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
30	B	628	LMT	C1'-O5'-C5'	-3.18	107.59	113.73
22	B	608	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
25	D	410	DGD	O3G-C3G-C2G	-3.17	103.44	110.99
22	B	603	CLA	CBD-CHA-C1A	3.17	132.92	128.77
29	B	626	SQD	C3-C4-C5	3.16	115.85	110.17
24	j	102	BCR	C3-C4-C5	-3.15	108.63	113.81
22	B	612	CLA	CMB-C2B-C3B	3.15	131.09	125.16
26	c	519	LHG	C18-C17-C16	-3.14	103.97	112.94
22	b	616	CLA	CMB-C2B-C3B	3.13	131.07	125.16
29	b	602	SQD	C3-C4-C5	3.12	115.78	110.17
24	J	102	BCR	C27-C26-C25	3.12	126.98	122.86
24	a	409	BCR	C2-C1-C6	3.12	115.34	110.37
23	A	406	PL9	C22-C23-C24	-3.12	121.07	127.81
22	B	605	CLA	O2D-CGD-O1D	-3.11	117.54	123.79
25	b	624	DGD	O6D-C1D-O3G	-3.10	102.54	109.93
30	b	604	LMT	C1'-O5'-C5'	-3.10	107.73	113.73
26	C	519	LHG	C18-C17-C16	-3.10	104.09	112.94
22	c	507	CLA	CMB-C2B-C3B	3.09	130.99	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	C40-C39-C41	3.09	120.08	115.39
26	A	409	LHG	C9-C10-C11	-3.09	101.31	113.73
23	a	408	PL9	C22-C23-C24	-3.09	121.13	127.81
25	B	620	DGD	O6D-C1D-O3G	-3.09	102.58	109.93
25	c	517	DGD	C1D-C2D-C3D	-3.08	104.01	109.99
22	b	609	CLA	O2D-CGD-O1D	-3.08	117.60	123.79
22	B	603	CLA	O2D-CGD-O1D	-3.08	117.60	123.79
24	B	618	BCR	C2-C1-C6	3.08	115.28	110.37
22	b	607	CLA	CBD-CHA-C1A	3.07	132.78	128.77
25	c	516	DGD	O6D-C1D-O3G	-3.07	102.62	109.93
22	B	613	CLA	O2D-CGD-O1D	-3.06	117.64	123.79
24	j	102	BCR	C7-C8-C9	-3.06	121.63	126.22
29	A	413	SQD	C44-O6-C1	3.06	119.94	113.80
22	C	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
24	j	102	BCR	C27-C26-C25	3.04	126.88	122.86
26	a	411	LHG	C9-C10-C11	-3.04	101.48	113.73
22	c	504	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
24	J	102	BCR	C7-C8-C9	-3.04	121.67	126.22
25	B	625	DGD	C1D-C2D-C3D	-3.03	104.12	109.99
22	c	503	CLA	O2D-CGD-O1D	-3.03	117.70	123.79
24	b	622	BCR	C2-C1-C6	3.03	115.20	110.37
23	D	407	PL9	C22-C23-C24	-3.02	121.27	127.81
27	d	412	LMG	C38-C39-C40	-3.02	101.57	113.73
25	C	517	DGD	C1D-C2D-C3D	-3.02	104.14	109.99
23	D	407	PL9	C40-C39-C41	3.02	119.97	115.39
25	A	408	DGD	O6D-C1D-O3G	-3.01	102.75	109.93
22	b	617	CLA	O2D-CGD-O1D	-3.01	117.74	123.79
22	b	606	CLA	O2D-CGD-O1D	-3.01	117.75	123.79
27	D	412	LMG	C38-C39-C40	-3.00	101.64	113.73
25	C	516	DGD	O6D-C1D-O3G	-3.00	102.79	109.93
23	j	101	PL9	C27-C28-C29	-2.99	121.42	128.69
22	b	616	CLA	C4B-C3B-CAB	-2.98	121.14	127.18
22	c	507	CLA	O2D-CGD-O1D	-2.98	117.81	123.79
24	B	617	BCR	C33-C5-C6	-2.98	121.14	124.50
29	d	403	SQD	C3-C4-C5	2.97	115.51	110.17
22	b	607	CLA	O2D-CGD-O1D	-2.97	117.83	123.79
24	b	621	BCR	C33-C5-C6	-2.97	121.15	124.50
25	C	517	DGD	O5D-C6D-C5D	-2.96	103.82	108.96
22	C	505	CLA	O2D-CGD-O1D	-2.96	117.84	123.79
23	J	101	PL9	C27-C28-C29	-2.96	121.48	128.69
25	b	601	DGD	C1D-C2D-C3D	-2.96	104.26	109.99
22	b	611	CLA	CMB-C2B-C3B	2.96	130.73	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	517	DGD	O5D-C6D-C5D	-2.96	103.83	108.96
22	C	503	CLA	O2D-CGD-O1D	-2.96	117.85	123.79
22	c	504	CLA	O2D-CGD-O1D	-2.95	117.87	123.79
24	y	101	BCR	C27-C26-C25	2.95	126.75	122.86
22	B	608	CLA	O2D-CGD-O1D	-2.95	117.87	123.79
22	b	610	CLA	O2D-CGD-O1D	-2.95	117.87	123.79
22	C	502	CLA	O2D-CGD-O1D	-2.95	117.88	123.79
22	C	507	CLA	CMB-C2B-C3B	2.94	130.70	125.16
23	J	101	PL9	C22-C23-C24	-2.94	121.45	127.81
22	B	606	CLA	O2D-CGD-O1D	-2.93	117.90	123.79
30	B	624	LMT	C3'-C4'-C5'	-2.93	104.31	110.86
22	C	504	CLA	O2D-CGD-O1D	-2.93	117.91	123.79
22	B	612	CLA	C4B-C3B-CAB	-2.93	121.25	127.18
22	b	605	CLA	O2D-CGD-O1D	-2.92	117.92	123.79
22	C	511	CLA	C3D-C4D-CHA	2.92	112.85	108.16
23	d	407	PL9	C22-C23-C24	-2.92	121.49	127.81
27	d	408	LMG	C38-C39-C40	-2.92	102.00	113.73
22	c	501	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
22	B	610	CLA	CMB-C2B-C3B	2.91	130.65	125.16
22	B	602	CLA	CMB-C2B-C3B	2.91	130.65	125.16
27	d	408	LMG	O6-C1-O1	-2.91	103.00	109.93
27	e	101	LMG	C36-C37-C38	-2.91	102.04	113.73
24	g	101	BCR	C27-C26-C25	2.90	126.69	122.86
29	A	412	SQD	C3-C4-C5	2.90	115.38	110.17
22	b	606	CLA	CMB-C2B-C3B	2.90	130.63	125.16
23	j	101	PL9	C22-C23-C24	-2.90	121.54	127.81
24	F	102	BCR	C33-C5-C6	-2.90	121.22	124.50
24	c	521	BCR	C2-C1-C6	2.90	114.99	110.37
27	E	101	LMG	C36-C37-C38	-2.90	102.07	113.73
27	D	408	LMG	C38-C39-C40	-2.90	102.08	113.73
24	B	617	BCR	C15-C16-C17	-2.90	117.07	123.45
22	C	506	CLA	C3D-C4D-CHA	2.90	112.81	108.16
25	c	515	DGD	O6D-C1D-O3G	-2.89	103.04	109.93
24	H	102	BCR	C33-C5-C6	-2.89	121.23	124.50
34	F	101	HEM	CBD-CAD-C3D	-2.88	108.25	114.51
25	a	410	DGD	O6D-C1D-O3G	-2.88	103.06	109.93
22	b	611	CLA	O2D-CGD-O1D	-2.88	118.00	123.79
22	c	506	CLA	C3D-C4D-CHA	2.88	112.78	108.16
22	B	603	CLA	C3D-C4D-CHA	2.88	112.78	108.16
22	B	607	CLA	CMB-C2B-C3B	2.88	130.59	125.16
22	c	511	CLA	C3D-C4D-CHA	2.88	112.78	108.16
22	b	608	CLA	O2D-CGD-O1D	-2.87	118.02	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	CMB-C2B-C3B	2.87	130.57	125.16
25	b	601	DGD	C3G-C2G-C1G	-2.87	105.27	111.86
22	c	511	CLA	CBD-CHA-C1A	2.87	132.51	128.77
22	c	506	CLA	CMB-C2B-C3B	2.87	130.56	125.16
24	x	101	BCR	C33-C5-C6	-2.86	121.27	124.50
22	C	510	CLA	C3D-C4D-CHA	2.86	112.75	108.16
22	B	613	CLA	CMB-C2B-C3B	2.86	130.55	125.16
24	f	102	BCR	C33-C5-C6	-2.86	121.27	124.50
22	B	602	CLA	O2D-CGD-O1D	-2.86	118.05	123.79
22	c	510	CLA	C3D-C4D-CHA	2.86	112.74	108.16
29	a	415	SQD	C3-C4-C5	2.86	115.30	110.17
25	b	601	DGD	O3G-C3G-C2G	-2.85	104.20	110.99
22	c	507	CLA	C3D-C4D-CHA	2.86	112.74	108.16
22	B	604	CLA	O2D-CGD-O1D	-2.85	118.06	123.79
29	B	622	SQD	C3-C4-C5	2.85	115.29	110.17
22	b	608	CLA	CHD-C4C-NC	2.85	126.27	124.28
22	B	611	CLA	C2D-C3D-CAD	2.85	146.55	134.94
22	b	612	CLA	O2D-CGD-O1D	-2.85	118.08	123.79
26	c	519	LHG	O3-C3-C2	-2.84	99.36	108.54
30	b	627	LMT	C3'-C4'-C5'	-2.84	104.50	110.86
22	a	406	CLA	O2D-CGD-O1D	-2.84	118.08	123.79
24	J	102	BCR	C35-C13-C14	-2.84	118.87	122.92
22	c	505	CLA	O2D-CGD-O1D	-2.84	118.08	123.79
22	b	615	CLA	C2D-C3D-CAD	2.84	146.53	134.94
22	C	507	CLA	O2D-CGD-O1D	-2.84	118.08	123.79
25	C	515	DGD	O6D-C1D-O3G	-2.84	103.16	109.93
22	b	607	CLA	C3D-C4D-CHA	2.84	112.72	108.16
22	C	506	CLA	O2D-CGD-O1D	-2.84	118.09	123.79
22	D	405	CLA	C3D-C4D-CHA	2.84	112.71	108.16
22	c	505	CLA	C3D-C4D-CHA	2.84	112.71	108.16
26	A	409	LHG	O8-C23-C24	2.84	120.58	111.90
22	c	510	CLA	CMB-C2B-C3B	2.84	130.50	125.16
22	a	404	CLA	O2D-CGD-O1D	-2.83	118.10	123.79
24	b	621	BCR	C15-C16-C17	-2.83	117.21	123.45
29	A	413	SQD	C5-C6-S	-2.83	110.45	114.40
22	B	602	CLA	C3D-C4D-CHA	2.82	112.69	108.16
22	c	506	CLA	CBD-CHA-C1A	2.82	132.46	128.77
22	B	612	CLA	C3D-C4D-CHA	2.82	112.68	108.16
22	B	601	CLA	C3D-C4D-CHA	2.82	112.68	108.16
24	b	623	BCR	C2-C1-C6	2.82	114.86	110.37
25	B	625	DGD	C3G-C2G-C1G	-2.82	105.39	111.86
22	C	501	CLA	O2D-CGD-O1D	-2.82	118.14	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	520	CLA	O2D-CGD-O1D	-2.82	118.14	123.79
24	B	619	BCR	C2-C1-C6	2.82	114.86	110.37
22	C	505	CLA	CMB-C2B-C3B	2.82	130.47	125.16
22	B	607	CLA	O2D-CGD-O1D	-2.82	118.13	123.79
24	B	619	BCR	C3-C4-C5	-2.82	109.18	113.81
22	c	511	CLA	O2D-CGD-O1D	-2.82	118.14	123.79
22	C	501	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
22	b	617	CLA	CMB-C2B-C3B	2.81	130.46	125.16
22	C	510	CLA	O2D-CGD-O1D	-2.81	118.15	123.79
22	b	616	CLA	O2D-CGD-O1D	-2.81	118.16	123.79
22	c	501	CLA	O2D-CGD-O1D	-2.81	118.15	123.79
22	d	406	CLA	C2D-C3D-CAD	2.81	146.38	134.94
22	d	406	CLA	O2D-CGD-O1D	-2.81	118.15	123.79
22	c	506	CLA	O2D-CGD-O1D	-2.81	118.16	123.79
22	b	618	CLA	C3D-C4D-CHA	2.81	112.66	108.16
22	A	402	CLA	O2D-CGD-O1D	-2.80	118.16	123.79
27	m	101	LMG	C22-C21-C20	-2.80	104.94	112.94
22	A	403	CLA	O2D-CGD-O1D	-2.80	118.17	123.79
22	c	512	CLA	O2D-CGD-O1D	-2.80	118.16	123.79
24	b	623	BCR	C3-C4-C5	-2.80	109.21	113.81
22	c	510	CLA	CBD-CHA-C1A	2.80	132.43	128.77
22	c	510	CLA	O2D-CGD-O1D	-2.80	118.17	123.79
25	c	517	DGD	CDB-CCB-CBB	-2.80	99.70	114.56
22	b	614	CLA	CMB-C2B-C3B	2.80	130.44	125.16
22	a	407	CLA	CMB-C2B-C3B	2.80	130.44	125.16
25	C	517	DGD	CDB-CCB-CBB	-2.80	99.70	114.56
26	a	411	LHG	O8-C23-C24	2.80	120.46	111.90
22	b	615	CLA	CMB-C2B-C3B	2.79	130.43	125.16
22	D	406	CLA	C2D-C3D-CAD	2.79	146.33	134.94
22	C	505	CLA	C3D-C4D-CHA	2.80	112.64	108.16
22	b	613	CLA	O2D-CGD-O1D	-2.79	118.18	123.79
22	C	507	CLA	C3D-C4D-CHA	2.79	112.64	108.16
27	d	412	LMG	C22-C21-C20	-2.79	104.96	112.94
22	C	520	CLA	C3D-C4D-CHA	2.79	112.64	108.16
22	b	609	CLA	CHD-C4C-NC	2.79	126.23	124.28
22	a	404	CLA	C2D-C3D-CAD	2.79	146.32	134.94
25	A	408	DGD	O5D-C6D-C5D	-2.79	104.12	108.96
27	A	414	LMG	C22-C21-C20	-2.79	104.97	112.94
22	C	510	CLA	CBD-CHA-C1A	2.79	132.41	128.77
22	B	604	CLA	CHD-C4C-NC	2.79	126.23	124.28
24	B	617	BCR	C28-C27-C26	-2.79	109.23	113.81
22	B	601	CLA	O2D-CGD-O1D	-2.79	118.20	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C3D-C4D-CHA	2.78	112.63	108.16
22	b	605	CLA	C2D-C3D-CAD	2.78	146.29	134.94
22	H	101	CLA	O2D-CGD-O1D	-2.78	118.20	123.79
22	B	615	CLA	C2D-C3D-CAD	2.78	146.29	134.94
22	b	619	CLA	C2D-C3D-CAD	2.78	146.30	134.94
22	b	609	CLA	CBD-CHA-C1A	2.78	132.41	128.77
22	c	512	CLA	CMB-C2B-C3B	2.78	130.41	125.16
25	B	625	DGD	O3G-C3G-C2G	-2.78	104.37	110.99
24	f	102	BCR	C29-C30-C25	2.78	114.80	110.37
22	b	612	CLA	C3D-C4D-CHA	2.78	112.62	108.16
22	c	509	CLA	CHD-C4C-NC	2.78	126.22	124.28
27	a	402	LMG	C22-C21-C20	-2.78	105.00	112.94
27	D	412	LMG	C22-C21-C20	-2.78	105.00	112.94
22	b	613	CLA	CMB-C2B-C3B	2.78	130.39	125.16
22	b	613	CLA	C2D-C3D-CAD	2.78	146.26	134.94
22	C	510	CLA	CMB-C2B-C3B	2.77	130.39	125.16
22	B	605	CLA	C3D-C4D-CHA	2.77	112.61	108.16
27	D	408	LMG	O6-C1-O1	-2.77	103.33	109.93
22	c	502	CLA	C3D-C4D-CHA	2.77	112.61	108.16
22	b	614	CLA	C3D-C4D-CHA	2.77	112.61	108.16
22	c	505	CLA	CMB-C2B-C3B	2.77	130.38	125.16
22	B	609	CLA	O2D-CGD-O1D	-2.77	118.23	123.79
22	d	405	CLA	C2D-C3D-CAD	2.77	146.23	134.94
22	b	613	CLA	C3D-C4D-CHA	2.77	112.60	108.16
22	B	610	CLA	C2D-C3D-CAD	2.77	146.23	134.94
22	b	605	CLA	C3D-C4D-CHA	2.77	112.60	108.16
22	b	616	CLA	C3D-C4D-CHA	2.76	112.60	108.16
27	E	101	LMG	C22-C21-C20	-2.77	105.04	112.94
22	B	612	CLA	O2D-CGD-O1D	-2.77	118.24	123.79
22	b	611	CLA	C2D-C3D-CAD	2.77	146.22	134.94
22	A	403	CLA	CHB-C4A-NA	2.77	128.24	124.38
22	B	608	CLA	C3D-C4D-CHA	2.77	112.60	108.16
22	B	609	CLA	C2D-C3D-CAD	2.76	146.21	134.94
22	b	617	CLA	C2D-C3D-CAD	2.76	146.21	134.94
24	b	621	BCR	C28-C27-C26	-2.76	109.27	113.81
22	c	520	CLA	C2D-C3D-CAD	2.76	146.20	134.94
22	B	601	CLA	C2D-C3D-CAD	2.76	146.19	134.94
22	A	402	CLA	C2D-C3D-CAD	2.76	146.19	134.94
22	b	609	CLA	C3D-C4D-CHA	2.76	112.59	108.16
22	a	406	CLA	C2D-C3D-CAD	2.76	146.19	134.94
22	a	407	CLA	C2D-C3D-CAD	2.76	146.19	134.94
22	B	606	CLA	C2D-C3D-CAD	2.76	146.19	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	CLA	O2D-CGD-O1D	-2.76	118.25	123.79
22	b	610	CLA	C2D-C3D-CAD	2.76	146.18	134.94
22	B	603	CLA	CHB-C4A-NA	2.76	128.23	124.38
26	a	411	LHG	O3-C3-C2	-2.76	99.63	108.54
22	b	616	CLA	CBD-CHA-C1A	2.76	132.37	128.77
22	c	502	CLA	O2D-CGD-O1D	-2.76	118.26	123.79
22	b	614	CLA	C2D-C3D-CAD	2.76	146.18	134.94
27	M	101	LMG	C22-C21-C20	-2.76	105.06	112.94
22	C	502	CLA	C3D-C4D-CHA	2.75	112.58	108.16
22	C	505	CLA	C2D-C3D-CAD	2.75	146.17	134.94
22	B	615	CLA	C3D-C4D-CHA	2.75	112.58	108.16
22	c	507	CLA	C2D-C3D-CAD	2.75	146.17	134.94
22	b	615	CLA	C3D-C4D-CHA	2.75	112.57	108.16
22	A	405	CLA	CMB-C2B-C3B	2.75	130.34	125.16
22	A	405	CLA	C2D-C3D-CAD	2.75	146.16	134.94
