



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2018 – 06:25 PM EST

PDB ID : 4FBY
Title : fs X-ray diffraction of Photosystem II
Authors : Kern, J.; Alonso-Mori, R.; Hellmich, J.; Tran, R.; Hattne, J.; Laksmono, H.; Gloeckner, C.; Echols, N.; Sierra, R.G.; Sellberg, J.; Lassalle-Kaiser, B.; Gildea, R.J.; Glatzel, P.; Grosse-Kunstleve, R.W.; Latimer, M.J.; McQueen, T.A.; Difiore, D.; Fry, A.R.; Messerschmidt, M.M.; Miahnahri, A.; Schafer, D.W.; Seibert, M.M.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; White, W.E.; Adams, P.D.; Bogan, M.J.; Boutet, S.; Williams, G.J.; Messinger, J.; Sauter, N.K.; Zouni, A.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2012-05-23
Resolution : 6.56 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

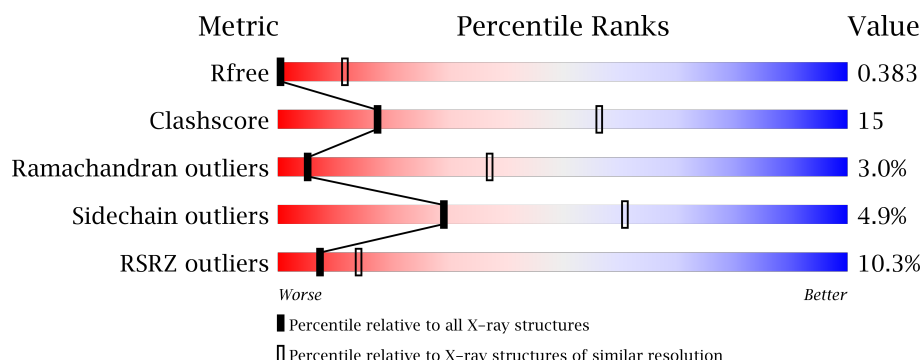
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1098 (9.00-3.70)
Clashscore	112137	1031 (9.00-3.80)
Ramachandran outliers	110173	1000 (9.00-3.76)
Sidechain outliers	110143	1096 (9.00-3.70)
RSRZ outliers	101464	1000 (9.00-3.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>8%</div> <div>62%</div> <div>33%</div> <div>• •</div> </div>
1	G	344	<div> <div>6%</div> <div>62%</div> <div>33%</div> <div>• •</div> </div>
2	B	510	<div> <div>11%</div> <div>69%</div> <div>24%</div> <div>• • •</div> </div>
2	N	510	<div> <div>13%</div> <div>71%</div> <div>23%</div> <div>• • •</div> </div>
3	C	461	<div> <div>5%</div> <div>61%</div> <div>32%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	461	
4	D	352	
4	Q	352	
5	E	83	
5	R	83	
6	F	44	
6	S	44	
7	H	65	
7	W	65	
8	I	38	
8	a	38	
9	J	39	
9	b	39	
10	K	37	
10	c	37	
11	L	37	
11	d	37	
12	M	36	
12	e	36	
13	O	246	
13	f	246	
14	T	32	
14	g	32	
15	U	104	
15	h	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	i	137	
17	m	46	
17	y	46	
18	X	40	
18	j	40	
19	Y	28	
19	k	28	
20	Z	62	
20	l	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	401	X	-	-	-
21	CLA	A	402	X	-	-	-
21	CLA	A	403	X	-	-	-
21	CLA	A	405	X	-	-	X
21	CLA	B	601	X	-	-	X
21	CLA	B	602	X	-	-	X
21	CLA	B	603	X	-	-	X
21	CLA	B	604	X	-	-	X
21	CLA	B	605	X	-	-	X
21	CLA	B	606	X	-	-	X
21	CLA	B	607	X	-	-	-
21	CLA	B	608	X	-	-	X
21	CLA	B	609	X	-	-	X
21	CLA	B	610	X	-	-	X
21	CLA	B	611	X	-	-	-
21	CLA	B	612	X	-	-	X
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	X
21	CLA	B	616	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	C	501	X	-	-	X
21	CLA	C	502	X	-	-	X
21	CLA	C	503	X	-	-	X
21	CLA	C	504	X	-	-	-
21	CLA	C	505	X	-	-	X
21	CLA	C	506	X	-	-	X
21	CLA	C	507	X	-	-	X
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	X
21	CLA	C	510	X	-	-	-
21	CLA	C	511	X	-	-	X
21	CLA	C	512	X	-	-	X
21	CLA	C	513	X	-	-	X
21	CLA	D	401	X	-	-	X
21	CLA	D	403	X	-	-	X
21	CLA	G	402	X	-	-	X
21	CLA	G	403	X	-	-	-
21	CLA	G	404	X	-	-	-
21	CLA	G	406	X	-	-	X
21	CLA	N	605	X	-	-	X
21	CLA	N	606	X	-	-	-
21	CLA	N	607	X	-	-	X
21	CLA	N	608	X	-	-	X
21	CLA	N	609	X	-	-	X
21	CLA	N	610	X	-	-	X
21	CLA	N	611	X	-	-	-
21	CLA	N	612	X	-	-	X
21	CLA	N	613	X	-	-	X
21	CLA	N	614	X	-	-	X
21	CLA	N	615	X	-	-	-
21	CLA	N	616	X	-	-	X
21	CLA	N	617	X	-	-	-
21	CLA	N	618	X	-	-	-
21	CLA	N	619	X	-	-	X
21	CLA	N	620	X	-	-	X
21	CLA	P	501	X	-	-	X
21	CLA	P	502	X	-	-	X
21	CLA	P	503	X	-	-	X
21	CLA	P	504	X	-	-	X
21	CLA	P	505	X	-	-	-
21	CLA	P	506	X	-	-	X
21	CLA	P	507	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	P	508	X	-	-	X
21	CLA	P	509	X	-	-	X
21	CLA	P	510	X	-	-	X
21	CLA	P	511	X	-	-	X
21	CLA	P	512	X	-	-	X
21	CLA	P	513	X	-	-	X
21	CLA	Q	402	X	-	-	X
21	CLA	Q	404	X	-	-	X
22	PHO	D	402	-	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	G	407	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	b	101	-	-	-	X
24	DGD	A	407	X	-	-	-
24	DGD	B	621	X	-	-	X
24	DGD	B	628	X	-	-	X
24	DGD	C	516	X	-	-	-
24	DGD	C	517	X	-	-	-
24	DGD	C	518	X	-	-	-
24	DGD	D	408	X	-	-	X
24	DGD	G	408	X	-	-	X
24	DGD	N	602	X	-	-	X
24	DGD	P	517	X	-	-	-
24	DGD	P	518	X	-	-	X
24	DGD	P	519	X	-	-	-
24	DGD	Q	409	X	-	-	X
24	DGD	W	102	X	-	-	-
25	LHG	A	411	-	-	-	X
25	LHG	G	412	-	-	-	X
26	SQD	A	414	-	-	-	X
26	SQD	B	624	-	-	-	X
26	SQD	B	627	-	-	-	X
26	SQD	F	101	-	-	-	X
26	SQD	N	601	-	-	-	X
26	SQD	Q	408	-	-	-	X
26	SQD	S	102	-	-	-	X
27	LMG	A	410	X	-	-	-
27	LMG	B	622	X	-	-	-
27	LMG	B	623	X	-	-	-
27	LMG	C	519	X	-	-	-
27	LMG	C	520	X	-	-	X
27	LMG	D	406	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	D	407	X	-	-	-
27	LMG	D	412	X	-	-	X
27	LMG	E	102	X	-	-	X
27	LMG	G	411	X	-	-	-
27	LMG	I	102	X	-	-	-
27	LMG	M	101	X	-	-	-
27	LMG	N	622	X	-	-	-
27	LMG	N	623	X	-	-	-
27	LMG	P	520	X	-	-	X
27	LMG	P	521	X	-	-	X
27	LMG	Q	401	X	-	-	X
27	LMG	Q	406	X	-	-	X
27	LMG	Q	407	X	-	-	-
27	LMG	R	102	X	-	-	X
27	LMG	a	102	X	-	-	-
27	LMG	e	102	X	-	-	-
28	OEC	A	412	-	-	-	X
28	OEC	G	413	-	-	-	X
30	BCR	B	620	-	-	-	X
30	BCR	C	514	-	-	-	X
30	BCR	C	515	-	-	-	X
30	BCR	D	405	-	-	-	X
30	BCR	H	101	-	-	-	X
30	BCR	I	101	-	-	-	X
30	BCR	J	102	-	-	-	X
30	BCR	K	101	-	-	-	X
30	BCR	P	514	-	-	-	X
30	BCR	P	515	-	-	-	X
30	BCR	P	516	-	-	-	X
30	BCR	S	101	-	-	-	X
30	BCR	T	103	-	-	-	X
30	BCR	W	101	-	-	-	X
30	BCR	Z	101	-	-	-	X
30	BCR	a	101	-	-	-	X
30	BCR	b	102	-	-	-	X
30	BCR	c	101	-	-	-	X
31	LMT	B	626	-	-	-	X
31	LMT	B	629	-	-	-	X
31	LMT	B	630	-	-	-	X
31	LMT	D	409	-	-	-	X
31	LMT	I	103	-	-	-	X
31	LMT	M	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	LMT	N	603	-	-	-	X
31	LMT	N	604	-	-	-	X
31	LMT	N	625	-	-	-	X
31	LMT	Q	410	-	-	-	X
31	LMT	a	103	-	-	-	X
31	LMT	e	101	-	-	-	X
32	BCT	Q	411	-	-	-	X
33	CL	D	411	-	-	-	X
33	CL	G	415	-	-	-	X
34	HEM	R	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	i	201	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem 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	G	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	N	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	P	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	Q	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	R	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	S	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	W	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	a	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	b	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	c	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	d	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	e	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	f	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	g	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	h	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	i	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	m	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

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

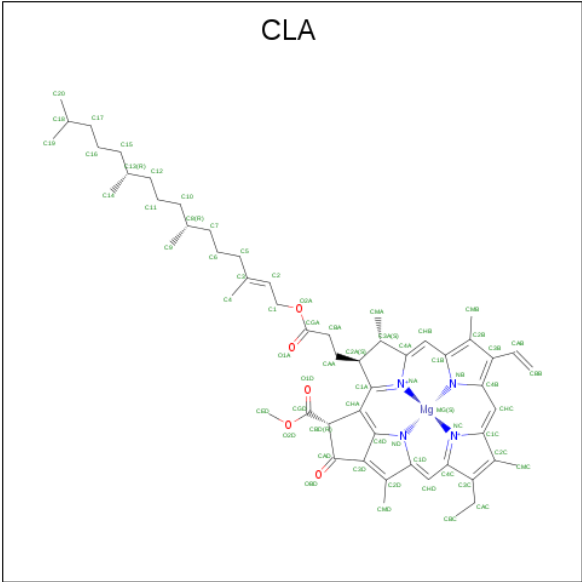
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	k	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	l	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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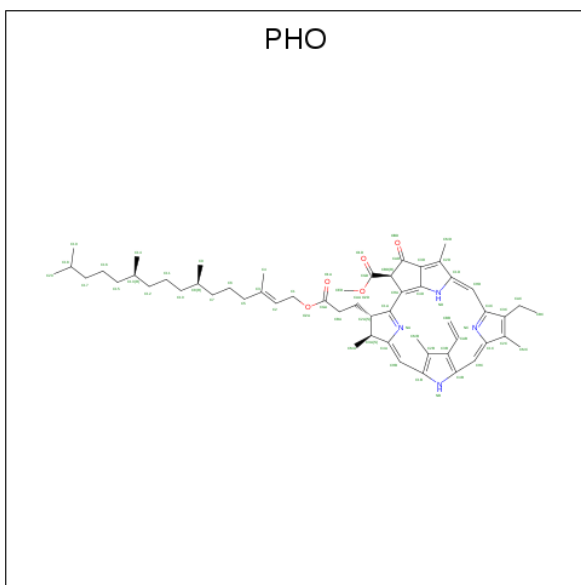
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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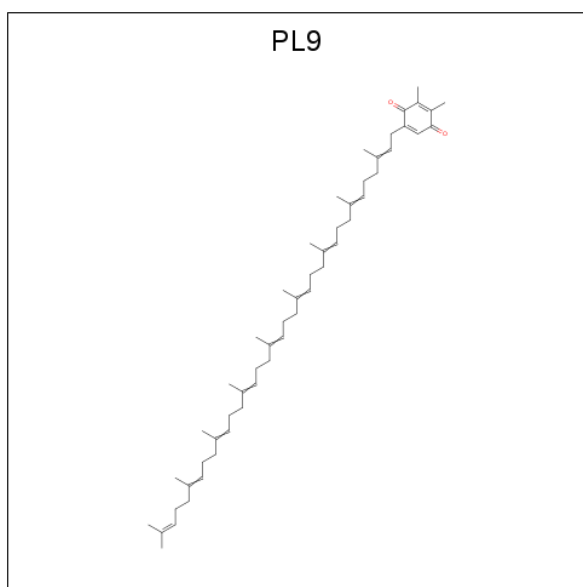
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