22	B	613	CLA	C2D-C3D-CAD	2.75	146.15	134.94
22	B	614	CLA	O2D-CGD-O1D	-2.75	118.27	123.79
22	C	509	CLA	C2D-C3D-CAD	2.75	146.15	134.94
22	D	405	CLA	C2D-C3D-CAD	2.75	146.15	134.94
22	A	404	CLA	C2D-C3D-CAD	2.75	146.15	134.94
22	c	505	CLA	C2D-C3D-CAD	2.75	146.14	134.94
22	B	614	CLA	C2D-C3D-CAD	2.75	146.14	134.94
25	c	516	DGD	CDB-CCB-CBB	-2.75	99.97	114.56
22	C	502	CLA	C2D-C3D-CAD	2.75	146.14	134.94
22	C	503	CLA	CMB-C2B-C3B	2.75	130.34	125.16
22	B	611	CLA	CMB-C2B-C3B	2.75	130.34	125.16
22	a	407	CLA	C3D-C4D-CHA	2.75	112.57	108.16
27	M	101	LMG	C1-C2-C3	-2.75	104.67	109.99
22	C	504	CLA	C3D-C4D-CHA	2.74	112.56	108.16
27	e	101	LMG	C22-C21-C20	-2.74	105.10	112.94
22	B	602	CLA	C4B-C3B-CAB	-2.74	121.62	127.18
22	c	511	CLA	C2D-C3D-CAD	2.74	146.13	134.94
22	C	520	CLA	O2D-CGD-O1D	-2.74	118.28	123.79
22	h	101	CLA	C3D-C4D-CHA	2.74	112.56	108.16
22	c	501	CLA	C2D-C3D-CAD	2.74	146.12	134.94
22	c	502	CLA	C2D-C3D-CAD	2.74	146.12	134.94
22	B	607	CLA	C2D-C3D-CAD	2.74	146.12	134.94
24	K	102	BCR	C2-C1-C6	2.74	114.74	110.37
22	c	503	CLA	C3D-C4D-CHA	2.74	112.56	108.16
26	C	519	LHG	O3-C3-C2	-2.74	99.70	108.54
24	j	102	BCR	C35-C13-C14	-2.74	119.02	122.92
22	c	509	CLA	C2D-C3D-CAD	2.74	146.11	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	C2D-C3D-CAD	2.74	146.11	134.94
22	B	604	CLA	C2D-C3D-CAD	2.74	146.10	134.94
22	C	501	CLA	C2D-C3D-CAD	2.74	146.10	134.94
22	b	606	CLA	C2D-C3D-CAD	2.74	146.10	134.94
22	B	614	CLA	C3D-C4D-CHA	2.74	112.55	108.16
22	b	617	CLA	C3D-C4D-CHA	2.74	112.55	108.16
22	B	608	CLA	C2D-C3D-CAD	2.74	146.10	134.94
22	b	612	CLA	C2D-C3D-CAD	2.74	146.10	134.94
22	D	406	CLA	O2D-CGD-O1D	-2.73	118.30	123.79
22	C	511	CLA	C2D-C3D-CAD	2.73	146.09	134.94
22	c	512	CLA	C2D-C3D-CAD	2.73	146.09	134.94
22	C	503	CLA	C3D-C4D-CHA	2.73	112.54	108.16
22	a	405	CLA	CHB-C4A-NA	2.73	128.19	124.38
22	B	611	CLA	C3D-C4D-CHA	2.73	112.54	108.16
22	C	512	CLA	CMB-C2B-C3B	2.73	130.30	125.16
22	B	610	CLA	C3D-C4D-CHA	2.73	112.53	108.16
22	b	607	CLA	CHB-C4A-NA	2.73	128.18	124.38
22	C	508	CLA	C2D-C3D-CAD	2.73	146.05	134.94
22	h	101	CLA	C2D-C3D-CAD	2.73	146.05	134.94
22	b	618	CLA	C2D-C3D-CAD	2.73	146.06	134.94
22	d	405	CLA	O2D-CGD-O1D	-2.72	118.32	123.79
22	b	619	CLA	C3D-C4D-CHA	2.72	112.53	108.16
22	C	512	CLA	C3D-C4D-CHA	2.72	112.53	108.16
24	B	618	BCR	C24-C23-C22	-2.72	122.14	126.22
25	C	516	DGD	CDB-CCB-CBB	-2.72	100.10	114.56
22	b	608	CLA	C2D-C3D-CAD	2.72	146.03	134.94
24	b	621	BCR	C15-C14-C13	-2.72	123.36	127.29
22	C	504	CLA	C2D-C3D-CAD	2.72	146.03	134.94
22	B	602	CLA	C2D-C3D-CAD	2.72	146.03	134.94
22	c	504	CLA	CBD-CHA-C1A	2.72	132.32	128.77
22	c	504	CLA	C2D-C3D-CAD	2.72	146.01	134.94
22	C	509	CLA	O2D-CGD-O1D	-2.72	118.34	123.79
22	A	404	CLA	O2D-CGD-O1D	-2.72	118.34	123.79
22	C	501	CLA	C3D-C4D-CHA	2.71	112.52	108.16
22	c	501	CLA	C3D-C4D-CHA	2.71	112.51	108.16
22	A	405	CLA	C3D-C4D-CHA	2.71	112.51	108.16
22	A	402	CLA	CHD-C4C-NC	2.71	126.18	124.28
22	H	101	CLA	C2D-C3D-CAD	2.71	146.01	134.94
22	A	403	CLA	C2D-C3D-CAD	2.71	146.01	134.94
22	c	511	CLA	CMB-C2B-C3B	2.71	130.27	125.16
31	D	402	PHO	O2D-CGD-O1D	-2.71	118.34	123.79
22	c	508	CLA	C2D-C3D-CAD	2.71	146.00	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	503	CLA	CMB-C2B-C3B	2.71	130.27	125.16
23	D	407	PL9	C27-C28-C29	-2.71	121.95	127.81
22	B	609	CLA	CMB-C2B-C3B	2.71	130.27	125.16
22	C	511	CLA	CBD-CHA-C1A	2.71	132.31	128.77
22	d	405	CLA	C3D-C4D-CHA	2.71	112.51	108.16
22	B	613	CLA	C3D-C4D-CHA	2.71	112.50	108.16
22	H	101	CLA	C3D-C4D-CHA	2.71	112.51	108.16
22	C	503	CLA	C2D-C3D-CAD	2.71	145.98	134.94
22	D	405	CLA	CMB-C2B-C3B	2.71	130.26	125.16
22	A	404	CLA	C3D-C4D-CHA	2.71	112.50	108.16
22	b	608	CLA	CHB-C4A-NA	2.70	128.15	124.38
22	c	503	CLA	CBD-CHA-C1A	2.70	132.30	128.77
22	C	506	CLA	CBD-CHA-C1A	2.70	132.31	128.77
22	D	406	CLA	CMB-C2B-C3B	2.70	130.24	125.16
22	c	504	CLA	C3D-C4D-CHA	2.70	112.49	108.16
22	c	520	CLA	C3D-C4D-CHA	2.70	112.48	108.16
22	C	512	CLA	C2D-C3D-CAD	2.70	145.94	134.94
22	C	520	CLA	C2D-C3D-CAD	2.69	145.93	134.94
22	B	609	CLA	C3D-C4D-CHA	2.69	112.48	108.16
22	C	504	CLA	CBD-CHA-C1A	2.69	132.29	128.77
22	C	506	CLA	CHB-C4A-NA	2.69	128.14	124.38
24	y	101	BCR	C7-C8-C9	-2.69	122.19	126.22
22	C	510	CLA	CHB-C4A-NA	2.69	128.13	124.38
24	j	102	BCR	C15-C14-C13	-2.69	123.40	127.29
22	B	605	CLA	CHD-C4C-NC	2.69	126.16	124.28
22	B	603	CLA	C1-C2-C3	-2.69	121.56	126.23
22	C	505	CLA	CHB-C4A-NA	2.69	128.13	124.38
22	c	502	CLA	CMB-C2B-C3B	2.69	130.23	125.16
22	b	607	CLA	C1-C2-C3	-2.69	121.56	126.23
22	b	616	CLA	C2D-C3D-CAD	2.69	145.90	134.94
22	C	502	CLA	CMB-C2B-C3B	2.69	130.23	125.16
22	b	614	CLA	O2D-CGD-O1D	-2.69	118.39	123.79
22	h	101	CLA	O2D-CGD-O1D	-2.69	118.39	123.79
22	B	606	CLA	C3D-C4D-CHA	2.69	112.47	108.16
22	B	602	CLA	CBD-CHA-C1A	2.69	132.28	128.77
22	C	508	CLA	C3D-C4D-CHA	2.69	112.47	108.16
22	b	606	CLA	C4B-C3B-CAB	-2.68	121.74	127.18
22	B	605	CLA	C2D-C3D-CAD	2.69	145.89	134.94
22	a	405	CLA	C2D-C3D-CAD	2.69	145.89	134.94
25	D	410	DGD	CDB-CCB-CBB	-2.68	100.31	114.56
22	c	509	CLA	C3D-C4D-CHA	2.68	112.47	108.16
22	C	520	CLA	CHB-C4A-NA	2.68	128.13	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	C7-C8-C9	-2.68	122.22	126.76
22	B	612	CLA	C2D-C3D-CAD	2.68	145.87	134.94
22	b	611	CLA	C3D-C4D-CHA	2.68	112.46	108.16
22	C	511	CLA	CMB-C2B-C3B	2.68	130.21	125.16
27	B	621	LMG	C1-C2-C3	-2.68	104.79	109.99
22	c	506	CLA	CHB-C4A-NA	2.68	128.12	124.38
24	c	514	BCR	C28-C27-C26	-2.68	109.41	113.81
24	F	102	BCR	C29-C30-C25	2.68	114.64	110.37
22	C	504	CLA	CHB-C4A-NA	2.68	128.12	124.38
27	A	410	LMG	C40-C41-C42	-2.68	102.96	113.73
22	b	609	CLA	CHB-C4A-NA	2.68	128.12	124.38
22	C	506	CLA	C2D-C3D-CAD	2.68	145.86	134.94
24	B	618	BCR	C29-C30-C25	2.68	114.64	110.37
22	c	506	CLA	C4B-C3B-CAB	-2.68	121.75	127.18
22	c	512	CLA	C3D-C4D-CHA	2.68	112.45	108.16
22	C	510	CLA	C2D-C3D-CAD	2.67	145.84	134.94
22	d	406	CLA	C3D-C4D-CHA	2.67	112.45	108.16
22	b	609	CLA	C2D-C3D-CAD	2.67	145.84	134.94
22	C	512	CLA	O2D-CGD-O1D	-2.67	118.42	123.79
22	c	508	CLA	C3D-C4D-CHA	2.67	112.45	108.16
22	C	506	CLA	C4B-C3B-CAB	-2.67	121.77	127.18
22	c	508	CLA	CBD-CHA-C1A	2.67	132.26	128.77
22	a	406	CLA	C3D-C4D-CHA	2.67	112.44	108.16
23	J	101	PL9	C7-C8-C9	-2.67	122.25	126.76
25	d	410	DGD	CDB-CCB-CBB	-2.67	100.39	114.56
22	b	607	CLA	C4B-C3B-CAB	-2.67	121.77	127.18
24	c	513	BCR	C11-C10-C9	-2.66	123.44	127.29
23	a	408	PL9	C27-C28-C29	-2.67	122.05	127.81
29	d	403	SQD	C44-O6-C1	2.67	119.15	113.80
22	b	617	CLA	C4B-C3B-CAB	-2.66	121.78	127.18
22	c	510	CLA	C2D-C3D-CAD	2.66	145.80	134.94
26	C	519	LHG	O8-C23-C24	2.66	120.04	111.90
23	A	406	PL9	C27-C28-C29	-2.66	122.06	127.81
22	B	610	CLA	O2D-CGD-O1D	-2.66	118.45	123.79
22	b	618	CLA	CBD-CHA-C1A	2.66	132.25	128.77
22	C	511	CLA	O2D-CGD-O1D	-2.66	118.45	123.79
22	c	506	CLA	C2D-C3D-CAD	2.66	145.78	134.94
30	M	102	LMT	C1'-O5'-C5'	-2.66	108.59	113.73
26	c	519	LHG	O8-C23-C24	2.66	120.03	111.90
23	a	408	PL9	C20-C19-C21	2.66	119.42	115.39
22	a	405	CLA	C3D-C4D-CHA	2.66	112.42	108.16
27	C	518	LMG	O6-C1-O1	-2.65	103.61	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	O2D-CGD-O1D	-2.65	118.46	123.79
22	A	403	CLA	C3D-C4D-CHA	2.65	112.42	108.16
23	d	407	PL9	C27-C28-C29	-2.65	122.07	127.81
22	B	612	CLA	CBD-CHA-C1A	2.65	132.24	128.77
22	B	604	CLA	CMB-C2B-C3B	2.65	130.15	125.16
22	c	503	CLA	C2D-C3D-CAD	2.65	145.75	134.94
22	b	608	CLA	C3D-C4D-CHA	2.65	112.41	108.16
23	j	101	PL9	C7-C8-C9	-2.65	122.28	126.76
22	B	607	CLA	C3D-C4D-CHA	2.65	112.41	108.16
24	C	514	BCR	C28-C27-C26	-2.65	109.46	113.81
25	C	517	DGD	C1D-O6D-C5D	-2.65	108.61	113.73
22	a	405	CLA	O2D-CGD-O1D	-2.65	118.47	123.79
22	d	405	CLA	CMB-C2B-C3B	2.65	130.15	125.16
22	c	511	CLA	CHB-C4A-NA	2.65	128.07	124.38
25	c	517	DGD	C1D-O6D-C5D	-2.64	108.62	113.73
24	J	102	BCR	C15-C14-C13	-2.64	123.47	127.29
22	c	520	CLA	CHB-C4A-NA	2.64	128.07	124.38
22	a	406	CLA	CHB-C4A-NA	2.64	128.07	124.38
31	D	401	PHO	O2D-CGD-O1D	-2.64	118.49	123.79
22	C	509	CLA	CHD-C4C-NC	2.64	126.13	124.28
22	B	603	CLA	C2D-C3D-CAD	2.64	145.71	134.94
27	B	621	LMG	C40-C41-C42	-2.64	103.11	113.73
22	b	607	CLA	C2D-C3D-CAD	2.64	145.71	134.94
27	i	101	LMG	O6-C1-O1	-2.64	103.65	109.93
24	y	101	BCR	C38-C26-C25	-2.64	121.52	124.50
22	B	605	CLA	CHB-C4A-NA	2.64	128.06	124.38
22	C	509	CLA	C3D-C4D-CHA	2.64	112.39	108.16
22	D	406	CLA	C3D-C4D-CHA	2.63	112.39	108.16
22	d	406	CLA	CMB-C2B-C3B	2.63	130.12	125.16
22	b	610	CLA	C3D-C4D-CHA	2.63	112.39	108.16
27	a	412	LMG	C40-C41-C42	-2.63	103.15	113.73
22	B	613	CLA	C4B-C3B-CAB	-2.63	121.85	127.18
26	A	409	LHG	O3-C3-C2	-2.63	100.05	108.54
30	B	623	LMT	C1'-O5'-C5'	-2.63	108.65	113.73
22	B	605	CLA	CMB-C2B-C3B	2.63	130.11	125.16
22	C	512	CLA	CHB-C4A-NA	2.63	128.04	124.38
29	f	103	SQD	C44-O6-C1	2.62	119.07	113.80
31	d	401	PHO	O2D-CGD-O1D	-2.62	118.53	123.79
24	g	101	BCR	C7-C8-C9	-2.62	122.29	126.22
22	C	501	CLA	CHB-C4A-NA	2.62	128.04	124.38
22	c	505	CLA	CHB-C4A-NA	2.62	128.04	124.38
22	b	608	CLA	CMB-C2B-C3B	2.62	130.10	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	CHB-C4A-NA	2.62	128.04	124.38
22	C	520	CLA	CBD-CHA-C1A	2.62	132.20	128.77
22	C	511	CLA	CHB-C4A-NA	2.62	128.03	124.38
22	B	605	CLA	CBD-CHA-C1A	2.62	132.19	128.77
22	B	608	CLA	CHB-C4A-NA	2.62	128.03	124.38
24	g	101	BCR	C38-C26-C25	-2.62	121.54	124.50
25	a	410	DGD	O5D-C6D-C5D	-2.62	104.42	108.96
23	D	407	PL9	C7-C8-C9	-2.62	122.34	126.76
22	D	405	CLA	C4B-C3B-CAB	-2.62	121.88	127.18
27	I	101	LMG	O6-C1-O1	-2.61	103.71	109.93
24	c	514	BCR	C11-C10-C9	-2.61	123.51	127.29
22	a	407	CLA	O2D-CGD-O1D	-2.61	118.55	123.79
23	D	407	PL9	C37-C38-C39	-2.61	122.17	127.81
23	D	407	PL9	C20-C19-C21	2.61	119.35	115.39
22	b	615	CLA	CHB-C4A-NA	2.61	128.02	124.38
22	B	611	CLA	CHB-C4A-NA	2.61	128.02	124.38
22	b	618	CLA	CHB-C4A-NA	2.61	128.02	124.38
22	c	502	CLA	CBD-CHA-C1A	2.61	132.18	128.77
24	c	521	BCR	C27-C26-C25	2.60	126.30	122.86
23	J	101	PL9	C20-C19-C21	2.60	119.34	115.39
22	c	504	CLA	CHB-C4A-NA	2.60	128.01	124.38
22	c	507	CLA	CHD-C4C-NC	2.60	126.10	124.28
22	B	614	CLA	CMB-C2B-C3B	2.60	130.05	125.16
27	b	625	LMG	C40-C41-C42	-2.60	103.28	113.73
22	a	407	CLA	CHB-C4A-NA	2.60	128.00	124.38
22	B	604	CLA	C3D-C4D-CHA	2.59	112.32	108.16
24	C	513	BCR	C24-C23-C22	-2.59	122.34	126.22
22	B	604	CLA	CHB-C4A-NA	2.59	127.99	124.38
24	K	102	BCR	C27-C26-C25	2.59	126.28	122.86
29	a	415	SQD	C5-C6-S	-2.59	110.78	114.40
23	A	406	PL9	C37-C38-C39	-2.59	122.39	128.69
27	C	518	LMG	C22-C21-C20	-2.59	105.54	112.94
24	b	622	BCR	C29-C30-C25	2.59	114.49	110.37
23	d	407	PL9	C20-C19-C21	2.59	119.32	115.39
22	b	619	CLA	O2D-CGD-O1D	-2.59	118.59	123.79
22	A	405	CLA	O2D-CGD-O1D	-2.59	118.60	123.79
22	B	610	CLA	CBD-CHA-C1A	2.59	132.15	128.77
24	B	618	BCR	C11-C10-C9	-2.59	123.55	127.29
22	c	510	CLA	CHB-C4A-NA	2.59	127.99	124.38
24	K	102	BCR	C15-C16-C17	-2.58	117.75	123.45
31	d	402	PHO	CMB-C2B-C3B	2.59	130.03	125.16
23	d	407	PL9	C37-C38-C39	-2.58	122.22	127.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	CBD-CHA-C1A	2.58	132.15	128.77
22	A	402	CLA	C3D-C4D-CHA	2.58	112.31	108.16
24	c	521	BCR	C15-C16-C17	-2.58	117.76	123.45
22	C	502	CLA	CBD-CHA-C1A	2.58	132.14	128.77
22	C	508	CLA	CHD-C4C-NC	2.58	126.09	124.28
22	c	501	CLA	CHB-C4A-NA	2.58	127.98	124.38
24	b	620	BCR	C33-C5-C6	-2.58	121.58	124.50
27	c	518	LMG	O6-C1-O1	-2.58	103.79	109.93
29	B	622	SQD	C44-O6-C1	2.58	118.97	113.80
22	b	618	CLA	CMB-C2B-C3B	2.58	130.02	125.16
22	B	609	CLA	CBD-CHA-C1A	2.58	132.14	128.77
27	c	518	LMG	C22-C21-C20	-2.58	105.58	112.94
22	A	404	CLA	CHB-C4A-NA	2.57	127.97	124.38
23	a	408	PL9	C7-C8-C9	-2.57	122.41	126.76
22	B	603	CLA	C4B-C3B-CAB	-2.57	121.97	127.18
22	b	607	CLA	CMB-C2B-C3B	2.57	130.01	125.16
22	B	614	CLA	CHB-C4A-NA	2.57	127.97	124.38
24	B	616	BCR	C33-C5-C6	-2.57	121.59	124.50
31	D	402	PHO	CMB-C2B-C3B	2.57	130.01	125.16
22	c	512	CLA	CHB-C4A-NA	2.57	127.97	124.38
22	B	609	CLA	CHB-C4A-NA	2.57	127.97	124.38
22	c	503	CLA	CHB-C4A-NA	2.57	127.97	124.38
22	B	612	CLA	CHB-C4A-NA	2.57	127.97	124.38
22	d	406	CLA	CHD-C4C-NC	2.57	126.08	124.28
22	b	606	CLA	CBD-CHA-C1A	2.57	132.12	128.77
22	C	504	CLA	C4A-NA-C1A	2.57	110.00	106.38
27	E	101	LMG	C1-C2-C3	-2.57	105.02	109.99
23	a	408	PL9	C37-C38-C39	-2.57	122.44	128.69
22	c	502	CLA	C4B-C3B-CAB	-2.57	121.98	127.18
22	C	520	CLA	CMB-C2B-C3B	2.56	129.99	125.16
22	B	606	CLA	CHB-C4A-NA	2.56	127.96	124.38
22	c	508	CLA	O2D-CGD-O1D	-2.56	118.65	123.79
22	H	101	CLA	CMB-C2B-C3B	2.56	129.99	125.16
22	C	507	CLA	CBD-CHA-C1A	2.56	132.12	128.77
24	C	514	BCR	C15-C16-C17	-2.56	117.81	123.45
22	C	508	CLA	CHB-C4A-NA	2.56	127.95	124.38
22	b	610	CLA	CHB-C4A-NA	2.56	127.95	124.38
22	a	404	CLA	C3D-C4D-CHA	2.56	112.27	108.16
22	d	405	CLA	C4B-C3B-CAB	-2.56	122.00	127.18
22	B	611	CLA	C4A-NA-C1A	2.56	109.99	106.38
27	b	625	LMG	C1-C2-C3	-2.56	105.03	109.99
25	d	410	DGD	C3G-C2G-C1G	-2.56	105.99	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	408	LMG	C22-C23-C24	-2.56	103.44	113.73
22	b	616	CLA	CHB-C4A-NA	2.56	127.95	124.38
22	D	405	CLA	O2D-CGD-O1D	-2.56	118.66	123.79
22	D	406	CLA	CHD-C4C-NC	2.55	126.07	124.28
22	B	607	CLA	CHB-C4A-NA	2.55	127.94	124.38
22	b	610	CLA	CMB-C2B-C3B	2.55	129.97	125.16
23	D	407	PL9	C32-C33-C34	-2.55	122.30	127.81
22	C	512	CLA	CBD-CHA-C1A	2.55	132.10	128.77
22	d	406	CLA	CHB-C4A-NA	2.55	127.94	124.38
22	c	503	CLA	CHD-C4C-NC	2.55	126.06	124.28
22	C	509	CLA	CMB-C2B-C3B	2.55	129.96	125.16
22	h	101	CLA	CMB-C2B-C3B	2.55	129.96	125.16
31	d	402	PHO	O2D-CGD-O1D	-2.55	118.68	123.79
22	a	404	CLA	CHB-C4A-NA	2.55	127.93	124.38
22	A	405	CLA	C4B-C3B-CAB	-2.54	122.03	127.18
22	B	614	CLA	CBD-CHA-C1A	2.54	132.09	128.77
30	b	626	LMT	C1'-O5'-C5'	-2.54	108.82	113.73
24	B	618	BCR	C15-C14-C13	-2.54	123.62	127.29
22	C	503	CLA	CBD-CHA-C1A	2.54	132.09	128.77
22	B	611	CLA	CBD-CHA-C1A	2.54	132.09	128.77
22	B	608	CLA	CBD-CHA-C1A	2.54	132.09	128.77
27	a	402	LMG	O6-C1-O1	-2.54	103.88	109.93
22	H	101	CLA	CBD-CHA-C1A	2.54	132.09	128.77
22	C	503	CLA	C4B-C3B-CAB	-2.54	122.04	127.18
24	A	407	BCR	C27-C26-C25	2.54	126.21	122.86
29	b	602	SQD	C4-C3-C2	2.53	115.47	110.80
30	M	103	LMT	C1'-O5'-C5'	-2.53	108.83	113.73
22	A	403	CLA	CMB-C2B-C3B	2.54	129.94	125.16
24	B	619	BCR	C7-C8-C9	-2.53	122.42	126.22
22	c	504	CLA	C4A-NA-C1A	2.53	109.95	106.38
22	c	520	CLA	CBD-CHA-C1A	2.53	132.08	128.77
22	a	405	CLA	CMB-C2B-C3B	2.53	129.93	125.16
22	b	609	CLA	CMB-C2B-C3B	2.53	129.93	125.16
24	g	101	BCR	C33-C5-C6	-2.53	121.64	124.50
22	c	520	CLA	CMB-C2B-C3B	2.53	129.92	125.16
22	B	607	CLA	C4B-C3B-CAB	-2.53	122.06	127.18
22	c	509	CLA	CMB-C2B-C3B	2.52	129.92	125.16
22	B	603	CLA	C4A-NA-C1A	2.52	109.94	106.38
22	A	402	CLA	CHB-C4A-NA	2.52	127.90	124.38
22	B	613	CLA	CHB-C4A-NA	2.52	127.90	124.38
22	D	406	CLA	CHB-C4A-NA	2.52	127.90	124.38
22	c	508	CLA	CHD-C4C-NC	2.52	126.04	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	617	CLA	CHB-C4A-NA	2.52	127.90	124.38
22	c	502	CLA	CHB-C4A-NA	2.52	127.89	124.38
22	C	503	CLA	CHB-C4A-NA	2.52	127.89	124.38
22	A	404	CLA	CMB-C2B-C3B	2.52	129.91	125.16
22	B	611	CLA	CHD-C4C-NC	2.52	126.04	124.28
22	b	615	CLA	CBD-CHA-C1A	2.52	132.06	128.77
22	b	614	CLA	CBD-CHA-C1A	2.52	132.06	128.77
22	a	407	CLA	CHD-C4C-NC	2.52	126.04	124.28
24	b	623	BCR	C27-C26-C25	2.51	126.18	122.86
22	A	405	CLA	CHB-C4A-NA	2.52	127.89	124.38
22	B	615	CLA	O2D-CGD-O1D	-2.51	118.74	123.79
24	a	409	BCR	C27-C26-C25	2.51	126.18	122.86
22	B	603	CLA	CMB-C2B-C3B	2.51	129.89	125.16
24	C	514	BCR	C11-C10-C9	-2.51	123.66	127.29
24	J	102	BCR	C38-C26-C25	-2.51	121.66	124.50
22	h	101	CLA	CHB-C4A-NA	2.51	127.88	124.38
22	b	612	CLA	CBD-CHA-C1A	2.51	132.05	128.77
22	A	405	CLA	CBD-CHA-C1A	2.50	132.04	128.77
24	B	619	BCR	C27-C26-C25	2.50	126.17	122.86
22	B	611	CLA	C4B-C3B-CAB	-2.50	122.11	127.18
22	C	502	CLA	C4B-C3B-CAB	-2.50	122.11	127.18
22	d	406	CLA	C1-C2-C3	-2.50	121.89	126.23
24	b	623	BCR	C7-C8-C9	-2.50	122.47	126.22
26	C	519	LHG	C27-C28-C29	-2.50	103.67	113.73
22	b	611	CLA	CHB-C4A-NA	2.50	127.87	124.38
22	C	509	CLA	CBD-CHA-C1A	2.50	132.04	128.77
22	a	407	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
22	B	602	CLA	CHB-C4A-NA	2.50	127.87	124.38
22	b	605	CLA	CMB-C2B-C3B	2.50	129.87	125.16
31	D	401	PHO	CBD-CHA-C1A	2.50	131.00	126.67
22	c	510	CLA	C4B-C3B-CAB	-2.50	122.12	127.18
30	M	102	LMT	C3'-C4'-C5'	-2.49	105.28	110.86
22	C	510	CLA	CHD-C4C-NC	2.49	126.03	124.28
22	c	503	CLA	C4B-C3B-CAB	-2.49	122.13	127.18
22	c	507	CLA	CHB-C4A-NA	2.49	127.86	124.38
22	a	404	CLA	CHD-C4C-NC	2.49	126.02	124.28
23	j	101	PL9	C20-C19-C21	2.49	119.17	115.39
22	C	505	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
24	c	521	BCR	C15-C14-C13	-2.49	123.69	127.29
30	D	411	LMT	C1'-O5'-C5'	-2.49	108.92	113.73
24	C	514	BCR	C29-C30-C25	2.49	114.34	110.37
24	B	617	BCR	C15-C14-C13	-2.49	123.70	127.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	CHD-C4C-NC	2.49	126.02	124.28
24	b	622	BCR	C11-C10-C9	-2.48	123.70	127.29
22	b	615	CLA	CHD-C4C-NC	2.49	126.02	124.28
22	c	511	CLA	CMD-C2D-C3D	2.48	129.84	125.16
24	C	514	BCR	C15-C14-C13	-2.49	123.70	127.29
22	B	606	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
22	b	615	CLA	C4A-NA-C1A	2.48	109.88	106.38
22	H	101	CLA	CHB-C4A-NA	2.48	127.84	124.38
22	B	605	CLA	C4B-C3B-CAB	-2.48	122.15	127.18
31	D	401	PHO	CMB-C2B-C3B	2.48	129.83	125.16
31	d	401	PHO	CBD-CHA-C1A	2.48	130.97	126.67
27	e	101	LMG	C1-C2-C3	-2.48	105.19	109.99
22	h	101	CLA	CBD-CHA-C1A	2.48	132.01	128.77
22	b	612	CLA	CMB-C2B-C3B	2.48	129.83	125.16
22	b	615	CLA	O2D-CGD-O1D	-2.48	118.81	123.79
22	b	614	CLA	CMD-C2D-C3D	2.48	129.83	125.16
22	a	404	CLA	CMB-C2B-C3B	2.48	129.83	125.16
22	C	502	CLA	CHB-C4A-NA	2.48	127.83	124.38
24	C	513	BCR	C15-C14-C13	-2.48	123.71	127.29
22	b	612	CLA	CHB-C4A-NA	2.48	127.83	124.38
22	C	504	CLA	C4B-C3B-CAB	-2.47	122.17	127.18
22	b	609	CLA	C4A-NA-C1A	2.47	109.87	106.38
22	c	507	CLA	CBD-CHA-C1A	2.47	132.00	128.77
22	c	509	CLA	CBD-CHA-C1A	2.47	132.00	128.77
31	d	402	PHO	O1D-CGD-CBD	2.47	129.50	124.45
22	C	512	CLA	C4B-C3B-CAB	-2.47	122.17	127.18
22	b	608	CLA	CBD-CHA-C1A	2.47	132.00	128.77
24	K	102	BCR	C24-C23-C22	-2.47	122.52	126.22
27	A	414	LMG	O6-C1-O1	-2.47	104.05	109.93
22	C	505	CLA	CBD-CHA-C1A	2.47	132.00	128.77
22	b	611	CLA	C4B-C3B-CAB	-2.47	122.18	127.18
22	c	509	CLA	CHB-C4A-NA	2.47	127.82	124.38
22	C	510	CLA	C4A-NA-C1A	2.47	109.86	106.38
26	c	519	LHG	C27-C28-C29	-2.47	103.81	113.73
24	c	514	BCR	C29-C30-C25	2.47	114.30	110.37
23	A	406	PL9	C7-C8-C9	-2.47	122.59	126.76
31	D	402	PHO	O1D-CGD-CBD	2.47	129.49	124.45
22	b	606	CLA	CHB-C4A-NA	2.47	127.82	124.38
22	b	609	CLA	C4B-C3B-CAB	-2.47	122.18	127.18
22	C	504	CLA	CMD-C2D-C3D	2.46	129.81	125.16
22	C	511	CLA	CMD-C2D-C3D	2.46	129.81	125.16
22	B	608	CLA	CMB-C2B-C3B	2.47	129.81	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	412	SQD	O48-C23-C24	2.46	119.44	111.90
24	j	102	BCR	C38-C26-C25	-2.46	121.72	124.50
30	M	103	LMT	C3'-C4'-C5'	-2.46	105.35	110.86
23	d	407	PL9	C32-C33-C34	-2.46	122.48	127.81
24	y	101	BCR	C33-C5-C6	-2.46	121.72	124.50
22	b	607	CLA	C4A-NA-C1A	2.46	109.85	106.38
25	D	410	DGD	CFB-CEB-CDB	-2.46	101.50	114.56
22	C	509	CLA	CHB-C4A-NA	2.46	127.81	124.38
27	d	408	LMG	C22-C23-C24	-2.46	103.84	113.73
22	C	501	CLA	CHD-C4C-NC	2.46	126.00	124.28
22	C	510	CLA	C4B-C3B-CAB	-2.46	122.20	127.18
22	C	504	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	b	615	CLA	C4B-C3B-CAB	-2.46	122.20	127.18
22	b	613	CLA	CHB-C4A-NA	2.46	127.81	124.38
22	C	507	CLA	CHB-C4A-NA	2.46	127.81	124.38
22	c	507	CLA	C4B-C3B-CAB	-2.46	122.20	127.18
22	H	101	CLA	C4B-C3B-CAB	-2.45	122.21	127.18
25	c	515	DGD	C3G-C2G-C1G	-2.45	106.22	111.86
22	b	614	CLA	C1-C2-C3	-2.45	121.97	126.23
22	b	610	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
27	m	101	LMG	O2-C2-C1	-2.46	104.70	110.03
22	B	601	CLA	CMB-C2B-C3B	2.45	129.78	125.16
22	a	406	CLA	CMB-C2B-C3B	2.45	129.78	125.16
22	c	512	CLA	C4B-C3B-CAB	-2.45	122.21	127.18
25	c	516	DGD	C3G-C2G-C1G	-2.45	106.23	111.86
22	A	403	CLA	CHD-C4C-NC	2.45	126.00	124.28
22	a	407	CLA	C4B-C3B-CAB	-2.45	122.21	127.18
22	C	508	CLA	CMB-C2B-C3B	2.45	129.78	125.16
22	B	606	CLA	CMB-C2B-C3B	2.45	129.78	125.16
22	A	405	CLA	CHD-C4C-NC	2.45	125.99	124.28
22	C	508	CLA	CBD-CHA-C1A	2.45	131.97	128.77
22	h	101	CLA	C4B-C3B-CAB	-2.45	122.22	127.18
22	C	501	CLA	C4A-NA-C1A	2.45	109.83	106.38
22	A	402	CLA	CMB-C2B-C3B	2.44	129.76	125.16
25	C	515	DGD	C3G-C2G-C1G	-2.44	106.25	111.86
29	B	626	SQD	C4-C3-C2	2.44	115.30	110.80
24	C	514	BCR	C33-C5-C6	-2.44	121.74	124.50
24	C	513	BCR	C15-C16-C17	-2.44	118.08	123.45
22	a	406	CLA	CBD-CHA-C1A	2.44	131.96	128.77
27	A	410	LMG	O3-C3-C2	-2.44	104.91	110.36
29	a	401	SQD	C5-C6-S	-2.43	111.00	114.40
25	C	516	DGD	C3G-C2G-C1G	-2.43	106.27	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	CBD-CHA-C1A	2.43	131.95	128.77
22	B	604	CLA	CBD-CHA-C1A	2.43	131.95	128.77
22	c	505	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
27	A	410	LMG	C1-C2-C3	-2.43	105.28	109.99
22	b	617	CLA	CBD-CHA-C1A	2.43	131.95	128.77
22	B	615	CLA	CHB-C4A-NA	2.43	127.77	124.38
22	B	610	CLA	C1-C2-C3	-2.43	122.01	126.23
22	A	403	CLA	C4A-NA-C1A	2.43	109.80	106.38
22	a	407	CLA	CBD-CHA-C1A	2.43	131.94	128.77
22	c	508	CLA	CMB-C2B-C3B	2.43	129.73	125.16
30	b	603	LMT	C1'-O5'-C5'	-2.43	109.04	113.73
29	B	622	SQD	O48-C23-C24	2.43	119.33	111.90
22	C	508	CLA	O2D-CGD-O1D	-2.43	118.92	123.79
31	d	401	PHO	O1D-CGD-CBD	2.42	129.41	124.45
22	A	403	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
22	c	503	CLA	C4A-NA-C1A	2.42	109.80	106.38
22	a	405	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	c	501	CLA	CBD-CHA-C1A	2.42	131.93	128.77
22	b	606	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	B	612	CLA	CHD-C4C-NC	2.42	125.97	124.28
25	B	620	DGD	C1D-C2D-C3D	-2.42	105.30	109.99
22	b	610	CLA	CBD-CHA-C1A	2.42	131.93	128.77
22	C	501	CLA	CBD-CHA-C1A	2.42	131.93	128.77
25	d	410	DGD	CFB-CEB-CDB	-2.42	101.72	114.56
22	c	501	CLA	CHD-C4C-NC	2.42	125.97	124.28
29	a	401	SQD	O48-C23-C24	2.42	119.30	111.90
24	c	514	BCR	C33-C5-C6	-2.42	121.77	124.50
25	D	410	DGD	C3G-C2G-C1G	-2.42	106.31	111.86
22	B	608	CLA	C1-C2-C3	-2.41	122.04	126.23
22	C	512	CLA	CHD-C4C-NC	2.41	125.97	124.28
23	A	406	PL9	C20-C19-C21	2.41	119.05	115.39
22	B	615	CLA	CMB-C2B-C3B	2.41	129.71	125.16
27	D	408	LMG	O2-C2-C1	-2.41	104.79	110.03
22	b	616	CLA	C4A-NA-C1A	2.41	109.78	106.38
27	d	412	LMG	C38-C37-C36	-2.41	101.77	114.56
29	F	103	SQD	C44-O6-C1	2.41	118.64	113.80
22	B	608	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	a	405	CLA	C4A-NA-C1A	2.41	109.78	106.38
22	b	619	CLA	CMB-C2B-C3B	2.41	129.70	125.16
22	C	520	CLA	C4A-NA-C1A	2.41	109.77	106.38
22	c	501	CLA	C4A-NA-C1A	2.40	109.77	106.38
24	c	513	BCR	C7-C8-C9	-2.40	122.62	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	CMB-C2B-C3B	2.40	129.69	125.16
22	b	608	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	c	511	CLA	C4B-C3B-CAB	-2.40	122.31	127.18