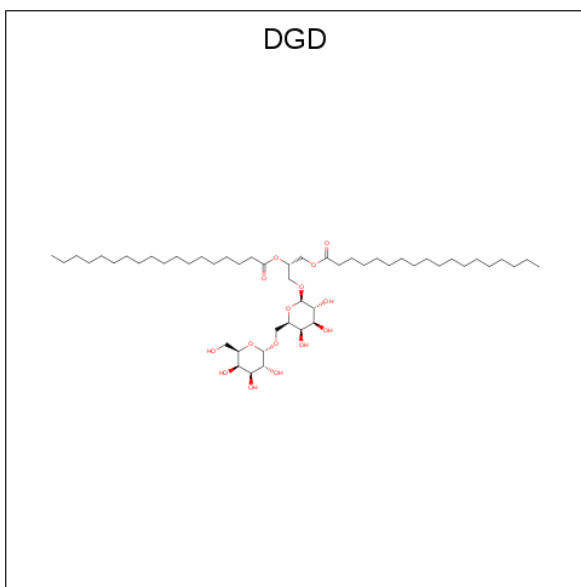
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		
22	G	1	Total	C	N	O	0	0
			64	55	4	5		
22	Q	1	Total	C	N	O	0	0
			64	55	4	5		

- 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: $C_{53}H_{80}O_2$).



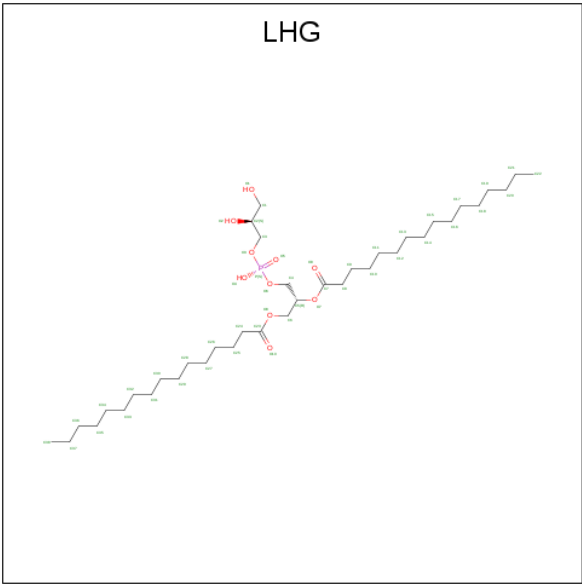
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	G	1	Total	C	O	0	0
			45	43	2		
23	Q	1	Total	C	O	0	0
			55	53	2		
23	b	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



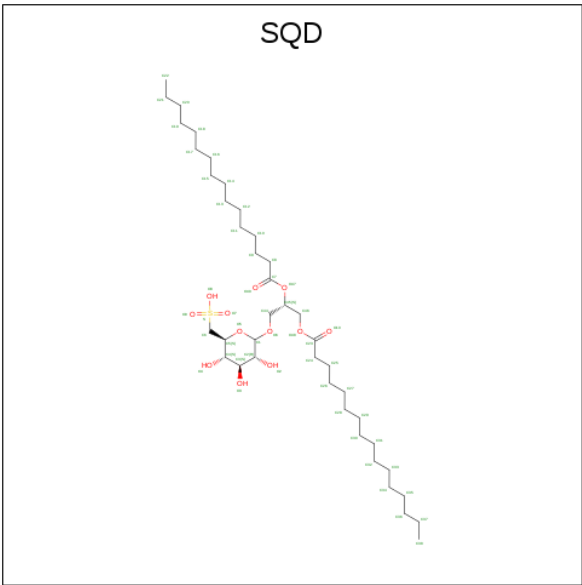
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			56	41	15		
24	B	1	Total	C	O	0	0
			58	43	15		
24	B	1	Total	C	O	0	0
			52	37	15		
24	C	1	Total	C	O	0	0
			53	38	15		
24	C	1	Total	C	O	0	0
			62	47	15		
24	C	1	Total	C	O	0	0
			66	51	15		
24	D	1	Total	C	O	0	0
			63	48	15		
24	G	1	Total	C	O	0	0
			56	41	15		
24	N	1	Total	C	O	0	0
			52	37	15		
24	P	1	Total	C	O	0	0
			53	38	15		
24	P	1	Total	C	O	0	0
			62	47	15		
24	P	1	Total	C	O	0	0
			66	51	15		
24	Q	1	Total	C	O	0	0
			63	48	15		
24	W	1	Total	C	O	0	0
			58	43	15		

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



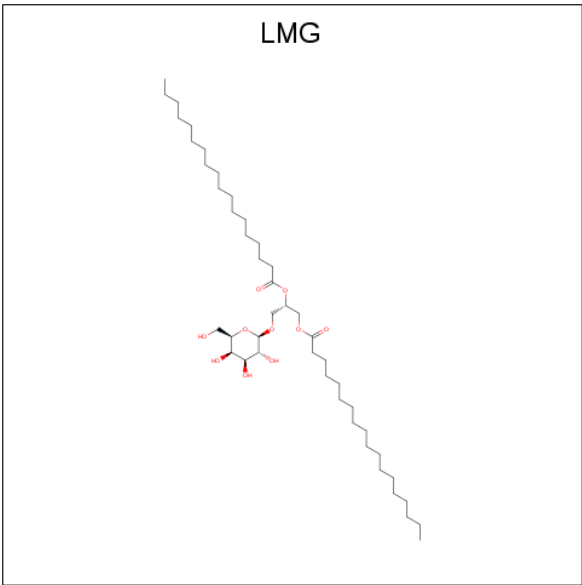
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	P	0	0
			39	28	10	1		
25	A	1	Total	C	O	P	0	0
			37	26	10	1		
25	G	1	Total	C	O	P	0	0
			39	28	10	1		
25	G	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			51	38	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			43	30	12	1		
26	B	1	Total	C	O	S	0	0
			47	34	12	1		
26	F	1	Total	C	O	S	0	0
			45	32	12	1		
26	G	1	Total	C	O	S	0	0
			54	41	12	1		
26	G	1	Total	C	O	S	0	0
			51	38	12	1		
26	N	1	Total	C	O	S	0	0
			47	34	12	1		
26	Q	1	Total	C	O	S	0	0
			43	30	12	1		
26	S	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



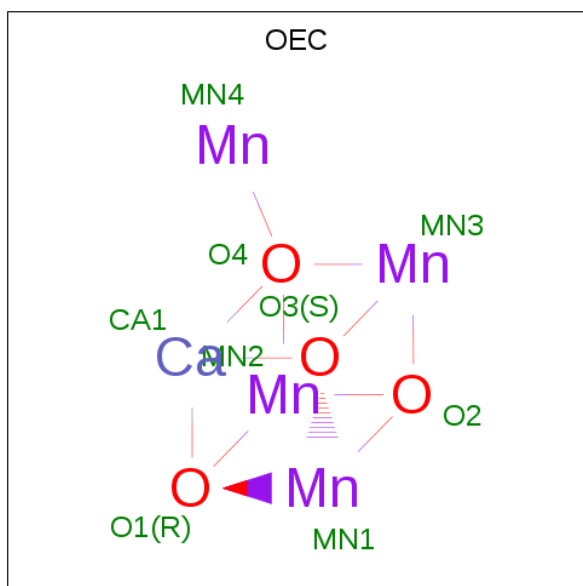
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			42	32	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	G	1	Total	C	O	0	0
			51	41	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	N	1	Total	C	O	0	0
			49	39	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	P	1	Total	C	O	0	0
			48	38	10		
27	P	1	Total	C	O	0	0
			45	35	10		
27	Q	1	Total	C	O	0	0
			42	32	10		
27	Q	1	Total	C	O	0	0
			48	38	10		
27	Q	1	Total	C	O	0	0
			46	36	10		
27	R	1	Total	C	O	0	0
			44	34	10		
27	a	1	Total	C	O	0	0
			43	33	10		
27	e	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).

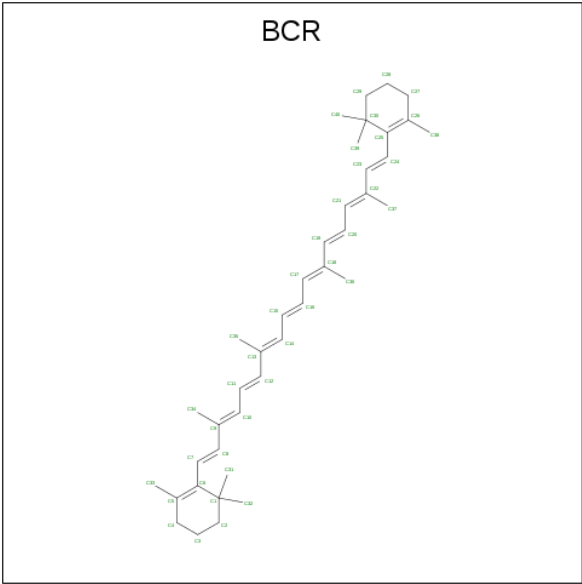


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	0	0
			5	1	4		
28	G	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total Fe 1 1	0	0
29	A	1	Total Fe 1 1	0	0

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



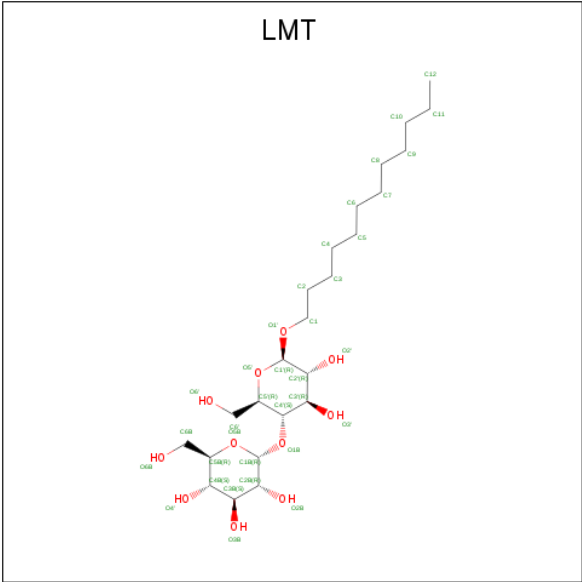
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	D	1	Total C 40 40	0	0
30	H	1	Total C 40 40	0	0
30	I	1	Total C 40 40	0	0
30	J	1	Total C 40 40	0	0

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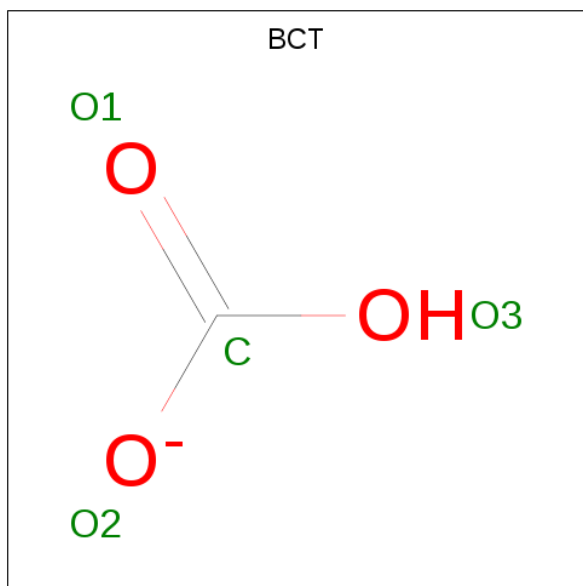
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	Z	1	Total C 40 40	0	0
30	N	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	S	1	Total C 40 40	0	0
30	W	1	Total C 40 40	0	0
30	a	1	Total C 40 40	0	0
30	b	1	Total C 40 40	0	0
30	c	1	Total C 40 40	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	N	1	Total	C	O	0	0
			35	24	11		
31	Q	1	Total	C	O	0	0
			31	20	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	e	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

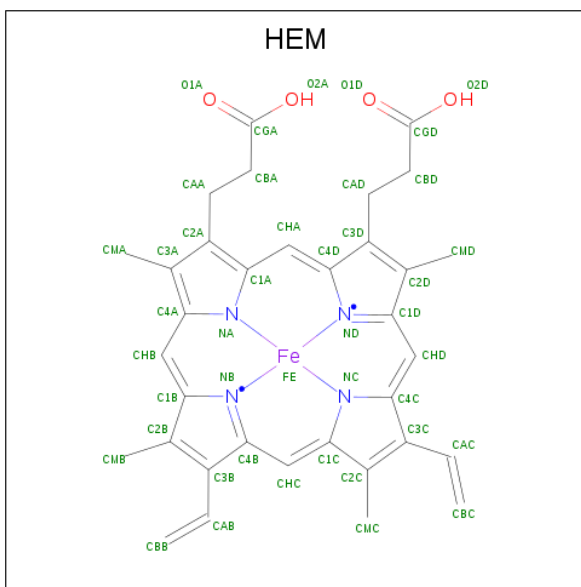


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	Q	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	G	1	Total	Cl	0	0
			1	1		
33	D	1	Total	Cl	0	0
			1	1		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

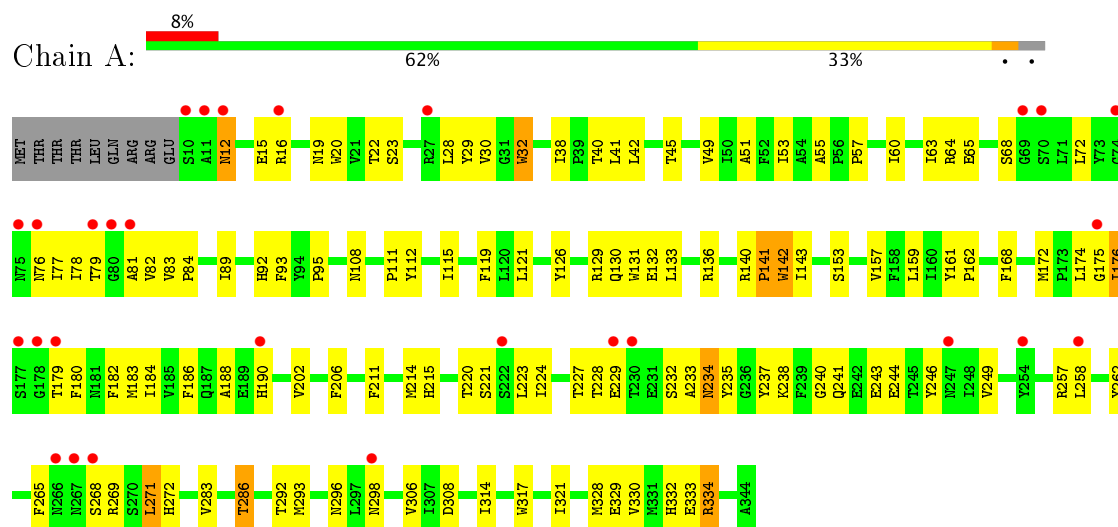
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	O	1	Total Ca 1 1	0	0
35	f	1	Total Ca 1 1	0	0