22	a	405	CLA	CHD-C4C-NC	2.40	125.96	124.28
22	B	605	CLA	C4A-NA-C1A	2.40	109.77	106.38
24	c	513	BCR	C15-C14-C13	-2.40	123.82	127.29
27	d	409	LMG	C38-C37-C36	-2.40	101.81	114.56
27	m	101	LMG	C1-C2-C3	-2.40	105.33	109.99
22	B	611	CLA	O2D-CGD-O1D	-2.40	118.97	123.79
27	C	521	LMG	O2-C2-C1	-2.40	104.81	110.03
22	b	605	CLA	CBD-CHA-C1A	2.40	131.91	128.77
22	b	612	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	B	611	CLA	CMD-C2D-C3D	2.40	129.68	125.16
24	b	620	BCR	C2-C1-C6	2.40	114.19	110.37
25	a	410	DGD	CBB-CAB-C9B	-2.40	101.83	114.56
31	D	401	PHO	O1D-CGD-CBD	2.40	129.35	124.45
27	D	412	LMG	C38-C37-C36	-2.40	101.83	114.56
24	c	514	BCR	C15-C16-C17	-2.40	118.17	123.45
22	C	511	CLA	C4B-C3B-CAB	-2.40	122.33	127.18
22	C	511	CLA	CHD-C4C-NC	2.40	125.96	124.28
22	C	505	CLA	CHD-C4C-NC	2.39	125.96	124.28
30	B	627	LMT	C1'-O5'-C5'	-2.40	109.10	113.73
22	A	403	CLA	CBD-CHA-C1A	2.40	131.90	128.77
22	b	615	CLA	CMD-C2D-C3D	2.39	129.67	125.16
27	i	101	LMG	O1-C1-C2	-2.39	105.08	108.15
27	i	101	LMG	O2-C2-C1	-2.39	104.83	110.03
24	B	618	BCR	C15-C16-C17	-2.39	118.17	123.45
27	A	410	LMG	C40-C39-C38	-2.39	101.86	114.56
22	B	602	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	c	504	CLA	C4B-C3B-CAB	-2.39	122.33	127.18
22	C	507	CLA	C4B-C3B-CAB	-2.39	122.33	127.18
22	A	404	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	b	608	CLA	C4B-C3B-CAB	-2.39	122.33	127.18
22	b	619	CLA	CHB-C4A-NA	2.39	127.72	124.38
27	D	412	LMG	C1-C2-C3	-2.39	105.36	109.99
22	b	618	CLA	C4A-NA-C1A	2.39	109.75	106.38
22	D	405	CLA	CBD-CHA-C1A	2.39	131.89	128.77
22	C	511	CLA	C4A-NA-C1A	2.39	109.75	106.38
24	b	623	BCR	C11-C10-C9	-2.39	123.84	127.29
25	b	624	DGD	C1D-C2D-C3D	-2.39	105.36	109.99
31	D	402	PHO	CBD-CHA-C1A	2.39	130.81	126.67
22	A	405	CLA	C1B-CHB-C4A	-2.39	125.39	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C15-C14-C13	-2.38	123.84	127.29
31	d	402	PHO	C2D-C3D-CAD	2.39	144.67	134.94
24	b	622	BCR	C15-C14-C13	-2.39	123.84	127.29
25	A	408	DGD	CBB-CAB-C9B	-2.39	101.89	114.56
22	a	404	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	D	406	CLA	C4B-C3B-CAB	-2.38	122.36	127.18
22	B	610	CLA	CMD-C2D-C3D	2.38	129.65	125.16
22	a	406	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	c	502	CLA	CMD-C2D-C3D	2.38	129.64	125.16
30	d	411	LMT	C3'-C4'-C5'	-2.38	105.54	110.86
27	I	101	LMG	O2-C2-C1	-2.38	104.87	110.03
27	a	412	LMG	O3-C3-C2	-2.38	105.05	110.36
25	c	516	DGD	O6E-C1E-O5D	-2.38	104.27	109.93
22	b	608	CLA	C4A-NA-C1A	2.38	109.73	106.38
22	B	606	CLA	C4A-NA-C1A	2.38	109.73	106.38
29	a	415	SQD	O48-C23-C24	2.37	119.16	111.90
30	i	102	LMT	C1'-O5'-C5'	-2.37	109.14	113.73
22	b	605	CLA	CHB-C4A-NA	2.37	127.69	124.38
24	B	617	BCR	C29-C30-C25	2.37	114.15	110.37
24	b	621	BCR	C29-C30-C25	2.37	114.16	110.37
31	D	402	PHO	C2D-C3D-CAD	2.37	144.62	134.94
22	c	520	CLA	C4A-NA-C1A	2.37	109.72	106.38
25	C	515	DGD	C6B-C7B-C8B	-2.37	104.19	113.73
22	A	402	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	C	506	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	c	515	DGD	O5D-C6D-C5D	-2.37	104.85	108.96
24	b	621	BCR	C35-C13-C14	-2.37	119.54	122.92
24	B	616	BCR	C27-C26-C25	2.37	125.99	122.86
22	c	507	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
24	b	620	BCR	C11-C10-C9	-2.37	123.86	127.29
22	B	601	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	b	611	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
24	y	101	BCR	C1-C6-C5	-2.37	119.16	122.59
25	C	516	DGD	O6E-C1E-O5D	-2.37	104.29	109.93
26	c	519	LHG	C11-C10-C9	-2.37	101.99	114.56
22	A	405	CLA	C4A-NA-C1A	2.37	109.72	106.38
22	c	511	CLA	C4A-NA-C1A	2.37	109.72	106.38
22	b	613	CLA	C4B-C3B-CAB	-2.37	122.39	127.18
22	C	520	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
27	d	408	LMG	O2-C2-C1	-2.37	104.89	110.03
22	B	604	CLA	C4B-C3B-CAB	-2.36	122.39	127.18
22	H	101	CLA	C1B-CHB-C4A	-2.36	125.44	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	C4B-C3B-CAB	-2.36	122.39	127.18
22	B	603	CLA	O1D-CGD-CBD	2.36	129.28	124.45
22	h	101	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	B	601	CLA	CHB-C4A-NA	2.36	127.67	124.38
22	b	616	CLA	C2B-C3B-CAB	2.36	132.15	127.33
27	E	101	LMG	O6-C1-O1	-2.36	104.31	109.93
22	C	512	CLA	C4A-NA-C1A	2.36	109.70	106.38
22	c	512	CLA	CBD-CHA-C1A	2.36	131.85	128.77
25	c	515	DGD	C6B-C7B-C8B	-2.36	104.25	113.73
22	B	615	CLA	CBD-CHA-C1A	2.36	131.85	128.77
27	d	412	LMG	C1-C2-C3	-2.36	105.42	109.99
22	B	615	CLA	C4A-NA-C1A	2.36	109.70	106.38
22	B	613	CLA	CBD-CHA-C1A	2.35	131.85	128.77
22	B	614	CLA	C4A-NA-C1A	2.35	109.70	106.38
22	C	503	CLA	CHD-C4C-NC	2.35	125.93	124.28
31	d	401	PHO	CMB-C2B-C3B	2.35	129.59	125.16
22	b	613	CLA	CBD-CHA-C1A	2.35	131.84	128.77
27	c	522	LMG	O6-C1-O1	-2.35	104.33	109.93
24	b	620	BCR	C27-C26-C25	2.35	125.96	122.86
22	c	512	CLA	CHD-C4C-NC	2.35	125.92	124.28
27	D	412	LMG	O3-C3-C2	-2.35	105.11	110.36
31	d	401	PHO	C2D-C3D-CAD	2.35	144.52	134.94
22	b	619	CLA	CBD-CHA-C1A	2.35	131.84	128.77
27	a	412	LMG	C1-C2-C3	-2.35	105.44	109.99
25	B	620	DGD	CBB-CAB-C9B	-2.35	102.10	114.56
22	B	612	CLA	C4A-NA-C1A	2.35	109.69	106.38
22	B	615	CLA	CHD-C4C-NC	2.35	125.92	124.28
27	D	409	LMG	C38-C37-C36	-2.35	102.10	114.56
24	B	616	BCR	C11-C10-C9	-2.35	123.90	127.29
27	d	408	LMG	C38-C37-C36	-2.35	102.10	114.56
22	d	405	CLA	CBD-CHA-C1A	2.35	131.84	128.77
22	d	406	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
22	C	506	CLA	C4A-NA-C1A	2.34	109.69	106.38
22	c	501	CLA	C4B-C3B-CAB	-2.34	122.43	127.18
22	B	601	CLA	CBD-CHA-C1A	2.34	131.83	128.77
27	D	409	LMG	O6-C1-C2	-2.34	105.50	110.30
22	B	613	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	a	410	DGD	C1D-C2D-C3D	-2.34	105.45	109.99
25	b	624	DGD	CBB-CAB-C9B	-2.34	102.13	114.56
25	C	515	DGD	C1D-C2D-C3D	-2.34	105.45	109.99
22	d	405	CLA	CMD-C2D-C3D	2.34	129.57	125.16
26	C	519	LHG	C11-C10-C9	-2.34	102.14	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
24	c	513	BCR	C27-C26-C25	2.34	125.95	122.86
22	c	504	CLA	CMB-C2B-C3B	2.34	129.57	125.16
22	c	506	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
27	a	412	LMG	C40-C39-C38	-2.34	102.15	114.56
24	C	513	BCR	C27-C26-C25	2.34	125.94	122.86
22	c	506	CLA	C4A-NA-C1A	2.34	109.67	106.38
29	d	403	SQD	O48-C23-C24	2.34	119.05	111.90
24	b	622	BCR	C15-C16-C17	-2.33	118.31	123.45
29	a	401	SQD	C1-O5-C5	2.34	118.25	113.73
27	B	621	LMG	O6-C1-O1	-2.33	104.37	109.93
24	C	513	BCR	C3-C4-C5	-2.34	109.97	113.81
22	b	617	CLA	C4A-NA-C1A	2.33	109.67	106.38
30	d	411	LMT	C1'-O5'-C5'	-2.33	109.22	113.73
22	b	605	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
34	v	201	HEM	C3A-C4A-NA	-2.33	107.94	109.50
24	j	102	BCR	C15-C16-C17	-2.33	118.31	123.45
22	b	619	CLA	CHD-C4C-NC	2.33	125.91	124.28
27	C	521	LMG	C40-C39-C38	-2.33	102.19	114.56
22	C	505	CLA	C4A-NA-C1A	2.33	109.67	106.38
22	a	406	CLA	C4A-NA-C1A	2.33	109.67	106.38
25	C	517	DGD	CFB-CEB-CDB	-2.33	102.19	114.56
22	a	407	CLA	CMD-C2D-C3D	2.33	129.55	125.16
22	b	616	CLA	CHD-C4C-NC	2.33	125.91	124.28
24	c	514	BCR	C15-C14-C13	-2.33	123.92	127.29
22	A	404	CLA	CBD-CHA-C1A	2.33	131.81	128.77
22	c	504	CLA	CMD-C2D-C3D	2.33	129.55	125.16
22	c	510	CLA	C4A-NA-C1A	2.33	109.66	106.38
22	b	610	CLA	C4B-C3B-CAB	-2.33	122.46	127.18
27	c	522	LMG	O2-C2-C1	-2.33	104.98	110.03
25	c	517	DGD	CFB-CEB-CDB	-2.33	102.21	114.56
22	c	504	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	B	604	CLA	C4A-NA-C1A	2.32	109.65	106.38
27	D	409	LMG	C22-C23-C24	-2.32	104.38	113.73
22	C	507	CLA	C4A-NA-C1A	2.32	109.65	106.38
22	c	507	CLA	CMD-C2D-C3D	2.32	129.54	125.16
24	c	513	BCR	C15-C16-C17	-2.32	118.34	123.45
24	c	513	BCR	C24-C23-C22	-2.32	122.74	126.22
31	D	401	PHO	C2D-C3D-CAD	2.32	144.40	134.94
22	a	405	CLA	CBD-CHA-C1A	2.32	131.80	128.77
29	B	626	SQD	O48-C23-C24	2.32	119.00	111.90
22	c	505	CLA	C4A-NA-C1A	2.32	109.65	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	C31-C32-C33	-2.32	105.05	111.64
22	C	503	CLA	C4A-NA-C1A	2.32	109.65	106.38
22	C	507	CLA	C1-C2-C3	-2.32	122.21	126.23
22	a	407	CLA	C4A-NA-C1A	2.32	109.65	106.38
27	A	410	LMG	C22-C23-C24	-2.32	104.41	113.73
27	d	409	LMG	C22-C23-C24	-2.32	104.41	113.73
22	D	405	CLA	CMD-C2D-C3D	2.32	129.52	125.16
27	c	522	LMG	C40-C39-C38	-2.31	102.28	114.56
25	A	408	DGD	C3G-C2G-C1G	-2.31	106.55	111.86
30	D	411	LMT	C3'-C4'-C5'	-2.31	105.69	110.86
22	D	405	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	D	407	PL9	C12-C13-C14	-2.31	122.81	127.81
22	B	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	B	608	CLA	CMD-C2D-C3D	2.31	129.51	125.16
24	B	616	BCR	C2-C1-C6	2.31	114.05	110.37
29	A	413	SQD	O48-C23-C24	2.31	118.96	111.90
22	B	614	CLA	C4B-C3B-CAB	-2.31	122.50	127.18
25	c	516	DGD	CFB-CEB-CDB	-2.31	102.32	114.56
22	B	605	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
27	b	625	LMG	O2-C2-C1	-2.30	105.03	110.03
29	F	103	SQD	C5-C6-S	-2.30	111.18	114.40
27	C	521	LMG	O6-C1-O1	-2.30	104.44	109.93
22	b	619	CLA	C4A-NA-C1A	2.31	109.63	106.38
22	c	505	CLA	CHD-C4C-NC	2.30	125.89	124.28
25	c	516	DGD	O3D-C3D-C4D	-2.30	105.21	110.36
22	c	506	CLA	C3A-C4A-CHB	-2.30	119.54	124.33
25	C	516	DGD	O3D-C3D-C4D	-2.30	105.21	110.36
22	D	406	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	D	408	LMG	C38-C37-C36	-2.30	102.34	114.56
27	e	101	LMG	O6-C1-O1	-2.30	104.45	109.93
24	f	102	BCR	C27-C26-C25	2.30	125.90	122.86
22	h	101	CLA	C4A-NA-C1A	2.30	109.62	106.38
22	B	613	CLA	C4A-NA-C1A	2.30	109.62	106.38
24	j	102	BCR	C29-C30-C25	2.30	114.03	110.37
22	C	506	CLA	C3A-C4A-CHB	-2.30	119.55	124.33
27	a	412	LMG	C22-C23-C24	-2.29	104.50	113.73
22	b	617	CLA	CMD-C2D-C3D	2.30	129.49	125.16
22	B	607	CLA	C4A-NA-C1A	2.30	109.62	106.38
25	a	410	DGD	C3G-C2G-C1G	-2.29	106.59	111.86
22	H	101	CLA	C4A-NA-C1A	2.29	109.61	106.38
24	g	101	BCR	C1-C6-C5	-2.29	119.27	122.59
22	B	603	CLA	C1B-CHB-C4A	-2.29	125.57	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	BCR	C3-C4-C5	-2.29	110.04	113.81
27	M	101	LMG	O2-C2-C1	-2.29	105.05	110.03
22	B	608	CLA	C4A-NA-C1A	2.29	109.61	106.38
22	B	607	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
24	F	102	BCR	C27-C26-C25	2.29	125.88	122.86
24	B	619	BCR	C11-C10-C9	-2.29	123.98	127.29
22	d	406	CLA	C4B-C3B-CAB	-2.29	122.54	127.18
22	c	505	CLA	C4B-C3B-CAB	-2.29	122.55	127.18
22	B	609	CLA	C4A-NA-C1A	2.29	109.60	106.38
27	A	410	LMG	C38-C37-C36	-2.29	102.42	114.56
27	i	101	LMG	O1-C7-C8	-2.29	105.55	110.99
22	B	607	CLA	CBD-CHA-C1A	2.29	131.76	128.77
24	F	102	BCR	C11-C10-C9	-2.29	123.99	127.29
22	b	610	CLA	C4A-NA-C1A	2.29	109.60	106.38
27	d	408	LMG	O3-C3-C2	-2.29	105.25	110.36
22	C	502	CLA	CMD-C2D-C3D	2.28	129.46	125.16
31	d	402	PHO	C3D-C4D-ND	2.28	109.68	106.81
22	B	609	CLA	C4B-C3B-CAB	-2.28	122.56	127.18
27	A	410	LMG	O1-C1-C2	-2.28	105.23	108.15
25	c	515	DGD	C1D-C2D-C3D	-2.28	105.57	109.99
22	A	404	CLA	C4A-NA-C1A	2.28	109.59	106.38
22	b	612	CLA	CMD-C2D-C3D	2.28	129.46	125.16
22	c	502	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
34	V	201	HEM	C3A-C4A-NA	-2.28	107.98	109.50
22	c	507	CLA	C4A-NA-C1A	2.27	109.59	106.38
30	I	102	LMT	C1'-O5'-C5'	-2.28	109.33	113.73
22	c	508	CLA	C4A-NA-C1A	2.27	109.58	106.38
25	B	620	DGD	C3G-C2G-C1G	-2.27	106.64	111.86
31	d	402	PHO	CBD-CHA-C1A	2.27	130.61	126.67
22	c	502	CLA	C4A-NA-C1A	2.27	109.58	106.38
27	C	518	LMG	C38-C37-C36	-2.27	102.49	114.56
22	B	612	CLA	C2B-C3B-CAB	2.27	131.97	127.33
22	b	618	CLA	C4B-C3B-CAB	-2.27	122.58	127.18
22	C	511	CLA	O2A-CGA-O1A	-2.27	117.55	123.48