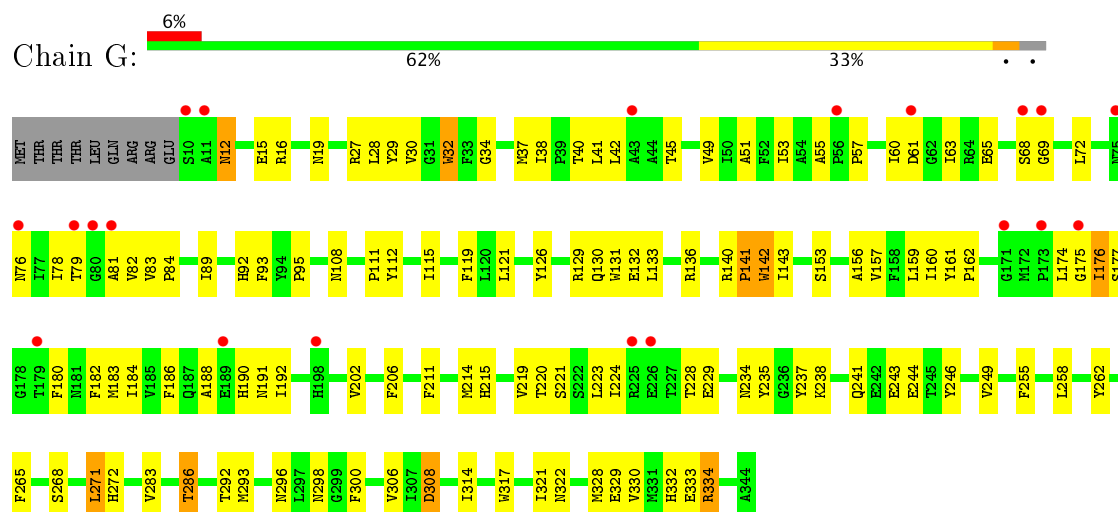
3 Residue-property plots

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

• Molecule 1: Photosystem Q(B) protein 1

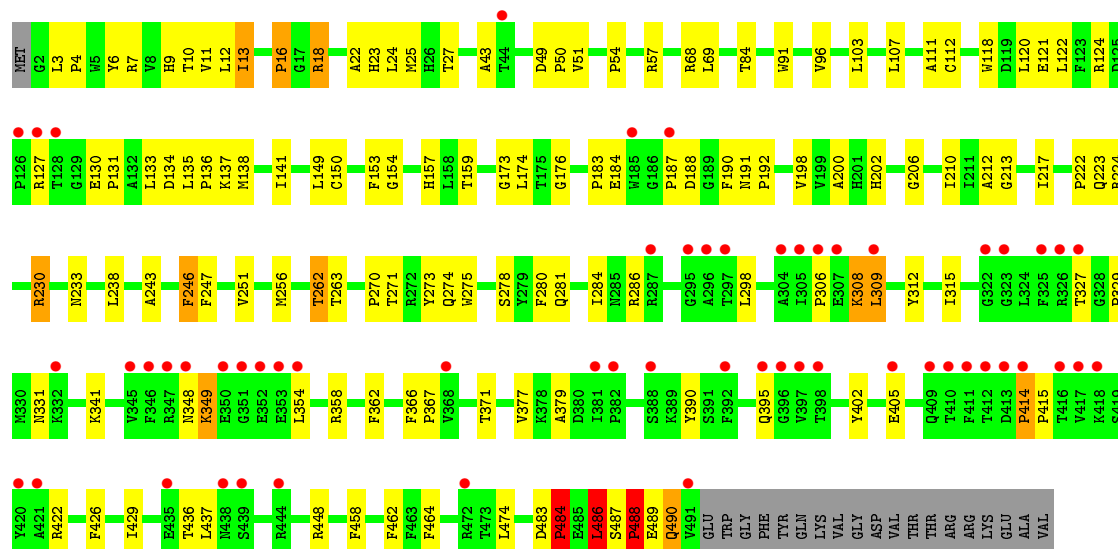


• Molecule 1: Photosystem Q(B) protein 1

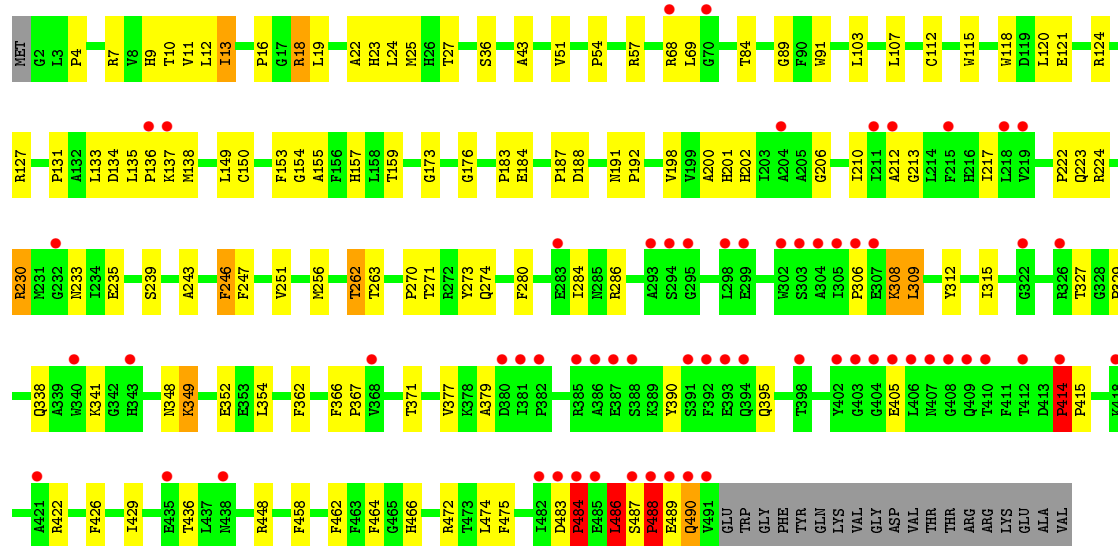


• Molecule 2: Photosystem II core light harvesting protein

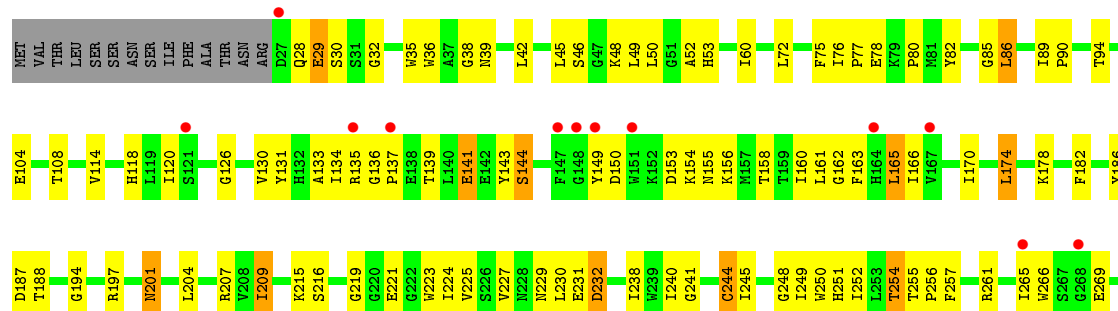


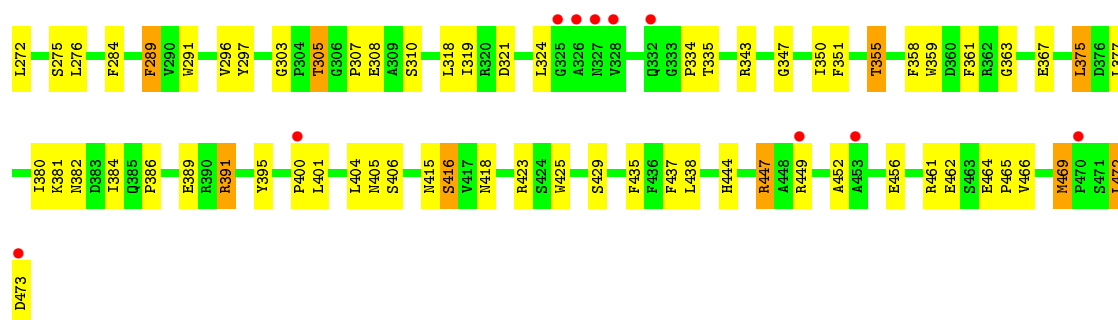


• Molecule 2: Photosystem II core light harvesting protein

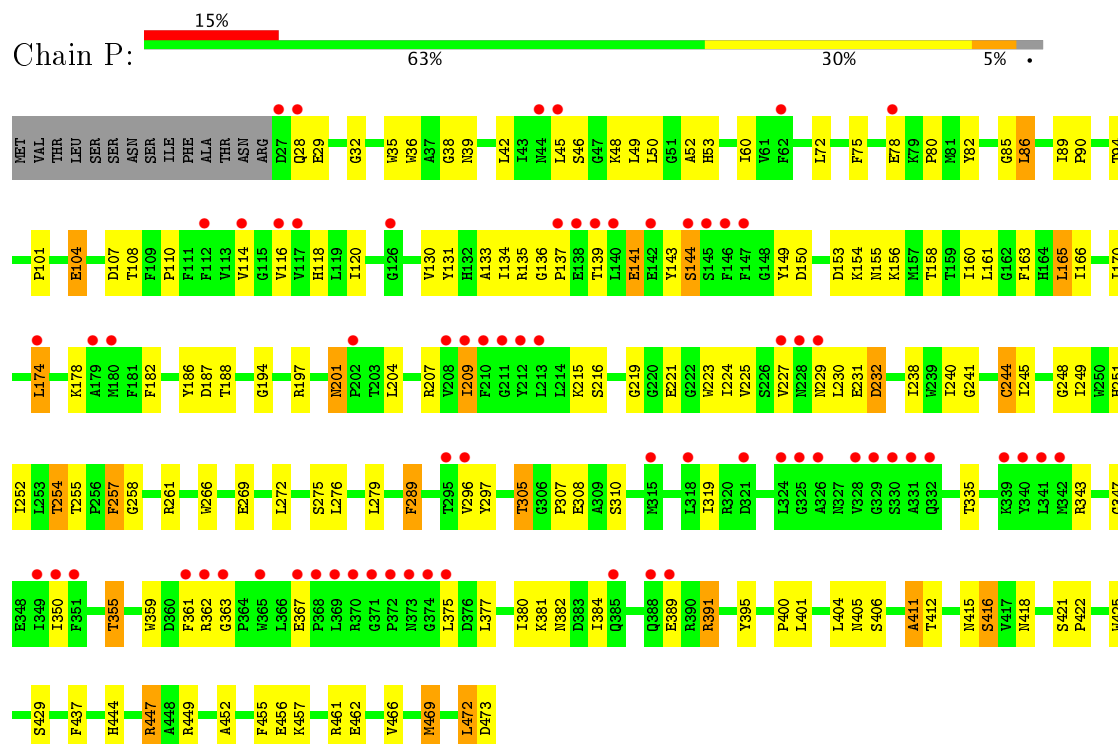


• Molecule 3: Photosystem II CP43 protein

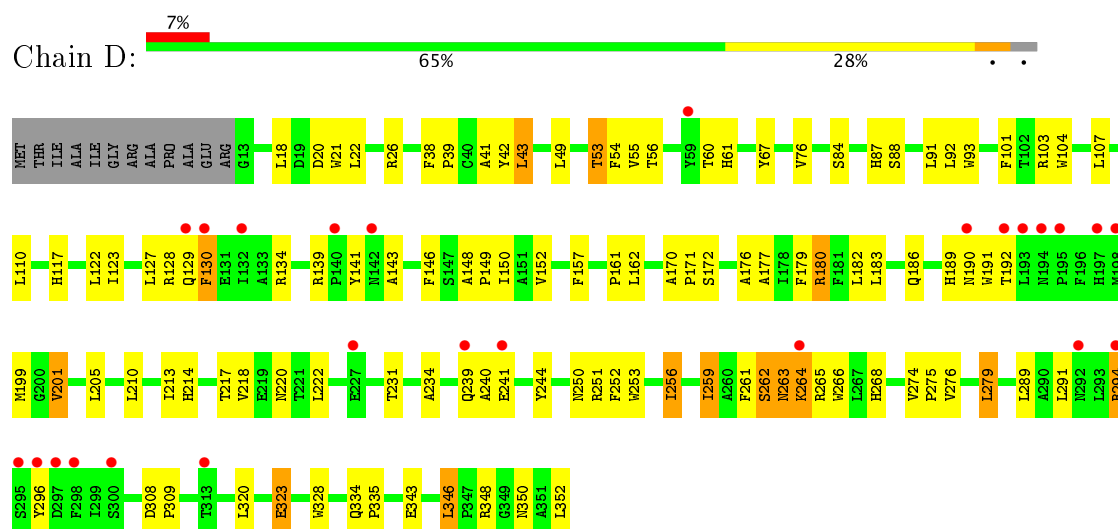




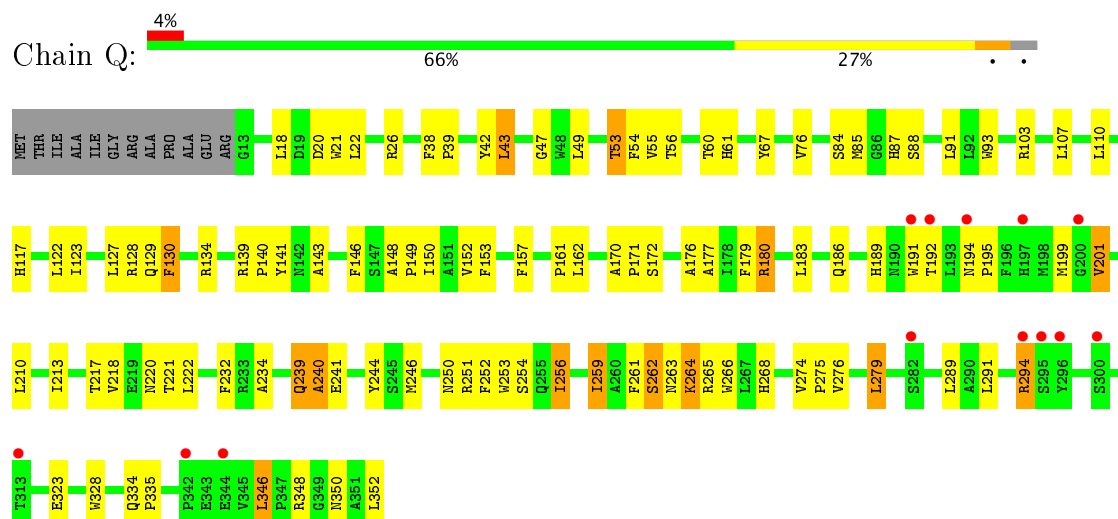
• Molecule 3: Photosystem II CP43 protein



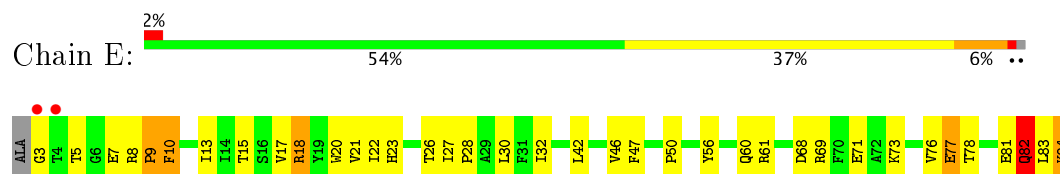
• Molecule 4: Photosystem II D2 protein



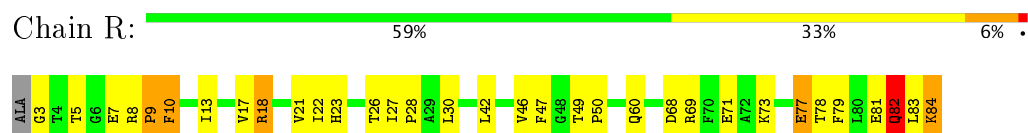
- Molecule 4: Photosystem II D2 protein



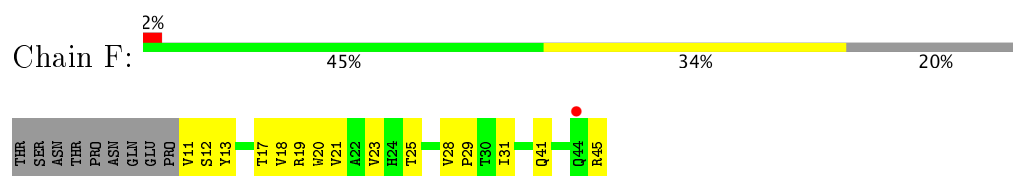
- Molecule 5: Cytochrome b559 subunit alpha



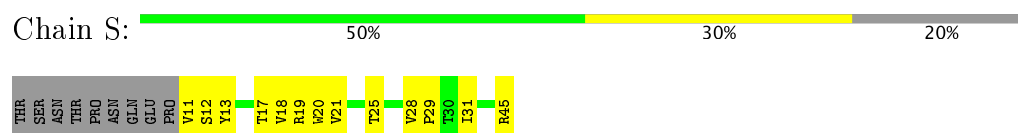
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

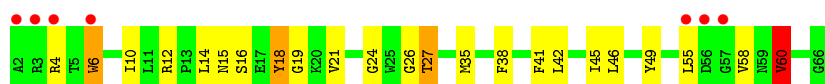


- Molecule 6: Cytochrome b559 subunit beta

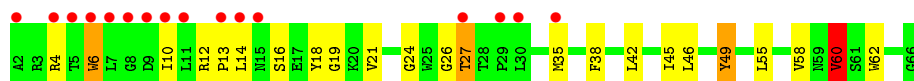


- Molecule 7: Photosystem II reaction center protein H

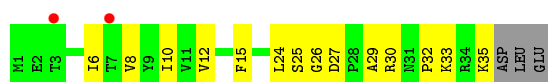




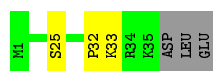
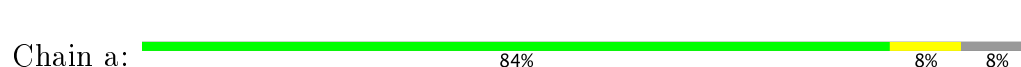
- Molecule 7: Photosystem II reaction center protein H



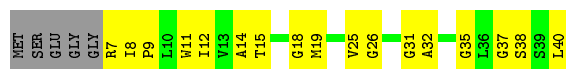
- Molecule 8: Photosystem II reaction center protein I



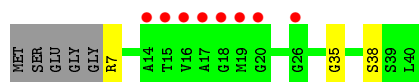
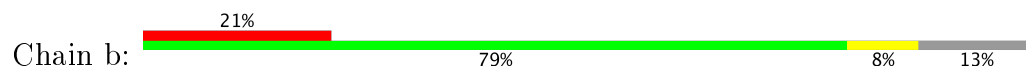
- Molecule 8: Photosystem II reaction center protein I



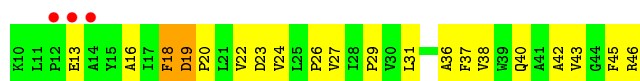
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

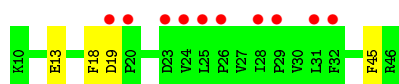


- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

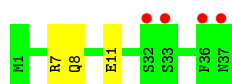




- Molecule 11: Photosystem II reaction center protein L



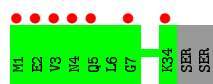
- Molecule 11: Photosystem II reaction center protein L



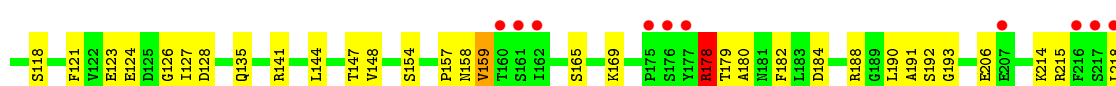
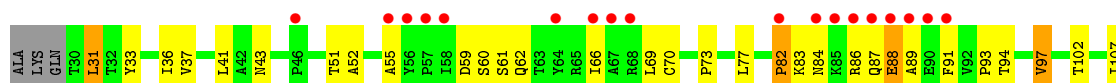
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

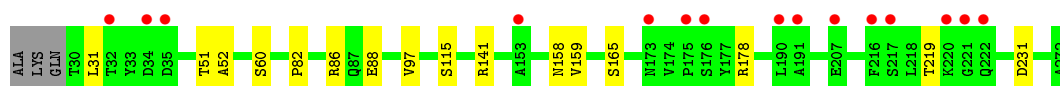


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





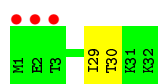
- Molecule 14: Photosystem II reaction center protein T

Chain T: 63% 34% .