22	c	510	CLA	CHD-C4C-NC	2.27	125.87	124.28
22	c	512	CLA	C4A-NA-C1A	2.27	109.58	106.38
22	b	617	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	b	613	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
24	C	513	BCR	C11-C10-C9	-2.27	124.01	127.29
24	K	102	BCR	C11-C10-C9	-2.26	124.02	127.29
25	d	410	DGD	C3D-C4D-C5D	-2.27	106.10	110.17
24	J	102	BCR	C20-C21-C22	-2.26	124.02	127.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	CHD-C4C-NC	2.26	125.86	124.28
22	c	520	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
29	a	415	SQD	C4-C3-C2	2.26	114.97	110.80
25	c	515	DGD	C9B-C8B-C7B	-2.26	106.47	112.94
27	d	412	LMG	O6-C1-O1	-2.26	104.55	109.93
22	B	602	CLA	C4A-NA-C1A	2.26	109.57	106.38
22	C	502	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	D	405	CLA	C4A-NA-C1A	2.26	109.56	106.38
27	D	408	LMG	O3-C3-C2	-2.26	105.31	110.36
27	B	621	LMG	C40-C39-C38	-2.26	102.58	114.56
22	c	512	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
27	b	625	LMG	O6-C1-O1	-2.26	104.56	109.93
27	c	518	LMG	C38-C37-C36	-2.26	102.58	114.56
29	b	602	SQD	O48-C23-C24	2.26	118.80	111.90
24	J	102	BCR	C29-C30-C25	2.26	113.97	110.37
22	b	616	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
24	j	102	BCR	C20-C21-C22	-2.26	124.03	127.29
27	b	625	LMG	O3-C3-C2	-2.26	105.31	110.36
27	c	518	LMG	O2-C2-C1	-2.26	105.13	110.03
22	c	504	CLA	CBA-CAA-C2A	2.26	119.47	113.95
27	C	518	LMG	O2-C2-C1	-2.26	105.13	110.03
27	B	621	LMG	O3-C3-C2	-2.26	105.32	110.36
25	C	516	DGD	CFB-CEB-CDB	-2.26	102.58	114.56
27	a	402	LMG	O3-C3-C2	-2.26	105.31	110.36
22	b	607	CLA	O1D-CGD-CBD	2.26	129.06	124.45
22	d	406	CLA	C4A-NA-C1A	2.25	109.56	106.38
22	c	509	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
27	I	101	LMG	O3-C3-C2	-2.25	105.33	110.36
22	b	611	CLA	CMD-C2D-C3D	2.25	129.41	125.16
29	B	622	SQD	C5-C6-S	-2.25	111.25	114.40
22	B	607	CLA	CMD-C2D-C3D	2.25	129.40	125.16
22	C	501	CLA	C4B-C3B-CAB	-2.25	122.62	127.18
25	C	515	DGD	O5D-C6D-C5D	-2.25	105.06	108.96
25	b	601	DGD	O6D-C1D-O3G	-2.25	104.58	109.93
27	d	412	LMG	O3-C3-C2	-2.25	105.34	110.36
29	A	413	SQD	O6-C1-C2	2.25	111.03	108.15
22	B	609	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
27	i	101	LMG	C20-C21-C22	-2.25	104.70	113.73
22	C	512	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	b	609	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
22	C	506	CLA	CMD-C2D-C3D	2.24	129.39	125.16
24	f	102	BCR	C11-C10-C9	-2.24	124.05	127.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
22	C	520	CLA	CHD-C4C-NC	2.24	125.85	124.28
30	B	624	LMT	O1'-C1'-C2'	2.24	111.02	108.15
22	b	607	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
22	h	101	CLA	CMD-C2D-C3D	2.24	129.38	125.16
27	a	412	LMG	C38-C37-C36	-2.24	102.68	114.56
22	B	601	CLA	CMD-C2D-C3D	2.24	129.37	125.16
27	i	101	LMG	C23-C22-C21	-2.24	106.55	112.94
23	j	101	PL9	C12-C13-C14	-2.24	122.97	127.81
22	b	611	CLA	C4A-NA-C1A	2.24	109.53	106.38
25	b	624	DGD	C3G-C2G-C1G	-2.24	106.73	111.86
22	C	508	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
27	b	625	LMG	C40-C39-C38	-2.23	102.70	114.56
22	B	602	CLA	CMD-C2D-C3D	2.23	129.37	125.16
27	a	412	LMG	O2-C2-C1	-2.23	105.18	110.03
22	b	617	CLA	CHD-C4C-NC	2.23	125.84	124.28
22	B	603	CLA	CMD-C2D-C3D	2.23	129.36	125.16
27	d	412	LMG	O2-C2-C1	-2.23	105.19	110.03
27	A	410	LMG	O2-C2-C1	-2.23	105.19	110.03
25	A	408	DGD	C1D-C2D-C3D	-2.23	105.67	109.99
22	B	608	CLA	C4B-C3B-CAB	-2.23	122.66	127.18
22	C	508	CLA	C4A-NA-C1A	2.23	109.52	106.38
22	A	403	CLA	C3A-C4A-CHB	-2.23	119.69	124.33
22	a	405	CLA	C3A-C4A-CHB	-2.23	119.69	124.33
24	B	616	BCR	C15-C14-C13	-2.23	124.07	127.29
29	F	103	SQD	O48-C23-C24	2.23	118.71	111.90
22	D	406	CLA	CMD-C2D-C3D	2.22	129.35	125.16
24	c	521	BCR	C11-C10-C9	-2.23	124.07	127.29
24	b	620	BCR	C15-C14-C13	-2.22	124.08	127.29
22	C	506	CLA	CHD-C4C-NC	2.22	125.84	124.28
22	c	510	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
27	a	402	LMG	O1-C7-C8	-2.23	105.69	110.99
27	B	621	LMG	O2-C2-C1	-2.22	105.20	110.03
22	c	511	CLA	CHD-C4C-NC	2.22	125.84	124.28
22	B	606	CLA	C1-C2-C3	-2.22	122.37	126.23
22	B	606	CLA	C4B-C3B-CAB	-2.22	122.68	127.18
22	c	501	CLA	CMB-C2B-C3B	2.22	129.35	125.16
22	b	605	CLA	CMD-C2D-C3D	2.22	129.34	125.16
22	C	502	CLA	C4A-NA-C1A	2.22	109.51	106.38
22	c	507	CLA	C1-C2-C3	-2.22	122.37	126.23
27	a	402	LMG	O2-C2-C1	-2.22	105.21	110.03
30	B	624	LMT	C1'-O5'-C5'	-2.22	109.44	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	103	SQD	C3-C4-C5	2.22	114.15	110.17
23	J	101	PL9	C12-C13-C14	-2.22	123.01	127.81
22	c	506	CLA	CHD-C4C-NC	2.22	125.83	124.28
27	m	101	LMG	C1-O6-C5	-2.22	109.44	113.73
22	A	402	CLA	CBD-CHA-C1A	2.22	131.67	128.77
22	C	510	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
24	B	617	BCR	C35-C13-C14	-2.22	119.76	122.92
29	f	103	SQD	C3-C4-C5	2.22	114.15	110.17
22	b	612	CLA	C4B-C3B-CAB	-2.22	122.69	127.18
22	b	614	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
22	B	606	CLA	CHD-C4C-NC	2.22	125.83	124.28
23	D	407	PL9	C31-C32-C33	-2.21	105.35	111.64
25	C	515	DGD	C9B-C8B-C7B	-2.21	106.61	112.94
27	c	522	LMG	O3-C3-C2	-2.21	105.42	110.36
22	C	502	CLA	C1-C2-C3	-2.21	122.39	126.23
22	A	402	CLA	C4A-NA-C1A	2.21	109.50	106.38
27	C	521	LMG	C38-C37-C36	-2.21	102.82	114.56
27	D	412	LMG	O6-C1-O1	-2.21	104.66	109.93
22	B	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	b	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	C	511	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
27	C	521	LMG	O3-C3-C2	-2.21	105.42	110.36
27	i	101	LMG	O3-C3-C2	-2.21	105.42	110.36
22	C	509	CLA	C4A-NA-C1A	2.21	109.49	106.38
22	D	406	CLA	C1-C2-C3	-2.21	122.40	126.23
24	a	409	BCR	C33-C5-C6	-2.20	122.01	124.50
22	c	509	CLA	C4A-NA-C1A	2.21	109.49	106.38
22	c	505	CLA	C3A-C4A-CHB	-2.20	119.75	124.33
22	B	613	CLA	CMD-C2D-C3D	2.20	129.31	125.16
22	C	501	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
22	C	510	CLA	C3A-C4A-CHB	-2.20	119.75	124.33
31	d	401	PHO	C3D-C4D-ND	2.20	109.58	106.81
27	I	101	LMG	C20-C21-C22	-2.20	104.88	113.73
22	b	618	CLA	CHD-C4C-NC	2.20	125.82	124.28
22	C	505	CLA	C3A-C4A-CHB	-2.20	119.75	124.33
22	C	507	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
22	A	404	CLA	C4B-C3B-CAB	-2.20	122.72	127.18
27	e	101	LMG	O3-C3-C2	-2.20	105.44	110.36
22	D	406	CLA	C4A-NA-C1A	2.20	109.48	106.38
23	d	407	PL9	C12-C13-C14	-2.20	123.06	127.81
22	b	613	CLA	C4A-NA-C1A	2.20	109.48	106.38
22	c	501	CLA	C1B-CHB-C4A	-2.20	125.77	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	405	CLA	CHB-C4A-NA	2.20	127.44	124.38
27	C	521	LMG	C20-C21-C22	-2.20	104.89	113.73
22	B	601	CLA	C4A-NA-C1A	2.20	109.47	106.38
24	B	617	BCR	C11-C10-C9	-2.20	124.12	127.29
22	d	406	CLA	CMD-C2D-C3D	2.19	129.30	125.16
27	A	414	LMG	O3-C3-C2	-2.20	105.45	110.36
22	C	501	CLA	CMD-C2D-C3D	2.19	129.29	125.16
27	b	625	LMG	C38-C37-C36	-2.19	102.91	114.56
22	d	405	CLA	C4A-NA-C1A	2.19	109.47	106.38
22	C	504	CLA	CBA-CAA-C2A	2.19	119.31	113.95
22	A	405	CLA	CMD-C2D-C3D	2.19	129.29	125.16
27	e	101	LMG	O1-C7-C8	-2.19	105.77	110.99
27	I	101	LMG	C23-C22-C21	-2.19	106.67	112.94
27	c	518	LMG	O3-C3-C2	-2.19	105.46	110.36
27	C	521	LMG	C23-C22-C21	-2.19	106.68	112.94
24	c	521	BCR	C24-C23-C22	-2.19	122.94	126.22
22	b	606	CLA	CMD-C2D-C3D	2.19	129.28	125.16
24	b	622	BCR	C7-C8-C9	-2.19	122.94	126.22
27	D	412	LMG	O2-C2-C1	-2.19	105.28	110.03
24	A	407	BCR	C15-C14-C13	-2.19	124.12	127.29
24	b	622	BCR	C27-C26-C25	2.19	125.75	122.86
22	C	503	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
29	A	412	SQD	C5-C6-S	-2.19	111.35	114.40
24	K	102	BCR	C33-C5-C6	-2.18	122.03	124.50
22	b	605	CLA	C4A-NA-C1A	2.18	109.46	106.38
27	a	412	LMG	O1-C1-C2	-2.18	105.36	108.15
22	b	613	CLA	CMD-C2D-C3D	2.18	129.27	125.16
22	c	511	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	c	511	CLA	O2A-CGA-O1A	-2.18	117.78	123.48
22	D	406	CLA	CBD-CHA-C1A	2.18	131.62	128.77
27	B	621	LMG	C23-C22-C21	-2.18	106.72	112.94
24	a	409	BCR	C15-C14-C13	-2.18	124.14	127.29
27	I	101	LMG	O1-C1-C2	-2.18	105.36	108.15
22	a	404	CLA	CBD-CHA-C1A	2.18	131.62	128.77
22	D	405	CLA	CHB-C4A-NA	2.17	127.41	124.38
22	b	612	CLA	C4A-NA-C1A	2.18	109.45	106.38
22	b	618	CLA	C3A-C4A-CHB	-2.17	119.81	124.33
31	D	401	PHO	C3D-C4D-ND	2.17	109.55	106.81
27	c	522	LMG	C23-C22-C21	-2.17	106.74	112.94
22	c	510	CLA	C3A-C4A-CHB	-2.17	119.81	124.33
24	a	409	BCR	C15-C16-C17	-2.17	118.67	123.45
22	B	611	CLA	C1B-CHB-C4A	-2.17	125.82	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
27	c	522	LMG	C38-C37-C36	-2.17	103.04	114.56
24	x	101	BCR	C29-C30-C25	2.17	113.83	110.37
27	E	101	LMG	O1-C7-C8	-2.17	105.83	110.99
30	b	627	LMT	C1'-O5'-C5'	-2.17	109.54	113.73
24	b	621	BCR	C7-C8-C9	-2.17	122.97	126.22
29	f	103	SQD	C5-C6-S	-2.17	111.37	114.40
31	D	402	PHO	C3D-C4D-ND	2.17	109.54	106.81
29	d	403	SQD	C6-C5-C4	-2.17	107.29	111.86
24	A	407	BCR	C33-C5-C6	-2.17	122.05	124.50
24	b	623	BCR	C24-C23-C22	-2.16	122.98	126.22
27	c	522	LMG	C20-C21-C22	-2.16	105.03	113.73
22	c	508	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
31	D	401	PHO	CHD-C4C-NC	-2.16	124.82	128.68
22	c	506	CLA	CMD-C2D-C3D	2.16	129.24	125.16
22	d	405	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	d	406	CLA	CBD-CHA-C1A	2.16	131.60	128.77
25	d	410	DGD	O5D-C1E-C2E	2.16	110.92	108.15
23	A	406	PL9	C12-C13-C14	-2.16	123.13	127.81
27	B	621	LMG	C38-C37-C36	-2.16	103.08	114.56
27	C	518	LMG	O3-C3-C2	-2.16	105.53	110.36
22	D	406	CLA	C3A-C4A-CHB	-2.16	119.84	124.33
22	B	605	CLA	O1D-CGD-CBD	2.16	128.86	124.45
22	b	606	CLA	C4A-NA-C1A	2.16	109.42	106.38
22	b	619	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
22	B	603	CLA	C3A-C4A-CHB	-2.16	119.84	124.33
22	a	404	CLA	C4A-NA-C1A	2.16	109.42	106.38
29	A	412	SQD	C4-C3-C2	2.16	114.78	110.80
24	C	513	BCR	C7-C8-C9	-2.16	122.99	126.22
22	d	406	CLA	C3A-C4A-CHB	-2.15	119.85	124.33
27	A	414	LMG	O1-C7-C8	-2.16	105.86	110.99
22	c	501	CLA	CMD-C2D-C3D	2.15	129.22	125.16
22	B	610	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
22	B	612	CLA	CMD-C2D-C3D	2.15	129.22	125.16
22	c	511	CLA	C3A-C4A-CHB	-2.15	119.85	124.33
31	D	402	PHO	CMB-C2B-C1B	-2.15	121.85	125.68
24	F	102	BCR	C7-C8-C9	-2.15	123.00	126.22
27	b	625	LMG	C23-C22-C21	-2.15	106.79	112.94
22	c	508	CLA	C3A-C4A-CHB	-2.15	119.86	124.33
22	B	614	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
25	B	625	DGD	O6D-C1D-O3G	-2.15	104.81	109.93
22	d	405	CLA	O1D-CGD-CBD	2.15	128.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	E	101	LMG	O3-C3-C2	-2.15	105.56	110.36
27	B	621	LMG	C20-C21-C22	-2.15	105.09	113.73
22	b	614	CLA	CHD-C4C-NC	2.15	125.78	124.28
23	a	408	PL9	C32-C33-C34	-2.15	123.17	127.81
23	d	407	PL9	C36-C34-C33	-2.15	116.94	121.06
27	d	409	LMG	O6-C1-O1	-2.15	104.82	109.93
25	C	516	DGD	C3D-C4D-C5D	-2.15	106.32	110.17
27	b	625	LMG	C20-C21-C22	-2.14	105.10	113.73
22	b	611	CLA	C3A-C4A-CHB	-2.14	119.87	124.33
22	c	520	CLA	CHD-C4C-NC	2.14	125.78	124.28
27	M	101	LMG	O3-C3-C2	-2.14	105.57	110.36
27	D	409	LMG	O6-C1-O1	-2.14	104.83	109.93
22	b	607	CLA	C3A-C4A-CHB	-2.14	119.88	124.33
22	b	611	CLA	CBD-CHA-C1A	2.14	131.57	128.77
22	a	406	CLA	C4B-C3B-CAB	-2.14	122.84	127.18
34	f	101	HEM	C3A-C4A-NA	-2.14	108.07	109.50
24	J	102	BCR	C15-C16-C17	-2.14	118.74	123.45
24	B	617	BCR	C7-C8-C9	-2.14	123.02	126.22
25	D	410	DGD	C3D-C4D-C5D	-2.14	106.33	110.17
25	a	410	DGD	CAB-C9B-C8B	-2.14	103.22	114.56
22	C	503	CLA	CMD-C2D-C3D	2.13	129.18	125.16