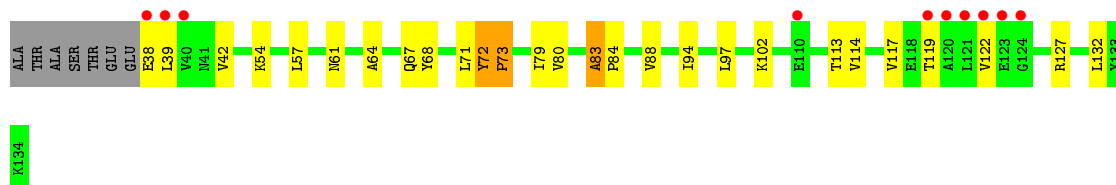
- Molecule 14: Photosystem II reaction center protein T

Chain g: 9% 94% 6%



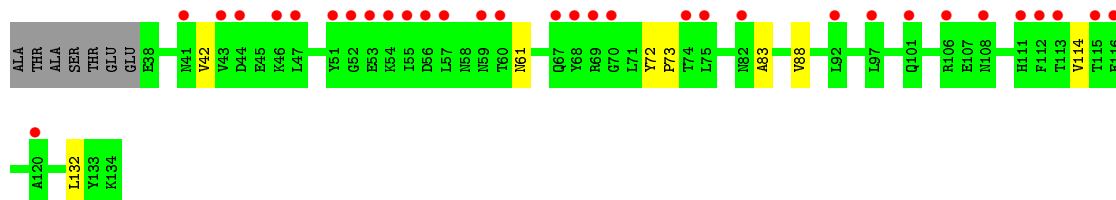
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 10% 67% 23% 7%



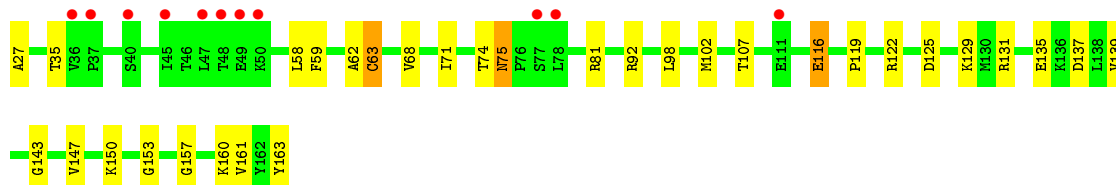
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain h: 31% 86% 8% 7%

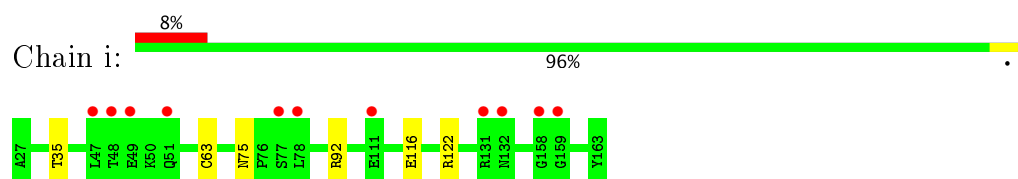


- Molecule 16: Cytochrome c-550

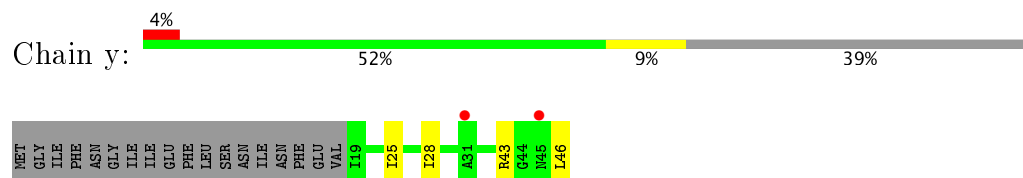
Chain V: 8% 77% 21%



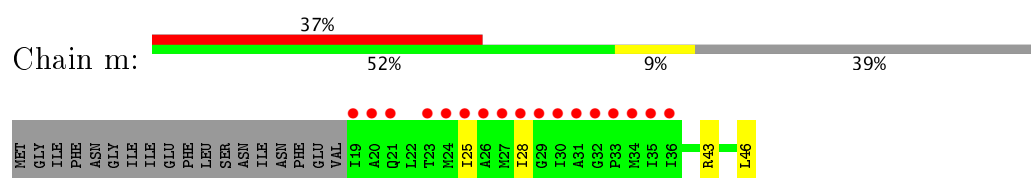
- Molecule 16: Cytochrome c-550



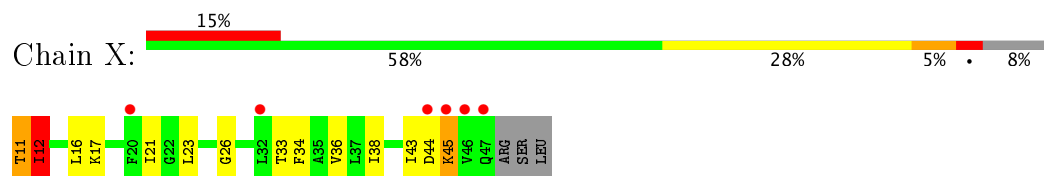
- Molecule 17: Photosystem II reaction center protein ycf12



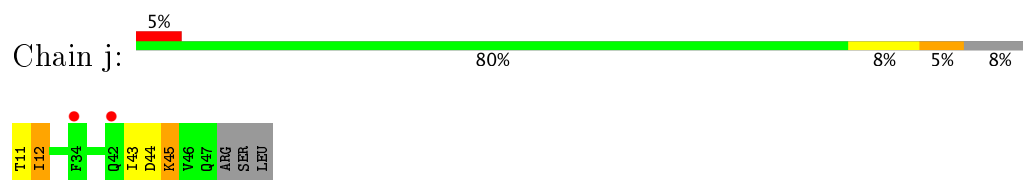
- Molecule 17: Photosystem II reaction center protein ycf12



- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Y



There are no outlier residues recorded for this chain.

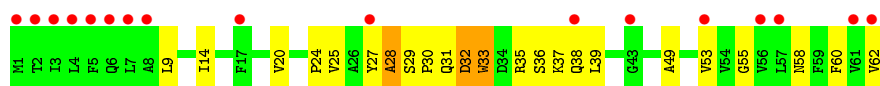
- Molecule 19: Photosystem II reaction center protein Y



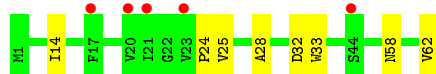
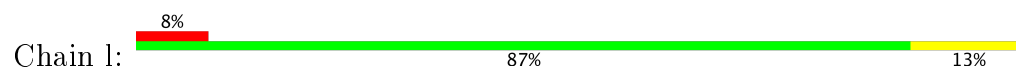
There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein 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, α , β , γ	130.78 Å 227.76 Å 308.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.89 – 6.56 85.88 – 6.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.89-6.56) 97.8 (85.88-6.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 6.72 Å)	Xtriage
Refinement program	PHENIX 1.7.3	Depositor
R, R_{free}	0.366 , 0.385 0.361 , 0.383	Depositor DCC
R_{free} test set	895 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	6.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2713	0.55	0/3700
1	G	0.26	0/2713	0.54	0/3700
2	B	0.26	0/3986	0.55	2/5433 (0.0%)
2	N	0.27	0/3986	0.56	2/5433 (0.0%)
3	C	0.25	0/3556	0.56	0/4842
3	P	0.25	0/3556	0.56	0/4842
4	D	0.26	0/2801	0.55	0/3818
4	Q	0.26	0/2801	0.54	0/3818
5	E	0.27	0/685	0.58	0/933
5	R	0.27	0/685	0.58	0/933
6	F	0.25	0/291	0.49	0/397
6	S	0.23	0/291	0.48	0/397
7	H	0.27	0/520	0.61	0/709
7	W	0.28	0/520	0.61	0/709
8	I	0.26	0/293	0.53	0/395
8	a	0.27	0/293	0.53	0/395
9	J	0.24	0/255	0.56	0/346
9	b	0.24	0/255	0.57	0/346
10	K	0.30	0/303	0.59	0/416
10	c	0.30	0/303	0.59	0/416
11	L	0.25	0/311	0.52	0/422
11	d	0.26	0/311	0.52	0/422
12	M	0.28	0/270	0.58	0/367
12	e	0.29	0/270	0.57	0/367
13	O	0.26	0/1876	0.60	1/2548 (0.0%)
13	f	0.26	0/1876	0.61	0/2548
14	T	0.27	0/284	0.53	0/381
14	g	0.27	0/284	0.53	0/381
15	U	0.27	0/785	0.61	0/1064
15	h	0.27	0/785	0.62	0/1064
16	V	0.24	0/1081	0.54	0/1468
16	i	0.24	0/1081	0.53	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	m	0.27	0/202	0.68	0/272
17	y	0.30	0/202	0.69	0/272
18	X	0.32	0/273	0.59	0/370
18	j	0.32	0/273	0.59	0/370
20	Z	0.28	0/490	0.62	0/669
20	l	0.28	0/490	0.62	0/669
All	All	0.26	0/41950	0.56	5/57100 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	LEU	CA-CB-CG	7.03	131.46	115.30
2	N	486	LEU	CA-CB-CG	6.79	130.91	115.30
2	N	484	PRO	N-CA-C	5.16	125.51	112.10
2	B	484	PRO	N-CA-C	5.05	125.24	112.10
13	O	178	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	98	0
1	G	2628	0	2524	97	0
2	B	3850	0	3718	107	0
2	N	3850	0	3718	105	0
3	C	3444	0	3365	127	0
3	P	3444	0	3365	111	0
4	D	2706	0	2608	98	0
4	Q	2706	0	2608	97	0
5	E	666	0	651	39	0
5	R	666	0	651	33	0
6	F	282	0	291	13	0
6	S	282	0	291	12	0
7	H	507	0	521	24	0
7	W	507	0	521	21	0
8	I	286	0	308	7	0
8	a	286	0	308	0	0
9	J	249	0	262	19	0
9	b	249	0	262	0	0
10	K	293	0	305	16	0
10	c	293	0	305	0	0
11	L	304	0	316	12	0
11	d	304	0	316	0	0
12	M	267	0	289	7	0
12	e	267	0	289	0	0
13	O	1845	0	1801	45	0
13	f	1845	0	1801	0	1
14	T	275	0	288	13	0
14	g	275	0	288	0	0
15	U	774	0	773	15	0
15	h	774	0	773	0	0
16	V	1060	0	1068	21	0
16	i	1060	0	1068	0	0
17	m	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	j	270	0	299	0	0
19	Y	140	0	32	0	0
19	k	140	0	32	0	0
20	Z	479	0	516	18	1
20	l	479	0	516	0	0
21	A	260	0	288	32	0
21	B	1040	0	1152	75	0
21	C	845	0	936	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	D	130	0	144	13	0
21	G	260	0	288	27	0
21	N	1040	0	1152	74	0
21	P	845	0	936	51	0
21	Q	130	0	144	14	0
22	A	64	0	74	7	0
22	D	64	0	74	4	0
22	G	64	0	74	7	0
22	Q	64	0	74	6	0
23	A	45	0	61	5	0
23	D	55	0	80	7	0
23	G	45	0	61	6	0
23	J	35	0	45	0	0
23	Q	55	0	80	6	0
23	b	35	0	45	0	0
24	A	56	0	70	1	0
24	B	110	0	136	5	0
24	C	181	0	245	16	0
24	D	63	0	87	0	0
24	G	56	0	70	2	0
24	N	52	0	62	4	0
24	P	181	0	245	12	0
24	Q	63	0	87	1	0
24	W	58	0	74	3	0
25	A	76	0	95	4	0
25	G	76	0	95	4	0
26	A	105	0	147	11	0
26	B	90	0	111	10	0
26	F	45	0	54	2	0
26	G	105	0	147	12	0
26	N	47	0	61	7	0
26	Q	43	0	50	3	0
26	S	45	0	54	0	0
27	A	51	0	72	2	0
27	B	98	0	136	2	0
27	C	93	0	126	4	0
27	D	136	0	182	15	0
27	E	44	0	58	3	0
27	G	51	0	72	0	0
27	I	43	0	56	4	0
27	M	42	0	54	3	0
27	N	98	0	136	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	P	93	0	126	4	0
27	Q	136	0	182	10	0
27	R	44	0	58	2	0
27	a	43	0	56	0	0
27	e	42	0	54	0	0
28	A	5	0	0	0	0
28	G	5	0	0	0	0
29	A	1	0	0	0	0
29	G	1	0	0	0	0
30	B	160	0	224	15	0
30	C	80	0	112	18	0
30	D	40	0	56	3	0
30	H	40	0	56	3	0
30	I	40	0	56	5	0
30	J	40	0	56	4	0
30	K	40	0	56	11	0
30	N	40	0	56	4	0
30	P	120	0	168	17	0
30	S	40	0	56	4	0
30	T	120	0	168	15	0
30	W	40	0	56	4	0
30	Z	40	0	56	3	0
30	a	40	0	56	0	0
30	b	40	0	56	0	0
30	c	40	0	56	0	0
31	B	140	0	184	7	0
31	D	31	0	35	1	0
31	I	35	0	46	2	0
31	M	35	0	46	1	0
31	N	140	0	184	9	0
31	Q	31	0	35	0	0
31	a	35	0	46	0	0
31	e	35	0	46	0	0
32	D	4	0	1	0	0
32	Q	4	0	1	0	0
33	D	1	0	0	0	0
33	G	1	0	0	0	0
34	E	43	0	30	7	0
34	R	43	0	30	6	0
34	V	43	0	30	4	0
34	i	43	0	30	0	0
35	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	f	1	0	0	0	0
All	All	50232	0	51376	1336	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:121:GLU:HG2	7:W:4:ARG:HG2	1.49	0.94
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.50	0.93
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.52	0.92
4:Q:26:ARG:HD3	6:S:18:VAL:HG11	1.54	0.88
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.54	0.88
3:C:39:ASN:HB2	21:C:508:CLA:HBA1	1.59	0.83
21:P:505:CLA:HBA1	21:P:505:CLA:HBD	1.63	0.80
7:H:38:PHE:HB2	30:H:101:BCR:H10C	1.64	0.80
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.64	0.80
1:A:40:THR:HG23	21:A:405:CLA:HBB1	1.62	0.80
21:N:612:CLA:H51	21:N:613:CLA:H101	1.64	0.79
7:W:38:PHE:HB2	30:W:101:BCR:H10C	1.63	0.79
1:G:129:ARG:HH21	4:Q:256:ILE:HD12	1.48	0.78
3:P:39:ASN:HB2	21:P:508:CLA:HBA1	1.64	0.77
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.66	0.76
1:G:174:LEU:HD22	22:G:405:PHO:H151	1.68	0.76
1:G:40:THR:HG23	21:G:406:CLA:HBB1	1.65	0.75
21:C:507:CLA:H112	30:C:515:BCR:H362	1.67	0.74
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.50	0.74
3:P:305:THR:HG23	3:P:307:PRO:HD2	1.68	0.74
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.69	0.73
23:Q:405:PL9:H13	27:Q:407:LMG:H132	1.71	0.73
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.69	0.73
21:C:505:CLA:HBA1	21:C:505:CLA:HBD	1.69	0.72
26:G:410:SQD:H311	21:P:508:CLA:H71	1.71	0.72
21:A:401:CLA:H152	22:A:404:PHO:H51	1.72	0.72
2:N:149:LEU:HG	21:N:607:CLA:HBC1	1.71	0.72
1:G:183:MET:HA	21:G:402:CLA:HMD2	1.71	0.72
21:G:402:CLA:H152	22:G:405:PHO:H51	1.72	0.72
21:B:608:CLA:H51	21:B:609:CLA:H101	1.71	0.72
1:G:45:THR:HG21	26:G:401:SQD:H201	1.72	0.71
13:O:230:VAL:HG12	13:O:231:ASP:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.72	0.71
2:B:490:GLN:NE2	2:B:490:GLN:O	2.17	0.71
30:C:514:BCR:H353	30:K:101:BCR:H321	1.72	0.71
3:C:254:THR:HG22	3:C:255:THR:H	1.56	0.71
25:A:411:LHG:H271	25:A:411:LHG:H101	1.73	0.70
2:B:149:LEU:HG	21:B:603:CLA:HBC1	1.72	0.70
21:P:503:CLA:HBB1	27:P:521:LMG:H201	1.73	0.70
3:P:254:THR:HG22	3:P:255:THR:H	1.56	0.70
26:A:409:SQD:H311	21:C:508:CLA:H71	1.74	0.70
1:A:174:LEU:HD22	22:A:404:PHO:H151	1.74	0.69
26:A:414:SQD:H311	30:I:101:BCR:H342	1.73	0.69
30:C:514:BCR:H11C	30:K:101:BCR:H322	1.73	0.69
21:P:507:CLA:H112	30:P:516:BCR:H362	1.74	0.69
21:C:503:CLA:HBB1	27:C:520:LMG:H201	1.72	0.69
14:T:18:PHE:HZ	2:N:112:CYS:HG	1.41	0.69
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.74	0.69
30:T:101:BCR:H383	26:N:601:SQD:H92	1.75	0.69
3:P:361:PHE:HA	24:P:517:DGD:HE61	1.75	0.69
1:A:183:MET:HA	21:A:401:CLA:HMD2	1.74	0.68
1:A:72:LEU:HD13	27:D:412:LMG:H111	1.76	0.68
21:N:612:CLA:H151	21:N:613:CLA:H203	1.75	0.68
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.28	0.68
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.76	0.68
4:D:279:LEU:HG	22:D:402:PHO:HBC3	1.74	0.68
1:G:82:VAL:HB	1:G:174:LEU:HB2	1.73	0.68
4:Q:279:LEU:HG	22:Q:403:PHO:HBC3	1.74	0.68
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.57	0.68
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.76	0.68
3:P:166:ILE:HG23	3:P:245:ILE:HG23	1.76	0.68
30:B:617:BCR:H383	26:B:627:SQD:H92	1.76	0.68
1:A:28:LEU:HB2	26:A:414:SQD:H91	1.74	0.67
23:D:404:PL9:H13	27:D:407:LMG:H132	1.76	0.67
21:B:606:CLA:H72	30:B:620:BCR:H311	1.77	0.67
21:D:403:CLA:H43	18:X:23:LEU:HA	1.76	0.67
4:D:214:HIS:ND1	23:D:404:PL9:O2	2.25	0.67
2:B:271:THR:HG22	2:B:273:TYR:H	1.59	0.67
2:N:271:THR:HG22	2:N:273:TYR:H	1.59	0.67
30:D:405:BCR:H403	9:J:25:VAL:HG21	1.77	0.67
21:P:508:CLA:HBC3	21:P:510:CLA:H92	1.77	0.66
30:K:101:BCR:H331	30:K:101:BCR:HC8	1.78	0.66
13:O:83:LYS:HG2	13:O:84:ASN:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:TRP:CZ3	4:Q:180:ARG:HD3	2.31	0.66
12:M:25:LEU:O	12:M:28:GLN:HG3	1.96	0.66
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.31	0.65
13:O:69:LEU:HD12	13:O:70:CYS:H	1.61	0.65