22	C	507	CLA	CMD-C2D-C3D	2.13	129.18	125.16
22	b	607	CLA	CMD-C2D-C3D	2.13	129.18	125.16
29	a	401	SQD	C6-C5-C4	-2.13	107.36	111.86
22	B	609	CLA	C3A-C4A-CHB	-2.13	119.89	124.33
27	d	409	LMG	O6-C1-C2	-2.13	105.94	110.30
22	c	505	CLA	CMD-C2D-C3D	2.13	129.18	125.16
31	d	402	PHO	CMB-C2B-C1B	-2.13	121.88	125.68
24	B	618	BCR	C7-C8-C9	-2.13	123.02	126.22
22	C	511	CLA	C3A-C4A-CHB	-2.13	119.90	124.33
22	C	510	CLA	CMD-C2D-C3D	2.13	129.17	125.16
22	c	503	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
22	b	610	CLA	C1-C2-C3	-2.13	122.53	126.23
22	b	618	CLA	CMD-C2D-C3D	2.13	129.17	125.16
24	C	514	BCR	C24-C23-C22	-2.13	123.03	126.22
22	C	520	CLA	C3A-C4A-CHB	-2.13	119.91	124.33
22	b	612	CLA	C1-C2-C3	-2.13	122.54	126.23
24	b	621	BCR	C11-C10-C9	-2.13	124.22	127.29
22	b	619	CLA	C4B-C3B-CAB	-2.13	122.87	127.18
25	c	516	DGD	CBB-CAB-C9B	-2.12	103.29	114.56
26	a	411	LHG	C27-C26-C25	-2.12	103.29	114.56
22	C	501	CLA	CMB-C2B-C3B	2.12	129.16	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	m	101	LMG	O3-C3-C2	-2.12	105.62	110.36
22	b	605	CLA	C1-C2-C3	-2.12	122.55	126.23
24	B	619	BCR	C24-C23-C22	-2.12	123.05	126.22
27	A	414	LMG	O2-C2-C1	-2.12	105.43	110.03
23	a	408	PL9	C12-C13-C14	-2.12	123.23	127.81
22	C	508	CLA	C3A-C4A-CHB	-2.12	119.93	124.33
25	c	516	DGD	O2D-C2D-C1D	-2.11	105.44	110.03
22	H	101	CLA	CMD-C2D-C3D	2.11	129.15	125.16
25	A	408	DGD	CAB-C9B-C8B	-2.12	103.33	114.56
25	C	516	DGD	CBB-CAB-C9B	-2.12	103.33	114.56
24	A	407	BCR	C15-C16-C17	-2.12	118.79	123.45
30	B	623	LMT	O1'-C1'-C2'	2.11	110.86	108.15
22	B	614	CLA	C3A-C4A-CHB	-2.11	119.94	124.33
24	c	521	BCR	C33-C5-C6	-2.11	122.11	124.50
22	B	607	CLA	C3A-C4A-CHB	-2.11	119.93	124.33
29	B	622	SQD	C6-C5-C4	-2.11	107.40	111.86
29	f	103	SQD	O48-C23-C24	2.11	118.37	111.90
24	B	616	BCR	C15-C16-C17	-2.11	118.80	123.45
24	b	623	BCR	C38-C26-C25	-2.11	122.11	124.50
24	c	514	BCR	C24-C23-C22	-2.11	123.06	126.22
25	C	517	DGD	CBB-CAB-C9B	-2.11	103.35	114.56
24	C	514	BCR	C38-C26-C25	-2.11	122.11	124.50
25	b	601	DGD	CBB-CAB-C9B	-2.10	103.38	114.56
22	c	504	CLA	O1D-CGD-CBD	2.10	128.75	124.45
22	C	512	CLA	C3A-C4A-CHB	-2.10	119.96	124.33
22	H	101	CLA	C1-C2-C3	-2.10	122.58	126.23
22	a	407	CLA	C3A-C4A-CHB	-2.10	119.96	124.33
24	B	619	BCR	C38-C26-C25	-2.10	122.13	124.50
22	B	612	CLA	C3A-C4A-CHB	-2.10	119.97	124.33
22	c	502	CLA	C1-C2-C3	-2.10	122.59	126.23
24	H	102	BCR	C29-C30-C25	2.10	113.71	110.37
24	b	623	BCR	C33-C5-C6	-2.09	122.13	124.50
22	B	614	CLA	CMD-C2D-C3D	2.10	129.11	125.16
25	a	410	DGD	CDA-CCA-CBA	-2.09	106.95	112.94
22	C	504	CLA	C3A-C4A-CHB	-2.09	119.97	124.33
22	C	520	CLA	CMD-C2D-C3D	2.10	129.11	125.16
23	d	407	PL9	C46-C47-C48	-2.09	105.69	111.64
25	C	516	DGD	CAB-C9B-C8B	-2.09	103.45	114.56
25	C	516	DGD	O2D-C2D-C1D	-2.09	105.48	110.03
27	d	408	LMG	O1-C1-C2	-2.09	105.47	108.15
22	C	512	CLA	CMD-C2D-C3D	2.09	129.10	125.16
24	F	102	BCR	C15-C16-C17	-2.09	118.85	123.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	C3A-C4A-CHB	-2.09	119.98	124.33
23	a	408	PL9	C31-C32-C33	-2.09	105.71	111.64
27	M	101	LMG	C1-O6-C5	-2.09	109.70	113.73
25	b	601	DGD	C9A-C8A-C7A	-2.09	106.98	112.94
22	B	615	CLA	C4B-C3B-CAB	-2.09	122.95	127.18
24	g	101	BCR	C3-C2-C1	-2.09	106.82	114.77
27	e	101	LMG	O2-C2-C1	-2.08	105.50	110.03
25	B	625	DGD	CBB-CAB-C9B	-2.08	103.51	114.56
23	D	407	PL9	C42-C43-C44	-2.08	123.31	127.81
25	c	517	DGD	CBB-CAB-C9B	-2.08	103.52	114.56
27	E	101	LMG	O2-C2-C1	-2.08	105.51	110.03
22	B	611	CLA	C1-C2-C3	-2.08	122.62	126.23
22	c	512	CLA	C3A-C4A-CHB	-2.08	120.01	124.33
22	b	609	CLA	O1D-CGD-CBD	2.08	128.69	124.45
24	B	618	BCR	C27-C26-C25	2.08	125.60	122.86
23	d	407	PL9	O2-C1-C2	-2.07	116.88	121.82
23	A	406	PL9	C32-C33-C34	-2.07	123.32	127.81
26	A	409	LHG	C27-C26-C25	-2.08	103.54	114.56
22	c	506	CLA	O2A-CGA-O1A	-2.07	118.06	123.48
22	b	616	CLA	CMD-C2D-C3D	2.07	129.06	125.16
24	a	409	BCR	C24-C23-C22	-2.07	123.11	126.22
22	B	610	CLA	C4B-CHC-C1C	-2.07	124.75	127.47
29	B	622	SQD	C4-C3-C2	2.07	114.62	110.80
23	j	101	PL9	O2-C1-C2	-2.07	116.89	121.82
22	B	610	CLA	CHB-C4A-NA	2.07	127.27	124.38
25	c	515	DGD	O2D-C2D-C1D	-2.07	105.54	110.03
22	c	520	CLA	C3A-C4A-CHB	-2.07	120.03	124.33
25	b	601	DGD	CAB-C9B-C8B	-2.07	103.58	114.56
22	b	614	CLA	CHB-C4A-NA	2.07	127.27	124.38
27	D	408	LMG	O1-C7-C8	-2.07	106.07	110.99
31	d	402	PHO	CHD-C4C-NC	-2.07	124.99	128.68
22	B	605	CLA	C3A-C4A-CHB	-2.07	120.03	124.33
22	C	503	CLA	C3A-C4A-CHB	-2.07	120.03	124.33
31	D	401	PHO	CMB-C2B-C1B	-2.06	122.00	125.68
22	B	607	CLA	CHD-C4C-NC	2.07	125.73	124.28
25	B	625	DGD	C9A-C8A-C7A	-2.06	107.04	112.94
22	B	605	CLA	CMD-C2D-C3D	2.06	129.05	125.16
30	b	627	LMT	O1'-C1'-C2'	2.06	110.80	108.15
25	C	517	DGD	O2D-C2D-C1D	-2.06	105.55	110.03
25	C	516	DGD	C1D-C2D-C3D	-2.06	105.99	109.99
22	b	618	CLA	O2A-CGA-O1A	-2.06	118.09	123.48
29	A	413	SQD	C1-O5-C5	2.06	117.72	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	C3A-C4A-CHB	-2.06	120.05	124.33
30	M	103	LMT	O1'-C1'-C2'	2.06	110.79	108.15
22	b	608	CLA	C3A-C4A-CHB	-2.06	120.04	124.33
22	C	505	CLA	CMD-C2D-C3D	2.06	129.04	125.16
22	b	613	CLA	CHD-C4C-NC	2.06	125.72	124.28
25	C	517	DGD	C3G-O3G-C1D	2.06	117.94	113.80
23	D	407	PL9	C46-C47-C48	-2.06	105.79	111.64
25	C	515	DGD	O3E-C3E-C2E	-2.06	105.76	110.36
22	c	501	CLA	C3A-C4A-CHB	-2.06	120.05	124.33
25	d	410	DGD	C5B-C4B-C3B	-2.06	103.64	114.56
22	b	611	CLA	CHD-C4C-NC	2.06	125.72	124.28
22	c	502	CLA	C3A-C4A-CHB	-2.06	120.05	124.33
24	H	102	BCR	C27-C26-C25	2.06	125.58	122.86
22	B	609	CLA	CMD-C2D-C3D	2.06	129.04	125.16
31	D	402	PHO	C4D-CHA-CBD	-2.06	105.64	107.88
24	b	622	BCR	C33-C5-C6	-2.06	122.17	124.50
29	A	413	SQD	C6-C5-C4	-2.05	107.53	111.86
25	c	517	DGD	CAB-C9B-C8B	-2.05	103.66	114.56
31	d	401	PHO	CHD-C4C-NC	-2.05	125.01	128.68
25	A	408	DGD	CDA-CCA-CBA	-2.06	107.07	112.94
22	c	510	CLA	CMD-C2D-C3D	2.05	129.03	125.16
24	C	514	BCR	C7-C8-C9	-2.05	123.14	126.22
31	D	401	PHO	C4D-CHA-CBD	-2.05	105.64	107.88
27	D	408	LMG	O1-C1-C2	-2.05	105.52	108.15
29	d	403	SQD	C4-C3-C2	2.05	114.59	110.80
22	c	512	CLA	CMD-C2D-C3D	2.05	129.03	125.16
24	f	102	BCR	C15-C16-C17	-2.05	118.93	123.45
27	D	409	LMG	O3-C3-C2	-2.05	105.77	110.36
24	K	102	BCR	C7-C8-C9	-2.05	123.15	126.22
22	B	614	CLA	CHD-C4C-NC	2.05	125.72	124.28
25	B	625	DGD	CAB-C9B-C8B	-2.05	103.68	114.56
24	c	514	BCR	C38-C26-C25	-2.05	122.19	124.50
24	B	619	BCR	C33-C5-C6	-2.05	122.18	124.50
22	c	503	CLA	CMD-C2D-C3D	2.05	129.02	125.16
31	d	401	PHO	C4D-CHA-CBD	-2.05	105.65	107.88
22	C	504	CLA	O1D-CGD-CBD	2.05	128.63	124.45
23	J	101	PL9	O2-C1-C2	-2.05	116.94	121.82
22	B	608	CLA	C3A-C4A-CHB	-2.04	120.08	124.33
22	c	520	CLA	CMD-C2D-C3D	2.04	129.00	125.16
25	c	516	DGD	C3D-C4D-C5D	-2.04	106.51	110.17
22	c	507	CLA	C3A-C4A-CHB	-2.04	120.08	124.33
26	C	519	LHG	C27-C26-C25	-2.04	103.73	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	C1-C2-C3	-2.04	122.69	126.23
22	b	614	CLA	C4B-CHC-C1C	-2.04	124.79	127.47
22	h	101	CLA	C3A-C4A-CHB	-2.04	120.09	124.33
22	C	501	CLA	C3A-C4A-CHB	-2.04	120.10	124.33
22	B	601	CLA	O2A-CGA-O1A	-2.04	118.16	123.48
31	d	401	PHO	C1-C2-C3	-2.04	122.70	126.23
22	b	609	CLA	C3A-C4A-CHB	-2.04	120.09	124.33
34	F	101	HEM	C3A-C4A-NA	-2.04	108.14	109.50
22	C	509	CLA	C4B-C3B-CAB	-2.04	123.05	127.18
24	y	101	BCR	C3-C2-C1	-2.04	107.01	114.77
25	D	410	DGD	C5B-C4B-C3B	-2.04	103.75	114.56
22	B	601	CLA	C3A-C4A-CHB	-2.03	120.10	124.33
24	b	621	BCR	C24-C23-C22	-2.03	123.17	126.22
25	C	515	DGD	O2D-C2D-C1D	-2.03	105.62	110.03
22	c	509	CLA	C3A-C4A-CHB	-2.03	120.10	124.33
22	B	603	CLA	O2A-CGA-O1A	-2.03	118.17	123.48
22	b	605	CLA	C3A-C4A-CHB	-2.03	120.11	124.33
22	B	610	CLA	CHD-C4C-NC	2.03	125.70	124.28
22	b	612	CLA	C3A-C4A-CHB	-2.03	120.11	124.33
22	a	406	CLA	C3A-C4A-CHB	-2.03	120.11	124.33
23	D	407	PL9	O2-C1-C2	-2.03	116.99	121.82
22	b	608	CLA	CMD-C2D-C3D	2.03	128.98	125.16
25	C	517	DGD	CAB-C9B-C8B	-2.03	103.79	114.56
22	B	615	CLA	CMD-C2D-C3D	2.03	128.98	125.16
24	H	102	BCR	C16-C15-C14	-2.03	118.98	123.45
31	d	402	PHO	C4D-CHA-CBD	-2.02	105.67	107.88
25	D	410	DGD	O5D-C1E-C2E	2.03	110.75	108.15
27	C	521	LMG	C1-C2-C3	-2.03	106.06	109.99
24	g	101	BCR	C15-C16-C17	-2.03	118.99	123.45
25	c	516	DGD	CAB-C9B-C8B	-2.02	103.81	114.56
23	A	406	PL9	O2-C1-C2	-2.02	117.00	121.82
22	c	510	CLA	C1-C2-C3	-2.02	122.72	126.23
22	B	606	CLA	CMD-C2D-C3D	2.02	128.97	125.16
22	b	619	CLA	CMD-C2D-C3D	2.02	128.97	125.16
24	H	102	BCR	C7-C8-C9	-2.02	123.19	126.22
23	a	408	PL9	O2-C1-C2	-2.02	117.00	121.82
22	c	503	CLA	C3A-C4A-CHB	-2.02	120.13	124.33
26	c	519	LHG	C27-C26-C25	-2.02	103.84	114.56
25	C	515	DGD	C5B-C4B-C3B	-2.02	103.85	114.56
25	b	601	DGD	O3E-C3E-C2E	-2.02	105.85	110.36
27	c	518	LMG	O1-C7-C8	-2.02	106.19	110.99
25	B	620	DGD	C4E-C3E-C2E	-2.02	107.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	404	CLA	CHD-C4C-NC	2.02	125.69	124.28
24	A	407	BCR	C38-C26-C25	-2.02	122.22	124.50
23	D	407	PL9	C36-C34-C33	-2.01	117.19	121.06
22	A	405	CLA	C3A-C4A-CHB	-2.01	120.14	124.33
25	c	515	DGD	C5B-C4B-C3B	-2.01	103.87	114.56
22	A	402	CLA	C3A-C4A-CHB	-2.01	120.14	124.33
27	A	414	LMG	C1-C2-C3	-2.01	106.09	109.99
23	A	406	PL9	C11-C12-C13	-2.01	105.92	111.64
27	a	412	LMG	C1-O6-C5	-2.01	109.84	113.73
24	B	616	BCR	C7-C8-C9	-2.01	123.21	126.22
22	C	502	CLA	C3A-C4A-CHB	-2.01	120.15	124.33
27	I	101	LMG	O1-C7-C8	-2.01	106.21	110.99
23	A	406	PL9	C31-C32-C33	-2.01	105.93	111.64
22	H	101	CLA	C3A-C4A-CHB	-2.01	120.15	124.33
22	c	509	CLA	CMD-C2D-C3D	2.01	128.95	125.16
23	d	407	PL9	C42-C43-C44	-2.01	123.47	127.81
22	b	616	CLA	C1-C2-C3	-2.00	122.75	126.23
22	c	509	CLA	O2A-CGA-O1A	-2.00	118.24	123.48
22	b	616	CLA	C3A-C4A-CHB	-2.00	120.17	124.33
25	D	410	DGD	O3E-C3E-C2E	-2.00	105.88	110.36
22	c	504	CLA	C3A-C4A-CHB	-2.00	120.17	124.33
22	B	602	CLA	O2A-CGA-O1A	-2.00	118.25	123.48
24	a	409	BCR	C38-C26-C25	-2.00	122.24	124.50
22	B	608	CLA	CHD-C4C-NC	2.00	125.68	124.28
22	A	404	CLA	C3A-C4A-CHB	-2.00	120.17	124.33
22	B	611	CLA	C3A-C4A-CHB	-2.00	120.17	124.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	B	622	SQD	C45-O47-C7-C8
29	d	403	SQD	C45-O47-C7-C8
25	C	516	DGD	C2G-O2G-C1B-C2B
25	c	516	DGD	C2G-O2G-C1B-C2B

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	335/344 (97%)	0.95	38 (11%) 6 10	178, 179, 180, 181	0
1	a	335/344 (97%)	1.11	65 (19%) 2 4	178, 179, 180, 181	0
2	B	490/510 (96%)	0.78	50 (10%) 7 12	178, 179, 180, 181	0
2	b	490/510 (96%)	0.92	72 (14%) 3 6	178, 179, 180, 181	0
3	C	447/461 (96%)	0.84	54 (12%) 5 9	178, 179, 180, 181	0
3	c	447/461 (96%)	0.79	47 (10%) 7 11	178, 180, 180, 181	0
4	D	340/352 (96%)	0.74	28 (8%) 12 16	177, 179, 180, 181	0
4	d	340/352 (96%)	0.80	42 (12%) 5 9	177, 179, 180, 181	0
5	E	82/84 (97%)	0.70	7 (8%) 11 15	178, 180, 180, 181	0
5	e	82/84 (97%)	0.66	6 (7%) 15 18	178, 180, 181, 181	0
6	F	35/45 (77%)	0.33	2 (5%) 23 23	179, 179, 180, 180	0
6	f	35/45 (77%)	0.31	4 (11%) 6 10	179, 180, 181, 181	0
7	H	65/66 (98%)	1.17	17 (26%) 1 3	179, 180, 180, 181	0
7	h	65/66 (98%)	1.42	24 (36%) 1 2	179, 180, 181, 181	0
8	I	35/38 (92%)	0.62	1 (2%) 49 41	178, 179, 180, 181	0
8	i	35/38 (92%)	0.66	2 (5%) 23 23	179, 179, 181, 181	0
9	J	34/40 (85%)	0.55	3 (8%) 10 15	178, 179, 180, 180	0
9	j	34/40 (85%)	0.04	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	0.23	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.95	8 (21%) 1 3	179, 180, 181, 181	0
11	L	37/37 (100%)	1.50	12 (32%) 1 3	178, 179, 180, 181	0