5:R:10:PHE:CE1	34:R:101:HEM:HBD2	2.31	0.65
21:B:612:CLA:H171	21:B:613:CLA:HBB2	1.79	0.65
26:N:601:SQD:H101	21:N:618:CLA:H2	1.77	0.65
6:S:17:THR:HG23	6:S:20:TRP:H	1.61	0.65
3:P:49:LEU:O	3:P:53:HIS:ND1	2.29	0.65
5:E:10:PHE:CE1	34:E:101:HEM:HBD2	2.32	0.65
2:N:414:PRO:HB2	2:N:415:PRO:HD3	1.79	0.65
27:D:412:LMG:H112	2:N:43:ALA:HA	1.78	0.65
2:N:490:GLN:NE2	2:N:490:GLN:O	2.16	0.65
4:Q:60:THR:HG23	4:Q:61:HIS:CD2	2.32	0.65
3:C:118:HIS:CE1	27:C:520:LMG:H192	2.32	0.64
21:C:501:CLA:HMB3	30:C:515:BCR:H403	1.79	0.64
2:N:379:ALA:HA	2:N:390:TYR:HB3	1.79	0.64
2:N:24:LEU:HD21	21:N:620:CLA:HAB	1.80	0.64
21:P:511:CLA:HMB2	30:P:514:BCR:H382	1.79	0.64
3:C:48:LYS:NZ	3:C:133:ALA:O	2.30	0.64
11:L:8:GLN:HE21	11:L:8:GLN:N	1.95	0.64
4:Q:129:GLN:NE2	4:Q:143:ALA:HA	2.13	0.64
16:V:62:ALA:O	34:V:201:HEM:HAB	1.96	0.64
30:C:514:BCR:H382	21:C:511:CLA:HMB2	1.80	0.64
30:T:102:BCR:H23C	30:T:102:BCR:H403	1.80	0.64
30:B:618:BCR:H23C	30:B:618:BCR:H403	1.79	0.64
21:C:508:CLA:HBC3	21:C:510:CLA:H92	1.79	0.64
3:P:150:ASP:HB3	3:P:153:ASP:HB2	1.79	0.64
2:B:43:ALA:HA	27:Q:401:LMG:H112	1.79	0.63
6:F:17:THR:HG23	6:F:20:TRP:H	1.63	0.63
21:N:616:CLA:H171	21:N:617:CLA:HBB2	1.81	0.63
2:N:120:LEU:HD13	21:N:620:CLA:HMD2	1.79	0.63
3:P:42:LEU:HD21	21:P:511:CLA:H2A	1.79	0.63
21:D:403:CLA:H42	18:X:26:GLY:HA3	1.79	0.63
3:C:361:PHE:HA	24:C:516:DGD:HE61	1.80	0.63
2:N:135:LEU:HA	2:N:138:MET:HE3	1.81	0.63
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.79	0.63
21:G:403:CLA:HED1	23:Q:405:PL9:H372	1.80	0.63
1:G:89:ILE:HD11	1:G:108:ASN:HB3	1.80	0.63
3:P:118:HIS:CE1	27:P:521:LMG:H192	2.32	0.63
2:B:124:ARG:HE	2:B:131:PRO:HD3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:10:PHE:HE1	34:R:101:HEM:HBD2	1.62	0.63
14:T:21:ILE:HD12	30:T:102:BCR:H332	1.81	0.63
3:C:224:ILE:O	3:C:227:VAL:HG23	1.98	0.63
21:B:603:CLA:H193	7:H:42:LEU:HD12	1.80	0.62
2:N:22:ALA:O	2:N:25:MET:HB3	2.00	0.62
30:B:618:BCR:H19C	30:B:619:BCR:H363	1.81	0.62
4:D:274:VAL:HA	23:D:404:PL9:H253	1.80	0.62
3:C:158:THR:O	3:C:251:HIS:HB3	1.99	0.62
2:N:327:THR:HG22	21:N:611:CLA:H12	1.81	0.62
2:B:188:ASP:HA	7:H:58:VAL:HG23	1.82	0.62
2:N:68:ARG:HH22	21:N:608:CLA:HED1	1.65	0.62
2:N:188:ASP:HA	7:W:58:VAL:HG23	1.81	0.62
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.81	0.62
21:N:607:CLA:H193	7:W:42:LEU:HD12	1.80	0.62
2:B:22:ALA:HB1	21:B:612:CLA:HBB1	1.81	0.62
21:B:603:CLA:H3A	21:B:603:CLA:CGA	2.30	0.62
2:B:458:PHE:HB3	21:B:604:CLA:HBC2	1.82	0.62
4:Q:274:VAL:HA	23:Q:405:PL9:H253	1.82	0.62
3:C:447:ARG:HH11	3:C:447:ARG:HG2	1.64	0.62
4:D:186:GLN:HB2	21:D:401:CLA:HBC1	1.81	0.62
2:B:327:THR:HG22	21:B:607:CLA:H12	1.82	0.62
3:C:42:LEU:HD21	21:C:511:CLA:H2A	1.81	0.62
30:T:103:BCR:H311	21:N:610:CLA:H72	1.81	0.62
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.65	0.61
2:B:68:ARG:HH22	21:B:604:CLA:HED1	1.65	0.61
4:Q:148:ALA:HB2	4:Q:276:VAL:HG13	1.82	0.61
21:P:501:CLA:HMB3	30:P:516:BCR:H403	1.82	0.61
26:N:601:SQD:H1	26:N:601:SQD:H462	1.81	0.61
21:N:612:CLA:HAB	4:Q:123:ILE:HG23	1.80	0.61
2:N:4:PRO:HD2	2:N:7:ARG:HD2	1.82	0.61
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.83	0.61
2:B:135:LEU:HA	2:B:138:MET:HE3	1.82	0.61
21:B:605:CLA:HBB1	21:B:606:CLA:H51	1.81	0.61
3:P:406:SER:O	3:P:418:ASN:ND2	2.33	0.61
9:J:26:GLY:HA3	21:Q:404:CLA:H42	117.21	0.61
21:N:609:CLA:HBB1	21:N:610:CLA:H51	1.83	0.61
2:N:9:HIS:ND1	21:N:616:CLA:HAB	2.16	0.61
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.81	0.61
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.66	0.61
7:H:12:ARG:HD3	7:H:12:ARG:O	2.01	0.61
3:P:75:PHE:HD1	3:P:86:LEU:HD21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R:101:HEM:HBB2	34:R:101:HEM:HHC	1.81	0.61
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.82	0.61
26:A:414:SQD:H321	30:I:101:BCR:H321	1.82	0.60
3:P:224:ILE:O	3:P:227:VAL:HG23	2.01	0.60
14:T:29:ILE:HD12	14:T:29:ILE:H	1.66	0.60
1:G:221:SER:HB3	4:Q:141:TYR:HB2	1.82	0.60
34:E:101:HEM:HHC	34:E:101:HEM:HBB2	1.83	0.60
2:N:270:PRO:HG3	2:N:312:TYR:HD2	1.67	0.60
7:W:12:ARG:O	7:W:12:ARG:HD3	2.02	0.60
3:P:48:LYS:NZ	3:P:133:ALA:O	2.35	0.60
21:B:608:CLA:H42	4:D:127:LEU:HD11	1.84	0.60
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.67	0.60
1:G:244:GLU:HG3	1:G:246:TYR:H	1.67	0.60
21:N:607:CLA:H3A	21:N:607:CLA:CGA	2.31	0.60
3:P:158:THR:O	3:P:251:HIS:HB3	2.02	0.60
5:E:18:ARG:HH11	5:E:18:ARG:HB3	1.65	0.60
3:P:343:ARG:NH1	3:P:347:GLY:O	2.35	0.59
3:P:447:ARG:HH11	3:P:447:ARG:HG2	1.65	0.59
5:R:18:ARG:HB3	5:R:18:ARG:HH11	1.67	0.59
3:C:114:VAL:HG22	27:C:520:LMG:H152	1.84	0.59
27:D:407:LMG:HC62	11:L:15:THR:HG21	1.85	0.59
1:G:63:ILE:HB	3:P:335:THR:HG21	1.84	0.59
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.83	0.59
21:P:504:CLA:H151	24:P:518:DGD:HBW1	1.83	0.59
21:N:608:CLA:HBB1	21:N:611:CLA:CBB	2.33	0.59
3:P:466:VAL:HG13	4:Q:251:ARG:HD2	1.84	0.59
2:B:247:PHE:HE1	21:B:602:CLA:H101	1.66	0.59
5:E:18:ARG:HD2	5:E:22:ILE:HD11	1.85	0.59
24:N:602:DGD:HA21	31:N:604:LMT:H121	1.83	0.59
4:Q:186:GLN:HB2	21:Q:402:CLA:HBC1	1.82	0.59
21:C:511:CLA:H171	20:Z:20:VAL:HA	1.85	0.59
1:A:15:GLU:O	1:A:19:ASN:ND2	2.35	0.59
2:B:103:LEU:HD21	21:B:605:CLA:HMC3	1.84	0.59
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.59
2:B:487:SER:N	2:B:488:PRO:HD2	2.18	0.58
26:B:627:SQD:H1	26:B:627:SQD:H462	1.83	0.58
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.84	0.58
4:Q:103:ARG:HG3	5:R:73:LYS:HG3	1.85	0.58
21:A:402:CLA:HED1	23:D:404:PL9:H372	1.85	0.58
2:N:103:LEU:HD21	21:N:609:CLA:HMC3	1.85	0.58
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:PRO:HA	1:G:112:TYR:CG	2.39	0.58
21:N:616:CLA:HMB3	21:N:617:CLA:HAA1	1.86	0.58
3:P:131:TYR:HE1	3:P:135:ARG:HD2	1.69	0.58
3:P:166:ILE:O	3:P:170:ILE:HG13	2.03	0.58
4:Q:87:HIS:HD2	4:Q:162:LEU:HD23	1.67	0.58
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.03	0.58
3:C:437:PHE:HZ	21:C:510:CLA:HMB3	1.69	0.58
2:N:487:SER:N	2:N:488:PRO:HD2	2.18	0.58
21:B:614:CLA:H2	26:B:627:SQD:H101	1.85	0.58
4:D:199:MET:HG2	23:D:404:PL9:H322	1.85	0.58
21:N:613:CLA:HMC2	30:W:101:BCR:H343	1.85	0.58
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.85	0.58
3:C:343:ARG:NH1	3:C:347:GLY:O	2.37	0.58
21:C:506:CLA:HMC2	21:C:507:CLA:H102	1.85	0.58
3:C:377:LEU:O	3:C:381:LYS:HB2	2.04	0.57
21:C:503:CLA:H172	21:C:510:CLA:HBB2	1.86	0.57
5:E:10:PHE:HE1	34:E:101:HEM:HBD2	1.68	0.57
1:A:244:GLU:HG3	1:A:246:TYR:H	1.69	0.57
21:B:608:CLA:HAB	4:D:123:ILE:HG23	1.85	0.57
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.04	0.57
1:G:317:TRP:HZ3	4:Q:180:ARG:HD3	1.67	0.57
3:C:137:PRO:HB2	3:C:139:THR:O	2.03	0.57
30:C:514:BCR:H341	30:K:101:BCR:H322	1.87	0.57
2:B:187:PRO:HB3	21:B:601:CLA:HMB2	1.87	0.57
5:E:81:GLU:O	5:E:83:LEU:N	2.35	0.57
2:N:341:LYS:HA	2:N:405:GLU:HB2	1.86	0.57
3:C:437:PHE:CZ	21:C:510:CLA:HMB3	2.39	0.57
2:N:247:PHE:HE1	21:N:606:CLA:H101	1.68	0.57
4:Q:87:HIS:ND1	24:W:102:DGD:HD2	2.20	0.57
20:Z:32:ASP:HB2	20:Z:35:ARG:HG2	1.86	0.57
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.86	0.57
2:N:458:PHE:HB3	21:N:608:CLA:HBC2	1.85	0.57
3:P:429:SER:HB3	24:P:518:DGD:HA81	1.87	0.57
27:A:410:LMG:H211	11:L:26:VAL:HG21	1.87	0.57
2:N:213:GLY:O	2:N:217:ILE:HG13	2.04	0.57
21:C:504:CLA:H202	24:C:518:DGD:HAF2	1.86	0.57
1:G:15:GLU:O	1:G:19:ASN:ND2	2.37	0.57
21:P:503:CLA:H172	21:P:510:CLA:HBB2	1.85	0.57
2:B:271:THR:HB	2:B:274:GLN:HG3	1.87	0.56
21:B:608:CLA:H151	21:B:609:CLA:H203	1.86	0.56
30:K:101:BCR:H331	30:K:101:BCR:C8	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:259:ILE:HG12	27:Q:407:LMG:H292	1.86	0.56
1:A:111:PRO:O	1:A:115:ILE:HG13	2.04	0.56
4:D:87:HIS:HD2	4:D:162:LEU:HD23	1.70	0.56
1:G:153:SER:HB3	21:G:402:CLA:HED1	1.88	0.56
3:P:377:LEU:O	3:P:381:LYS:HB2	2.05	0.56
2:B:371:THR:HG22	2:B:377:VAL:HA	1.86	0.56
24:B:628:DGD:HD3	31:B:630:LMT:H12	1.87	0.56
2:N:19:LEU:O	2:N:23:HIS:ND1	2.38	0.56
2:N:187:PRO:HB3	21:N:605:CLA:HMB2	1.87	0.56
4:Q:21:TRP:O	4:Q:26:ARG:NH2	2.35	0.56
3:C:449:ARG:HE	21:C:505:CLA:HED1	1.70	0.56
1:A:64:ARG:O	13:O:178:ARG:NH2	2.39	0.56
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.87	0.56
21:A:403:CLA:H142	21:D:401:CLA:H151	1.87	0.56
2:B:213:GLY:O	2:B:217:ILE:HG13	2.06	0.56
21:B:603:CLA:HBA2	21:B:604:CLA:HED3	1.87	0.56
2:B:462:PHE:CZ	21:B:613:CLA:HMB3	2.40	0.56
3:C:405:ASN:HD22	24:C:518:DGD:HD5	1.70	0.56
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.87	0.56
3:P:405:ASN:HD22	24:P:519:DGD:HD5	1.69	0.56
21:A:402:CLA:H203	22:A:404:PHO:H71	1.87	0.56
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.88	0.56