11	l	37/37 (100%)	1.00	6 (16%) 2 5	178, 179, 180, 181	0
12	M	34/36 (94%)	0.97	4 (11%) 5 10	178, 179, 180, 181	0
12	m	34/36 (94%)	0.63	1 (2%) 49 41	178, 179, 180, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	1.12	48 (19%) 2 4	177, 179, 180, 181	0
13	o	243/272 (89%)	1.13	48 (19%) 2 4	177, 179, 181, 181	0
14	T	32/32 (100%)	0.88	2 (6%) 19 21	178, 179, 181, 181	0
14	t	32/32 (100%)	1.36	7 (21%) 1 3	178, 179, 180, 181	0
15	U	97/134 (72%)	1.10	12 (12%) 5 9	178, 179, 180, 181	0
15	u	97/134 (72%)	1.54	35 (36%) 1 2	178, 179, 180, 181	0
16	V	137/163 (84%)	0.68	12 (8%) 10 15	178, 179, 180, 181	0
16	v	137/163 (84%)	0.82	19 (13%) 4 7	178, 180, 181, 181	0
17	g	28/46 (60%)	1.40	4 (14%) 3 6	179, 180, 181, 182	0
17	y	28/46 (60%)	0.59	2 (7%) 16 19	178, 180, 181, 181	0
18	X	37/41 (90%)	0.77	2 (5%) 25 24	179, 179, 181, 181	0
18	x	37/41 (90%)	1.13	7 (18%) 2 4	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.80	6 (9%) 8 13	179, 180, 181, 181	0
20	z	62/62 (100%)	1.12	8 (12%) 4 8	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.89	705 (13%) 4 7	177, 179, 180, 182	0

All (705) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	169	LYS	9.1
5	e	84	LYS	9.0
7	H	66	GLY	7.3
15	U	38	GLU	6.5
5	E	84	LYS	6.2
1	a	172	MET	6.1
14	t	32	LYS	6.0
3	C	149	TYR	5.7
2	B	69	LEU	5.7
1	a	239	PHE	5.6
13	O	244	GLU	5.6
13	o	153	ALA	5.6
17	g	27	MET	5.5
15	u	72	TYR	5.5
3	C	140	LEU	5.5
13	o	168	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	a	299	GLY	5.4
14	t	30	THR	5.3
13	o	111	LEU	5.3
1	A	198	HIS	5.3
1	a	137	LEU	5.3
13	O	223	ILE	5.1
1	a	183	MET	5.1
1	A	299	GLY	5.0
1	a	175	GLY	5.0
3	C	266	TRP	5.0
3	C	151	TRP	4.9
1	A	293	MET	4.9
5	e	82	GLN	4.8
10	k	10	LYS	4.8
2	b	229	LEU	4.8
1	a	190	HIS	4.8
4	d	295	SER	4.8
3	C	148	GLY	4.7
14	t	29	ILE	4.7
3	C	147	PHE	4.7
5	e	55	TYR	4.7
10	k	11	LEU	4.7
4	d	191	TRP	4.7
1	a	179	THR	4.7
3	C	139	THR	4.7
15	U	39	LEU	4.6
14	t	31	LYS	4.6
7	h	14	LEU	4.6
3	c	372	PRO	4.6
3	C	261	ARG	4.6
4	d	246	MET	4.5
1	a	198	HIS	4.5
20	Z	1	MET	4.5
13	o	112	LYS	4.5
2	b	122	LEU	4.4
13	o	110	GLU	4.4
4	D	199	MET	4.4
7	h	4	ARG	4.4
4	D	197	HIS	4.4
2	B	83	GLU	4.4
1	a	240	GLY	4.4
3	C	143	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	195	HIS	4.4
2	B	402	TYR	4.4
2	b	133	LEU	4.3
13	o	120	THR	4.3
13	O	225	LEU	4.3
4	d	197	HIS	4.3
3	C	152	LYS	4.2
2	b	218	LEU	4.2
4	D	24	ARG	4.2
2	B	70	GLY	4.2
1	A	262	TYR	4.2
1	a	286	THR	4.2
2	b	187	PRO	4.1
13	O	243	SER	4.1
9	J	7	ARG	4.1
15	u	57	LEU	4.0
7	H	64	ALA	4.0
1	a	187	GLN	4.0
2	b	228	ALA	4.0
3	C	212	TYR	4.0
2	b	173	GLY	4.0
3	c	260	ALA	4.0
11	l	8	GLN	4.0
18	x	11	THR	4.0
7	h	11	LEU	4.0
2	b	411	PHE	4.0
6	F	11	VAL	4.0
7	H	65	LEU	3.9
11	L	9	PRO	3.9
13	o	237	ILE	3.9
1	a	165	GLN	3.9
1	A	294	ALA	3.9
2	b	420	TYR	3.9
13	o	31	LEU	3.9
3	C	141	GLU	3.9
3	C	258	GLY	3.9
4	D	191	TRP	3.9
7	H	6	TRP	3.8
13	O	170	GLY	3.8
2	B	164	PRO	3.8
3	c	97	TRP	3.8
3	c	202	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	a	81	ALA	3.8
1	a	178	GLY	3.8
11	L	7	ARG	3.8
13	O	261	ILE	3.8
13	O	222	GLN	3.8
13	o	225	LEU	3.8
15	U	121	LEU	3.8
3	C	44	ASN	3.8
15	u	71	LEU	3.8
2	B	166	MET	3.8
13	O	169	LYS	3.7
15	u	116	GLU	3.7
15	U	92	LEU	3.7
4	d	199	MET	3.7
9	J	8	ILE	3.7
16	V	38	LEU	3.7
2	B	165	GLY	3.7
1	a	199	GLN	3.7
13	o	242	GLU	3.7
1	A	190	HIS	3.6
7	H	11	LEU	3.6
13	o	223	ILE	3.6
2	b	188	ASP	3.6
7	h	54	ILE	3.6
13	o	154	SER	3.6
15	u	75	LEU	3.6
16	V	96	GLU	3.6
2	b	69	LEU	3.6
1	a	224	ILE	3.5
2	b	490	GLN	3.5
3	C	142	GLU	3.5
1	a	191	ASN	3.5
2	b	301	ALA	3.5
13	O	91	PHE	3.5
4	d	194	ASN	3.5
3	c	264	PHE	3.5
13	o	124	GLU	3.5
16	V	95	ILE	3.5
3	C	402	GLY	3.5
10	k	15	TYR	3.5
18	x	16	LEU	3.5
3	C	262	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
15	u	58	ASN	3.5
13	o	229	LYS	3.5
1	a	192	ILE	3.5
3	C	257	PHE	3.5
4	d	195	PRO	3.5
10	k	12	PRO	3.5
7	H	63	LYS	3.5
2	b	226	TYR	3.4
2	b	309	LEU	3.4
2	B	343	HIS	3.4
5	e	56	TYR	3.4
13	O	242	GLU	3.4
2	B	338	GLN	3.4
2	b	482	ILE	3.4
20	z	4	LEU	3.4
1	a	176	ILE	3.4
11	L	8	GLN	3.4
7	h	55	LEU	3.4
1	A	165	GLN	3.4
13	o	238	ALA	3.4
3	C	154	LYS	3.4
1	A	192	ILE	3.4
18	x	47	GLN	3.4
2	B	420	TYR	3.4
15	u	65	PHE	3.4
2	b	137	LYS	3.4
1	A	179	THR	3.3
15	u	47	LEU	3.3
15	u	53	GLU	3.3
2	B	161	LEU	3.3
7	h	66	GLY	3.3
2	b	296	ALA	3.3
11	L	5	PRO	3.3
2	b	308	LYS	3.3
15	u	115	THR	3.3
10	k	14	ALA	3.3
11	l	34	TYR	3.3
16	v	47	LEU	3.3
4	d	221	THR	3.3
4	D	281	MET	3.3
1	a	238	LYS	3.2
5	E	17	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	137	PRO	3.2
18	x	12	ILE	3.2
15	u	107	GLU	3.2
13	O	224	SER	3.2
3	c	149	TYR	3.2
3	c	259	TRP	3.2
4	D	174	GLY	3.2
2	b	402	TYR	3.2
13	o	224	SER	3.2
13	o	121	PHE	3.2
1	A	175	GLY	3.2
7	h	15	ASN	3.2
2	B	476	ARG	3.2
2	B	185	TRP	3.2
3	C	146	PHE	3.1
2	B	411	PHE	3.1
1	a	149	ALA	3.1
2	b	120	LEU	3.1
1	a	195	HIS	3.1
4	d	200	GLY	3.1
1	a	150	PRO	3.1
3	c	95	LEU	3.1
15	u	103	GLN	3.1
15	u	76	ALA	3.1
2	B	179	GLN	3.1
4	D	198	MET	3.1
2	B	474	LEU	3.1
13	o	269	ILE	3.1
15	U	65	PHE	3.1
1	A	298	ASN	3.1
2	b	397	VAL	3.1
2	b	398	THR	3.0
15	u	51	TYR	3.0
3	C	183	GLY	3.0
7	h	8	GLY	3.0
12	m	1	MET	3.0
2	b	219	VAL	3.0
3	C	43	ILE	3.0
7	H	10	ILE	3.0
3	c	375	LEU	3.0
13	O	259	VAL	3.0
2	b	412	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	184	GLY	3.0
14	T	28	ARG	3.0
1	a	282	GLY	3.0
2	b	172	TYR	3.0
11	l	9	PRO	3.0
1	a	325	ASN	3.0
15	u	85	TYR	3.0
2	B	429	ILE	3.0
1	a	300	PHE	2.9
15	u	79	ILE	2.9
3	c	343	ARG	2.9
2	b	262	THR	2.9
14	t	28	ARG	2.9
2	b	267	LEU	2.9
7	H	7	LEU	2.9
11	L	34	TYR	2.9
13	o	267	ALA	2.9
4	d	198	MET	2.9
13	o	123	GLU	2.9
3	c	411	ALA	2.9
13	O	260	LYS	2.9
13	O	245	GLN	2.9
4	d	189	HIS	2.9
2	b	167	TRP	2.9
4	D	190	ASN	2.9
4	d	201	VAL	2.9
11	l	7	ARG	2.9
6	f	16	PHE	2.9
12	M	2	GLU	2.9
16	V	43	LYS	2.9
1	a	139	MET	2.9
13	O	262	GLN	2.9
2	B	8	VAL	2.9
13	o	170	GLY	2.9
3	C	237	HIS	2.9
1	A	261	GLN	2.9
4	D	171	PRO	2.9
2	b	123	PHE	2.9
1	a	173	PRO	2.8
16	V	94	ASN	2.8
7	H	27	THR	2.8
13	o	155	THR	2.8

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Mol	Chain	Res	Type	RSRZ
15	U	40	VAL	2.8
2	b	132	ALA	2.8
1	A	11	ALA	2.8
13	O	195	ASP	2.8
15	u	62	ILE	2.8
7	h	13	PRO	2.8
1	a	303	ASN	2.8
1	a	80	GLY	2.8
20	Z	57	LEU	2.8
3	c	203	THR	2.8
11	L	6	ASN	2.8
2	b	302	TRP	2.8
1	a	301	ASN	2.8
15	u	74	THR	2.8
2	b	312	TYR	2.8
3	C	457	LYS	2.8
3	c	266	TRP	2.8
10	k	43	VAL	2.8
15	u	114	VAL	2.8
1	A	212	CYS	2.8
3	c	371	GLY	2.8
15	u	117	VAL	2.8
16	v	104	ASN	2.8
1	a	133	LEU	2.8
7	H	56	ASP	2.8
8	I	34	ARG	2.8
2	b	417	VAL	2.8
3	c	112	PHE	2.8
2	b	393	GLU	2.8
13	O	126	GLY	2.8
2	b	261	ALA	2.8
11	L	30	LEU	2.8
1	a	201	GLY	2.7
3	C	260	ALA	2.7
16	v	138	LEU	2.7
16	V	37	PRO	2.7
7	h	18	TYR	2.7
4	d	242	GLU	2.7
4	D	228	GLY	2.7
7	H	14	LEU	2.7
7	h	56	ASP	2.7
7	H	5	THR	2.7

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Mol	Chain	Res	Type	RSRZ
13	o	119	LEU	2.7
3	C	202	PRO	2.7
3	C	150	ASP	2.7
13	O	90	GLU	2.7
15	U	102	LYS	2.7
1	A	10	SER	2.7
2	b	323	GLY	2.7
4	D	170	ALA	2.7
1	A	80	GLY	2.7
1	A	201	GLY	2.7
1	a	177	SER	2.7
2	b	121	GLU	2.7
2	b	217	ILE	2.7
3	c	99	VAL	2.7
16	v	103	LYS	2.7
2	B	477	ASP	2.7
4	d	137	GLY	2.7
4	d	278	GLY	2.7
13	O	127	ILE	2.7
16	v	141	ILE	2.7
13	o	64	TYR	2.7
11	L	1	MET	2.7
4	D	195	PRO	2.7
2	b	379	ALA	2.7
15	u	104	ILE	2.7
17	y	46	LEU	2.7
4	d	285	GLY	2.7
1	A	248	ILE	2.7
4	D	229	ALA	2.7
4	d	281	MET	2.7
20	z	17	PHE	2.7
13	O	190	LEU	2.7
2	b	68	ARG	2.6
2	b	78	TRP	2.6
2	b	166	MET	2.6
6	F	13	TYR	2.6
12	M	5	GLN	2.6
13	o	152	VAL	2.6
18	x	42	GLN	2.6
2	b	298	LEU	2.6
16	v	130	MET	2.6
5	e	83	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
13	o	88	GLU	2.6
3	c	204	LEU	2.6
15	u	46	LYS	2.6
2	b	292	LEU	2.6
20	z	62	VAL	2.6
16	v	74	THR	2.6
15	u	59	ASN	2.6
4	D	172	SER	2.6
4	D	227	GLU	2.6
3	C	97	TRP	2.6
3	C	135	ARG	2.6
4	D	14	TRP	2.6
15	U	62	ILE	2.6
2	B	122	LEU	2.6
2	B	401	PHE	2.6
3	c	370	ARG	2.6
15	u	106	ARG	2.6
20	z	21	ILE	2.6
4	D	296	TYR	2.6
3	c	256	PRO	2.6
2	b	406	LEU	2.6
5	E	82	GLN	2.6
20	z	1	MET	2.6
1	a	333	GLU	2.6
3	c	263	ALA	2.6
3	C	473	ASP	2.6
3	c	75	PHE	2.6
7	h	53	LEU	2.6
4	D	177	ALA	2.5
1	a	322	ASN	2.5
2	B	84	THR	2.5
13	O	56	TYR	2.5
3	c	405	ASN	2.5
1	a	138	GLY	2.5
1	A	137	LEU	2.5
1	A	183	MET	2.5
7	H	8	GLY	2.5
2	b	214	LEU	2.5
2	B	431	GLU	2.5
3	C	201	ASN	2.5
20	z	9	LEU	2.5
13	O	234	THR	2.5

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Mol	Chain	Res	Type	RSRZ
15	u	101	GLN	2.5
2	B	475	PHE	2.5
4	d	136	VAL	2.5
15	u	131	GLY	2.5
16	v	133	LEU	2.5
1	a	18	CYS	2.5
13	O	73	PRO	2.5
2	B	345	VAL	2.5
4	D	201	VAL	2.5
1	A	266	ASN	2.5
11	L	37	ASN	2.5
2	B	341	LYS	2.5
3	c	329	GLY	2.5
1	a	336	ALA	2.5
13	O	269	ILE	2.5
3	c	262	ARG	2.5
13	O	168	PHE	2.5
16	v	102	MET	2.5
2	B	289	GLN	2.5
4	d	217	THR	2.5
7	H	30	LEU	2.5
13	o	122	VAL	2.5
2	b	134	ASP	2.5
13	o	63	THR	2.5
18	X	42	GLN	2.5
1	A	196	PRO	2.5
4	d	262	SER	2.5
1	a	136	ARG	2.5
7	h	9	ASP	2.4
2	b	294	SER	2.4
7	h	58	VAL	2.4
13	O	107	ILE	2.4
3	c	200	THR	2.4
2	b	185	TRP	2.4
8	i	15	PHE	2.4
1	a	225	ARG	2.4
3	C	413	GLU	2.4
18	x	46	VAL	2.4
1	a	334	ARG	2.4
2	b	266	GLU	2.4
14	t	1	MET	2.4
7	h	7	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	a	298	ASN	2.4
7	H	3	ARG	2.4
13	O	251	MET	2.4
3	c	151	TRP	2.4
13	o	262	GLN	2.4
13	o	69	LEU	2.4
15	U	42	VAL	2.4
3	c	78	GLU	2.4
13	o	167	ASP	2.4
2	b	488	PRO	2.4
4	D	282	SER	2.4
4	d	58	TRP	2.4
1	A	342	ASP	2.4
3	C	269	GLU	2.4
16	V	97	GLY	2.4
1	a	182	PHE	2.4
13	O	119	LEU	2.4
4	d	138	VAL	2.4
1	A	191	ASN	2.4
7	H	55	LEU	2.4
16	V	47	LEU	2.4
13	O	84	ASN	2.4
13	O	69	LEU	2.4
15	u	70	GLY	2.4
14	T	27	PRO	2.4
2	b	138	MET	2.4
4	D	77	ALA	2.4
2	b	341	LYS	2.4
1	a	200	LEU	2.4
16	v	111	GLU	2.4
3	c	349	ILE	2.4
2	B	155	ALA	2.4
7	h	12	ARG	2.4
2	B	339	ALA	2.4
2	b	141	ILE	2.4
2	B	183	PRO	2.3
13	O	111	LEU	2.3
6	f	15	ILE	2.3
8	i	30	ARG	2.3
3	C	268	GLY	2.3
3	c	191	PRO	2.3
15	U	64	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
17	g	26	ALA	2.3
3	C	204	LEU	2.3
13	o	246	LEU	2.3
4	D	200	GLY	2.3
13	O	218	LEU	2.3
16	V	78	LEU	2.3
4	D	297	ASP	2.3
4	d	289	LEU	2.3
2	B	214	LEU	2.3
2	B	337	ALA	2.3
2	b	190	PHE	2.3
20	Z	35	ARG	2.3
2	B	410	THR	2.3
13	o	240	THR	2.3
16	v	52	TYR	2.3
2	B	133	LEU	2.3
13	O	175	PRO	2.3
13	O	233	ARG	2.3
2	b	227	LYS	2.3
3	C	105	VAL	2.3
4	D	189	HIS	2.3
4	d	294	ARG	2.3
13	O	229	LYS	2.3
3	C	42	LEU	2.3
6	f	13	TYR	2.3
3	c	373	ASN	2.3
6	f	11	VAL	2.3
7	h	62	TRP	2.3
1	A	250	ALA	2.3
3	c	324	LEU	2.3
13	o	66	ILE	2.3
17	g	30	ILE	2.3
4	D	194	ASN	2.3
1	A	161	TYR	2.3
2	b	409	GLN	2.3
1	A	172	MET	2.3
1	a	26	ASN	2.3
7	h	30	LEU	2.3
11	l	30	LEU	2.3
13	o	264	VAL	2.3
1	a	153	SER	2.3
3	C	27	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
13	O	58	ILE	2.3
2	b	340	TRP	2.3
1	A	204	GLY	2.3
4	d	275	PRO	2.3
13	o	239	GLY	2.3
20	Z	34	ASP	2.3
1	a	287	ALA	2.3
15	u	105	LEU	2.3
1	A	289	GLY	2.3
7	h	23	PRO	2.3
13	o	90	GLU	2.3
16	V	39	ASN	2.3
4	d	332	GLN	2.3
4	d	202	ALA	2.2
4	d	203	GLY	2.2
20	z	20	VAL	2.2
15	u	73	PRO	2.2
2	b	322	GLY	2.2
7	H	9	ASP	2.2
4	d	241	GLU	2.2
2	B	292	LEU	2.2
2	B	295	GLY	2.2
3	C	157	MET	2.2
4	D	226	GLY	2.2
4	d	205	LEU	2.2
20	Z	4	LEU	2.2
1	a	181	ASN	2.2
13	O	258	GLU	2.2
16	V	111	GLU	2.2
13	O	55	ALA	2.2
4	d	214	HIS	2.2
5	E	21	VAL	2.2
3	C	144	SER	2.2
4	d	219	GLU	2.2
4	d	220	ASN	2.2
13	O	202	GLN	2.2
3	C	98	GLY	2.2
4	d	245	SER	2.2
1	a	166	GLY	2.2
3	c	365	TRP	2.2
3	C	185	LEU	2.2
2	b	70	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	338	GLN	2.2
1	a	202	VAL	2.2
1	A	286	THR	2.2
5	E	15	THR	2.2
3	c	288	CYS	2.2
7	h	3	ARG	2.2
7	h	57	GLY	2.2
18	X	13	THR	2.2
3	c	364	PRO	2.2
11	L	33	SER	2.2
3	C	45	LEU	2.2
13	o	265	PHE	2.2
15	U	128	TYR	2.2
15	u	50	ALA	2.2
2	b	399	VAL	2.2
2	B	218	LEU	2.2
12	M	34	LYS	2.2
16	v	113	GLU	2.2
4	d	239	GLN	2.2
11	L	28	ALA	2.2
1	a	79	THR	2.2
16	V	116	GLU	2.2
2	B	3	LEU	2.2
12	M	4	ASN	2.2
20	z	52	LEU	2.2
3	C	153	ASP	2.2
16	v	51	GLN	2.2
2	b	354	LEU	2.2
3	c	105	VAL	2.2
13	O	31	LEU	2.2
18	x	13	THR	2.2
1	A	296	ASN	2.1
2	B	187	PRO	2.1
13	o	151	LEU	2.1
1	a	237	TYR	2.1
15	u	52	GLY	2.1
4	d	204	VAL	2.1
5	E	64	PRO	2.1
4	d	248	THR	2.1
15	u	133	TYR	2.1
3	c	185	LEU	2.1
5	e	49	THR	2.1

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Mol	Chain	Res	Type	RSRZ
15	u	92	LEU	2.1
2	B	180	PRO	2.1
13	o	228	ALA	2.1
2	b	474	LEU	2.1
16	v	78	LEU	2.1
20	Z	40	ILE	2.1
13	o	213	VAL	2.1
2	b	370	LEU	2.1
1	A	14	TRP	2.1
2	B	296	ALA	2.1
2	b	230	ARG	2.1
13	O	125	ASP	2.1
2	b	174	LEU	2.1
3	c	186	TYR	2.1
3	c	209	ILE	2.1
7	h	27	THR	2.1
16	v	145	ILE	2.1
2	B	91	TRP	2.1
3	c	357	ARG	2.1
13	O	48	LEU	2.1
13	o	263	GLY	2.1
11	L	4	ASN	2.1
1	A	199	GLN	2.1
1	a	335	ASN	2.1
4	d	59	TYR	2.1
13	O	146	PHE	2.1
1	a	170	ASP	2.1
3	c	403	SER	2.1
1	a	76	ASN	2.1
16	v	89	THR	2.1
1	A	229	GLU	2.1
1	A	300	PHE	2.1
1	a	188	ALA	2.1
16	v	142	ALA	2.1
2	B	409	GLN	2.1
3	C	145	SER	2.1
2	B	424	ALA	2.1
3	C	253	LEU	2.1
3	c	387	TRP	2.1
15	U	75	LEU	2.1
2	b	215	PHE	2.1
16	v	131	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
17	y	42	ARG	2.1
17	g	45	ASN	2.1
3	C	256	PRO	2.1
2	B	120	LEU	2.1
3	c	42	LEU	2.1
4	D	211	CYS	2.1
1	a	250	ALA	2.1
7	h	16	SER	2.1
2	B	314	TYR	2.1
4	d	310	GLU	2.1
5	E	18	ARG	2.1
1	a	328	MET	2.1
3	c	213	LEU	2.1
13	O	113	VAL	2.1
4	d	13	GLY	2.1
9	J	9	PRO	2.1
13	o	157	PRO	2.1
13	o	236	GLU	2.1
13	O	153	ALA	2.0
2	B	7	ARG	2.0
3	C	203	THR	2.0
1	a	186	PHE	2.0
3	C	403	SER	2.0
13	O	216	PHE	2.0
1	A	287	ALA	2.0
3	C	89	ILE	2.0
3	C	46	SER	2.0
2	b	485	GLU	2.0
2	B	67	ALA	2.0
4	d	282	SER	2.0
7	h	10	ILE	2.0
2	b	287	ARG	2.0
4	D	192	THR	2.0
13	o	84	ASN	2.0
1	a	324	ALA	2.0
3	C	265	ILE	2.0
10	k	17	ILE	2.0
16	v	58	LEU	2.0
1	A	152	ALA	2.0
13	o	226	ASN	2.0
10	k	44	GLY	2.0
1	a	156	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
14	t	2	GLU	2.0
13	O	78	VAL	2.0
15	u	113	THR	2.0
1	a	194	MET	2.0
2	B	326	ARG	2.0
2	B	347	ARG	2.0
13	o	104	LEU	2.0
3	c	328	VAL	2.0
3	c	452	ALA	2.0
4	d	218	VAL	2.0
2	b	295	GLY	2.0
3	c	388	GLN	2.0
11	l	31	PHE	2.0
13	O	177	TYR	2.0
15	u	118	GLU	2.0
1	a	75	ASN	2.0
3	c	207	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
27	LMG	i	101	43/55	0.65	8.15	177,180,182,184	0
24	BCR	c	521	40/40	1.73	6.78	178,179,181,181	0
35	CA	K	101	1/1	0.47	6.38	184,184,184,184	0
25	DGD	D	410	63/66	0.88	5.89	178,181,182,183	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	C	518	45/55	1.19	5.57	178,179,180,181	0
24	BCR	y	101	40/40	0.90	5.47	177,179,180,180	0
30	LMT	i	102	35/35	0.78	5.44	178,181,183,183	0
23	PL9	J	101	35/55	0.52	5.25	177,180,181,181	0
25	DGD	d	410	63/66	0.88	5.23	178,180,183,183	0
30	LMT	I	102	35/35	0.89	5.20	178,180,182,183	0
23	PL9	j	101	35/55	0.39	5.04	179,180,181,181	0
22	CLA	c	512	65/65	0.97	4.70	178,180,181,182	0
30	LMT	D	411	31/35	0.92	4.54	179,180,182,182	0
22	CLA	A	405	65/65	0.70	4.45	177,179,180,181	0
24	BCR	H	102	40/40	1.03	4.26	178,180,181,182	0
24	BCR	C	513	40/40	0.67	4.25	177,179,180,180	0
24	BCR	b	623	40/40	0.71	4.08	177,178,180,180	0
22	CLA	b	605	65/65	1.26	3.46	179,180,182,183	0
30	LMT	B	627	35/35	0.62	3.39	178,180,182,182	0
35	CA	o	301	1/1	0.67	3.27	184,184,184,184	0
22	CLA	c	511	65/65	0.91	3.24	178,180,181,182	0
27	LMG	I	101	43/55	0.74	3.21	178,180,181,182	0
24	BCR	B	619	40/40	0.67	3.07	178,179,180,180	0
24	BCR	C	514	40/40	0.93	3.05	178,179,180,181	0
24	BCR	g	101	40/40	0.89	3.00	178,179,180,180	0
27	LMG	c	518	45/55	1.11	3.00	178,180,181,181	0
25	DGD	b	601	52/66	0.59	2.90	178,180,181,182	0
22	CLA	B	601	65/65	0.99	2.78	177,180,181,182	0
24	BCR	J	102	40/40	0.40	2.78	178,180,181,181	0
24	BCR	c	514	40/40	1.00	2.76	177,179,180,180	0
24	BCR	K	102	40/40	1.06	2.72	178,180,181,182	0
24	BCR	A	407	40/40	0.57	2.61	177,179,180,180	0
30	LMT	b	603	35/35	0.57	2.55	178,179,181,182	0
24	BCR	a	409	40/40	0.66	2.52	177,178,180,180	0
22	CLA	D	406	65/65	0.51	2.51	177,179,180,181	0
35	CA	O	301	1/1	0.59	2.49	182,182,182,182	0
30	LMT	b	626	35/35	0.60	2.39	178,180,182,183	0
30	LMT	d	411	31/35	0.70	2.39	178,181,182,183	0
22	CLA	a	407	65/65	0.63	2.34	178,179,180,181	0
30	LMT	B	623	35/35	0.82	2.28	177,181,182,183	0
22	CLA	d	406	65/65	0.60	2.23	177,179,180,181	0
30	LMT	b	627	35/35	0.83	2.10	178,180,182,182	0
29	SQD	a	401	54/54	0.74	2.07	178,180,181,183	0
29	SQD	f	103	45/54	0.68	1.90	177,179,181,182	0
24	BCR	x	101	40/40	1.01	1.86	178,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	F	102	40/40	0.41	1.86	177,179,180,180	0
27	LMG	e	101	44/55	0.40	1.85	177,179,181,181	0
22	CLA	B	603	65/65	0.51	1.83	176,179,180,180	0
30	LMT	B	624	35/35	0.56	1.78	178,180,182,183	0
22	CLA	C	501	65/65	0.63	1.76	178,179,180,180	0
22	CLA	C	502	65/65	0.62	1.73	178,179,180,180	0
27	LMG	M	101	42/55	0.58	1.73	178,180,181,182	0
24	BCR	c	513	40/40	0.69	1.73	178,179,180,180	0
22	CLA	c	501	65/65	0.65	1.67	177,179,180,181	0
29	SQD	d	403	43/54	0.94	1.64	178,180,182,186	0
25	DGD	B	625	52/66	0.61	1.62	177,180,182,182	0
24	BCR	f	102	40/40	0.30	1.61	177,179,181,181	0
22	CLA	b	606	65/65	0.67	1.55	177,179,180,181	0
22	CLA	b	607	65/65	0.52	1.52	177,179,180,181	0
22	CLA	b	613	65/65	0.70	1.46	178,179,180,181	0
22	CLA	b	609	65/65	0.61	1.39	178,179,180,181	0
27	LMG	a	402	42/55	0.43	1.37	177,180,181,182	0
30	LMT	b	604	35/35	0.46	1.30	177,179,181,182	0
29	SQD	B	626	47/54	0.56	1.27	175,179,181,183	0
29	SQD	F	103	45/54	0.64	1.25	178,180,182,182	0
22	CLA	B	611	65/65	0.39	1.24	177,179,180,180	0
24	BCR	B	618	40/40	0.29	1.21	177,178,179,179	0
22	CLA	C	511	65/65	0.95	1.19	178,179,180,181	0
27	LMG	E	101	44/55	0.61	1.16	176,179,181,182	0
22	CLA	c	506	65/65	0.69	1.13	178,179,180,181	0
22	CLA	C	512	65/65	0.94	1.10	177,180,181,182	0
24	BCR	B	616	40/40	0.43	1.06	176,178,180,180	0
22	CLA	B	609	65/65	0.47	1.06	178,179,180,181	0
22	CLA	c	502	65/65	0.62	1.02	178,179,180,181	0
35	CA	k	101	1/1	0.29	1.00	180,180,180,180	0
24	BCR	B	617	40/40	0.44	1.00	177,179,180,180	0
27	LMG	A	414	42/55	0.48	0.99	177,179,182,182	0
22	CLA	B	614	65/65	0.69	0.97	177,179,180,181	0
22	CLA	C	510	65/65	0.54	0.94	177,179,180,181	0
22	CLA	C	503	65/65	0.49	0.93	177,179,180,180	0
22	CLA	B	604	65/65	0.57	0.91	177,179,180,180	0
22	CLA	b	608	65/65	0.49	0.86	178,179,180,181	0
22	CLA	c	510	65/65	0.50	0.86	178,179,181,181	0
22	CLA	b	618	65/65	0.88	0.85	177,179,180,180	0
25	DGD	A	408	56/66	0.44	0.83	178,179,181,182	0
29	SQD	B	622	43/54	0.55	0.82	177,180,182,185	0
22	CLA	b	615	65/65	0.38	0.79	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	HEM	V	201	43/43	0.43	0.78	176,178,180,180	0
22	CLA	B	608	65/65	0.51	0.77	177,179,180,180	0
22	CLA	c	505	65/65	0.64	0.75	177,179,180,181	0
22	CLA	c	508	65/65	0.48	0.72	177,179,180,181	0
22	CLA	C	508	65/65	0.68	0.71	177,179,180,180	0
22	CLA	b	611	65/65	0.45	0.71	177,179,180,180	0
22	CLA	c	503	65/65	0.52	0.69	177,179,180,181	0
34	HEM	v	201	43/43	0.54	0.67	177,179,180,180	0
22	CLA	B	615	65/65	0.66	0.63	176,179,180,181	0
22	CLA	h	101	65/65	0.45	0.60	176,179,180,181	0
29	SQD	A	413	54/54	0.35	0.60	178,180,182,184	0
22	CLA	C	506	65/65	0.58	0.59	177,179,180,180	0
22	CLA	B	605	65/65	0.66	0.56	178,179,180,180	0
25	DGD	b	624	58/66	0.38	0.53	177,178,180,180	0
24	BCR	b	621	40/40	0.38	0.52	178,178,179,179	0
24	BCR	j	102	40/40	0.33	0.49	179,180,182,183	0
22	CLA	b	612	65/65	0.56	0.47	176,179,181,181	0
25	DGD	a	410	56/66	0.37	0.47	178,180,181,182	0
29	SQD	b	602	47/54	0.44	0.44	176,179,182,185	0
23	PL9	A	406	45/55	0.44	0.43	177,179,180,180	0
22	CLA	b	619	65/65	0.69	0.39	177,179,180,181	0
24	BCR	b	620	40/40	0.37	0.39	177,179,179,180	0
23	PL9	a	408	45/55	0.30	0.39	176,179,180,180	0
30	LMT	B	628	35/35	0.45	0.38	177,180,182,183	0
27	LMG	m	101	42/55	0.45	0.38	175,179,181,181	0
27	LMG	a	412	51/55	0.34	0.33	177,179,180,180	0
22	CLA	C	504	65/65	0.37	0.33	177,179,180,180	0
22	CLA	B	602	65/65	0.49	0.33	176,178,180,180	0
22	CLA	a	404	65/65	0.68	0.32	177,178,180,180	0
34	HEM	f	101	43/43	0.35	0.25	178,180,180,181	0
22	CLA	C	509	65/65	0.39	0.23	177,179,180,180	0
22	CLA	H	101	65/65	0.36	0.23	177,179,180,181	0
22	CLA	B	607	65/65	0.36	0.22	178,179,180,181	0
22	CLA	a	405	65/65	0.67	0.21	174,178,179,180	0
27	LMG	d	412	46/55	0.26	0.17	177,178,180,180	0
24	BCR	b	622	40/40	0.37	0.16	176,178,179,179	0
27	LMG	C	521	48/55	0.31	0.15	177,179,180,181	0
22	CLA	B	613	65/65	0.46	0.10	177,179,180,180	0
23	PL9	d	407	55/55	0.50	0.08	177,179,180,181	0
22	CLA	b	617	65/65	0.43	0.06	178,179,180,182	0
31	PHO	d	401	64/64	0.49	-0.00	178,179,180,180	0
22	CLA	b	616	65/65	0.34	-0.01	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	C	505	65/65	0.38	-0.03	177,179,180,181	0
34	HEM	F	101	43/43	0.32	-0.05	178,180,181,182	0
22	CLA	c	509	65/65	0.32	-0.08	177,179,180,180	0
22	CLA	c	504	65/65	0.30	-0.09	177,179,180,180	0
22	CLA	C	507	65/65	0.37	-0.12	178,179,180,181	0
27	LMG	c	522	48/55	0.30	-0.14	178,180,180,181	0
22	CLA	b	614	65/65	0.30	-0.15	178,179,180,180	0
26	LHG	c	519	37/49	0.34	-0.17	178,180,183,187	0
23	PL9	D	407	55/55	0.35	-0.18	177,178,179,180	0
26	LHG	A	409	39/49	0.35	-0.22	178,179,181,181	0
22	CLA	A	402	65/65	0.45	-0.24	178,179,180,181	0
22	CLA	d	405	65/65	0.49	-0.24	177,178,179,180	0
27	LMG	D	409	48/55	0.27	-0.24	175,178,180,181	0
27	LMG	d	409	48/55	0.29	-0.30	177,179,180,180	0
22	CLA	B	610	65/65	0.37	-0.31	177,179,180,180	0
29	SQD	a	415	51/54	0.26	-0.31	178,179,181,182	0
25	DGD	B	620	58/66	0.28	-0.35	176,179,181,182	0
25	DGD	c	515	53/66	0.33	-0.39	176,179,181,182	0
31	PHO	D	401	64/64	0.34	-0.41	177,179,180,180	0
27	LMG	A	410	51/55	0.28	-0.48	177,178,180,181	0
30	LMT	M	103	35/35	0.47	-0.50	177,179,180,180	0
22	CLA	B	612	65/65	0.31	-0.54	176,178,180,181	0
28	OEX	A	411	10/10	0.43	-0.58	172,175,178,178	0
22	CLA	D	405	65/65	0.38	-0.60	177,179,180,180	0
25	DGD	c	517	66/66	0.34	-0.61	177,179,181,181	0
22	CLA	a	406	65/65	0.30	-0.62	177,179,180,181	0
25	DGD	C	515	53/66	0.30	-0.65	177,178,179,180	0
22	CLA	c	520	65/65	0.26	-0.67	177,179,180,181	0
22	CLA	A	403	65/65	0.39	-0.67	177,179,179,180	0
29	SQD	A	412	51/54	0.25	-0.70	178,179,180,181	0
27	LMG	D	408	49/55	0.29	-0.71	177,178,180,180	0
31	PHO	d	402	64/64	0.24	-0.72	178,179,180,181	0
22	CLA	c	507	65/65	0.26	-0.74	177,179,180,181	0
26	LHG	C	519	37/49	0.34	-0.74	176,180,184,188	0
31	PHO	D	402	64/64	0.30	-0.77	177,179,180,181	0
22	CLA	B	606	65/65	0.28	-0.79	177,179,180,180	0
26	LHG	a	411	39/49	0.28	-0.84	177,179,180,181	0
27	LMG	D	412	46/55	0.25	-0.95	178,179,180,181	0
22	CLA	C	520	65/65	0.31	-0.98	178,179,180,181	0
25	DGD	c	516	62/66	0.26	-1.02	178,179,180,181	0
27	LMG	d	408	49/55	0.20	-1.02	178,179,180,180	0
22	CLA	A	404	65/65	0.28	-1.06	176,178,180,181	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	b	610	65/65	0.25	-1.06	177,179,180,180	0
25	DGD	C	517	66/66	0.26	-1.19	177,179,180,181	0
25	DGD	C	516	62/66	0.26	-1.20	177,179,180,181	0
33	BCT	D	404	4/4	0.20	-1.27	178,179,179,179	0
27	LMG	B	621	49/55	0.23	-1.33	177,179,180,180	0
28	OEX	a	414	10/10	0.42	-1.43	174,177,179,182	0
27	LMG	b	625	49/55	0.24	-1.46	178,179,180,180	0
30	LMT	M	102	35/35	0.31	-1.50	178,179,181,182	0
33	BCT	d	404	4/4	0.13	-1.52	178,180,180,180	0
21	FE2	a	403	1/1	0.06	-1.85	182,182,182,182	0
32	CL	a	413	1/1	0.24	-1.94	177,177,177,177	0
21	FE2	A	401	1/1	0.18	-3.53	176,176,176,176	0
32	CL	D	403	1/1	0.16	-3.53	180,180,180,180	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.