21:B:609:CLA:HMC2	30:H:101:BCR:H343	1.87	0.56
2:N:124:ARG:HE	2:N:131:PRO:HD3	1.71	0.56
3:P:114:VAL:HG22	27:P:521:LMG:H152	1.88	0.56
3:C:156:LYS:O	3:C:160:ILE:HG13	2.06	0.56
13:O:240:THR:HA	13:O:264:VAL:HA	1.86	0.56
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.88	0.56
1:G:28:LEU:HB2	26:G:401:SQD:H91	1.87	0.56
4:Q:148:ALA:HB3	4:Q:149:PRO:HD3	1.88	0.56
4:Q:192:THR:HG23	21:Q:402:CLA:HBC2	1.88	0.56
5:R:84:LYS:HB2	5:R:84:LYS:NZ	2.21	0.56
4:D:259:ILE:HG12	27:D:407:LMG:H292	1.88	0.55
5:E:84:LYS:NZ	5:E:84:LYS:HB2	2.22	0.55
1:G:40:THR:HG21	1:G:121:LEU:HD23	1.88	0.55
4:Q:87:HIS:CD2	4:Q:162:LEU:HA	2.42	0.55
5:R:18:ARG:HD2	5:R:22:ILE:HD11	1.86	0.55
27:D:407:LMG:H111	11:L:19:LEU:HD21	1.89	0.55
1:G:32:TRP:CE3	1:G:32:TRP:HA	2.42	0.55
30:P:515:BCR:H24C	21:P:513:CLA:HAB	1.88	0.55
27:D:407:LMG:H392	30:T:102:BCR:HC32	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:612:CLA:H42	4:Q:127:LEU:HD11	1.88	0.55
7:W:55:LEU:HB2	7:W:58:VAL:HG12	1.88	0.55
1:A:38:ILE:HG12	26:A:414:SQD:H142	1.88	0.55
21:B:604:CLA:HBB1	21:B:607:CLA:HBB2	1.89	0.55
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.87	0.55
2:N:348:ASN:HB3	2:N:354:LEU:HD21	1.87	0.55
2:N:371:THR:HG22	2:N:377:VAL:HA	1.87	0.55
4:D:266:TRP:CD1	27:D:407:LMG:HC3	2.42	0.55
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.39	0.55
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.88	0.55
20:Z:36:SER:HA	20:Z:39:LEU:HG	1.88	0.55
21:P:504:CLA:H202	24:P:519:DGD:HAF2	1.88	0.55
3:C:166:ILE:O	3:C:170:ILE:HG13	2.07	0.55
3:C:241:GLY:O	3:C:245:ILE:HG13	2.07	0.55
1:G:60:ILE:HD12	1:G:84:PRO:HD2	1.88	0.55
21:N:608:CLA:HBB1	21:N:611:CLA:HBB2	1.86	0.55
26:B:624:SQD:H241	26:B:624:SQD:H111	1.89	0.55
5:E:18:ARG:O	5:E:22:ILE:HG13	2.07	0.55
21:C:504:CLA:H151	24:C:517:DGD:HBW1	1.87	0.54
4:D:21:TRP:O	4:D:26:ARG:NH2	2.38	0.54
4:D:199:MET:HB3	23:D:404:PL9:H28	1.88	0.54
12:M:31:SER:HB3	27:M:101:LMG:HC71	1.88	0.54
2:N:89:GLY:HA2	24:N:602:DGD:HD5	1.88	0.54
3:P:137:PRO:HB2	3:P:139:THR:O	2.07	0.54
5:R:60:GLN:OE1	5:R:84:LYS:NZ	2.40	0.54
1:A:238:LYS:O	1:A:241:GLN:HG3	2.07	0.54
1:A:22:THR:HG21	8:I:30:ARG:HD3	1.88	0.54
3:P:437:PHE:CZ	21:P:510:CLA:HMB3	2.42	0.54
21:G:403:CLA:HHC	21:G:403:CLA:HBB1	1.88	0.54
3:P:174:LEU:HD12	21:P:512:CLA:H71	1.89	0.54
21:A:402:CLA:HBB1	21:A:402:CLA:HHC	1.89	0.54
26:A:414:SQD:H332	21:N:610:CLA:H203	1.89	0.54
4:D:192:THR:HG23	21:D:401:CLA:HBC2	1.88	0.54
2:N:150:CYS:HA	21:N:607:CLA:HBC2	1.89	0.54
2:N:150:CYS:HB2	21:N:607:CLA:HMC3	1.89	0.54
2:N:222:PRO:HG3	7:W:27:THR:H	1.73	0.54
3:C:429:SER:HB3	24:C:517:DGD:HA81	1.89	0.54
15:U:54:LYS:HB2	15:U:113:THR:HG23	1.88	0.54
5:E:15:THR:HG23	9:J:8:ILE:O	2.08	0.54
1:G:72:LEU:HD13	27:Q:401:LMG:H111	1.88	0.54
1:A:63:ILE:HB	3:C:335:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:215:LYS:HB3	3:P:223:TRP:HA	1.90	0.54
3:C:174:LEU:HD12	21:C:512:CLA:H71	1.89	0.54
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.43	0.54
2:N:18:ARG:NH2	26:N:601:SQD:O9	2.41	0.54
21:B:614:CLA:H61	27:E:102:LMG:H181	54.54	0.54
24:C:518:DGD:HD2	9:J:32:ALA:O	2.08	0.54
16:V:59:PHE:HA	16:V:63:CYS:SG	2.48	0.54
5:E:81:GLU:C	5:E:83:LEU:H	2.10	0.54
13:O:73:PRO:HG2	13:O:102:THR:HB	1.89	0.54
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.90	0.53
2:B:120:LEU:HD13	21:B:616:CLA:HMD2	1.89	0.53
4:Q:122:LEU:HD11	22:Q:403:PHO:H92	1.90	0.53
5:R:81:GLU:C	5:R:83:LEU:H	2.11	0.53
1:A:32:TRP:CE3	1:A:32:TRP:HA	2.43	0.53
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.90	0.53
1:G:332:HIS:CD2	1:G:333:GLU:HG3	2.43	0.53
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.37	0.53
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.11	0.53
1:A:45:THR:HG21	26:A:414:SQD:H201	1.91	0.53
3:C:466:VAL:HG13	4:D:251:ARG:HD2	1.89	0.53
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.91	0.53
2:N:256:MET:HA	2:N:263:THR:HG21	1.89	0.53
4:Q:43:LEU:HD23	4:Q:117:HIS:CE1	2.44	0.53
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.61	0.53
2:B:24:LEU:HD21	21:B:616:CLA:HAB	1.90	0.53
1:G:190:HIS:O	1:G:298:ASN:HB3	2.09	0.53
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.44	0.53
5:E:8:ARG:HB2	6:F:13:TYR:HB3	1.89	0.53
20:Z:49:ALA:O	20:Z:53:VAL:HG23	2.09	0.53
2:N:19:LEU:HG	2:N:23:HIS:CE1	2.44	0.53
4:Q:199:MET:HG2	23:Q:405:PL9:H322	1.90	0.53
1:G:111:PRO:O	1:G:115:ILE:HG13	2.08	0.53
21:G:402:CLA:H122	22:G:405:PHO:H3A	1.90	0.53
13:O:118:SER:HB3	13:O:157:PRO:HA	1.91	0.53
3:P:350:ILE:HG21	3:P:359:TRP:HB2	1.91	0.53
4:Q:49:LEU:O	4:Q:53:THR:HG23	2.09	0.53
21:B:604:CLA:HBB1	21:B:607:CLA:CBB	2.38	0.53
3:C:45:LEU:HD23	3:C:48:LYS:HD2	1.91	0.53
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.91	0.53
2:N:69:LEU:HD12	21:N:609:CLA:HBA1	1.90	0.53
3:P:187:ASP:HB2	3:P:230:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:503:CLA:H152	21:P:509:CLA:H2	1.90	0.53
4:Q:103:ARG:NH1	5:R:77:GLU:OE2	2.42	0.53
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.43	0.53
5:E:56:TYR:O	16:V:27:ALA:HB2	2.09	0.53
1:G:224:ILE:O	4:Q:265:ARG:NH2	2.40	0.53
2:N:462:PHE:CZ	21:N:617:CLA:HMB3	2.44	0.53
3:P:449:ARG:HE	21:P:505:CLA:HED1	1.74	0.53
23:A:406:PL9:H301	4:D:42:TYR:HA	1.91	0.52
5:R:8:ARG:NE	5:R:13:ILE:HG12	2.24	0.52
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	0.52
5:E:61:ARG:HH22	16:V:153:GLY:HA3	1.74	0.52
5:E:8:ARG:NE	5:E:13:ILE:HG12	2.24	0.52
1:G:93:PHE:CD2	1:G:95:PRO:HD3	2.44	0.52
6:S:21:VAL:O	6:S:25:THR:HG23	2.10	0.52
21:C:501:CLA:H171	21:C:507:CLA:HMB3	1.91	0.52
4:D:261:PHE:HB2	23:D:404:PL9:H522	1.91	0.52
2:N:135:LEU:HB2	2:N:136:PRO:HD3	1.91	0.52
24:N:602:DGD:HD3	31:N:604:LMT:H12	1.92	0.52
21:N:620:CLA:H72	21:N:620:CLA:H12	1.92	0.52
3:P:149:TYR:HA	3:P:156:LYS:HD3	1.90	0.52
3:P:156:LYS:O	3:P:160:ILE:HG13	2.10	0.52
1:G:328:MET:HE1	4:Q:183:LEU:HD22	1.92	0.52
27:D:406:LMG:O3	9:J:37:GLY:HA3	2.10	0.52
21:G:403:CLA:H203	22:G:405:PHO:H71	1.92	0.52
2:N:23:HIS:NE2	21:N:616:CLA:NB	2.58	0.52
1:A:140:ARG:HH22	25:A:408:LHG:P	2.32	0.52
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.90	0.52
2:B:329:PRO:HB3	21:B:607:CLA:HED1	1.92	0.52
4:D:266:TRP:HD1	27:D:407:LMG:HC3	1.75	0.52
10:K:26:PRO:O	10:K:29:PRO:HD2	2.10	0.52
2:N:9:HIS:HB2	21:N:615:CLA:HBA1	1.92	0.52
3:P:437:PHE:HZ	21:P:510:CLA:HMB3	1.73	0.52
21:G:404:CLA:H142	21:Q:402:CLA:H151	1.90	0.52
1:A:190:HIS:O	1:A:298:ASN:HB3	2.10	0.52
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.74	0.52
3:P:209:ILE:HG23	30:P:516:BCR:H382	1.91	0.52
3:P:240:ILE:O	3:P:244:CYS:HB2	2.10	0.52
4:Q:85:MET:HA	5:R:69:ARG:HB3	1.92	0.52
5:R:18:ARG:O	5:R:22:ILE:HG13	2.10	0.52
2:B:12:LEU:HB2	21:B:612:CLA:HMC2	1.92	0.52
3:P:216:SER:HB3	3:P:221:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:266:TRP:CD1	27:Q:407:LMG:HC3	2.45	0.52
1:A:131:TRP:CH2	21:C:505:CLA:HAA2	2.45	0.52
1:A:329:GLU:O	1:A:332:HIS:ND1	2.38	0.52
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.92	0.52
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.43	0.52
21:N:614:CLA:H152	21:N:619:CLA:HBD	1.92	0.52
5:R:8:ARG:HB2	6:S:13:TYR:HB3	1.91	0.52
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.91	0.52
21:B:614:CLA:H2	26:B:627:SQD:H112	1.93	0.51
2:B:489:GLU:HB2	5:E:3:GLY:N	2.25	0.51
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.10	0.51
3:P:241:GLY:O	3:P:245:ILE:HG13	2.10	0.51
5:R:81:GLU:O	5:R:83:LEU:N	2.36	0.51
1:G:238:LYS:O	1:G:241:GLN:HG3	2.10	0.51
1:G:38:ILE:HG12	26:G:401:SQD:H142	1.93	0.51
27:I:102:LMG:H181	31:I:103:LMT:H42	1.91	0.51
3:P:130:VAL:O	3:P:134:ILE:HG12	2.10	0.51
18:X:34:PHE:O	18:X:38:ILE:HG12	2.09	0.51
26:A:409:SQD:H241	25:A:411:LHG:HC81	1.91	0.51
21:B:616:CLA:H72	21:B:616:CLA:H12	1.91	0.51
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.92	0.51
1:G:119:PHE:HZ	21:G:402:CLA:H8	1.75	0.51
3:C:347:GLY:HA3	13:O:43:ASN:HB2	1.93	0.51
3:P:229:ASN:ND2	3:P:232:ASP:OD1	2.36	0.51
1:A:227:THR:HG21	1:A:233:ALA:HA	1.92	0.51
27:A:410:LMG:H292	11:L:20:GLY:HA2	1.93	0.51
2:B:9:HIS:HB2	21:B:611:CLA:HBA1	1.91	0.51
3:C:187:ASP:HB2	3:C:230:LEU:HD12	1.91	0.51
3:P:120:ILE:HD11	30:P:514:BCR:HC8	1.93	0.51
3:P:45:LEU:HD23	3:P:48:LYS:HD2	1.93	0.51
15:U:83:ALA:HB1	15:U:84:PRO:CD	2.38	0.51
2:B:256:MET:HA	2:B:263:THR:HG21	1.93	0.51
21:B:610:CLA:H152	21:B:615:CLA:HBD	1.93	0.51
1:G:140:ARG:HH22	25:G:409:LHG:P	2.33	0.51
21:P:501:CLA:H171	21:P:507:CLA:HMB3	1.93	0.51
26:A:409:SQD:H223	24:C:518:DGD:HAE1	1.93	0.51
2:B:280:PHE:O	2:B:284:ILE:HG13	2.11	0.51
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.93	0.51
3:P:248:GLY:O	3:P:252:ILE:HG12	2.11	0.51
3:P:52:ALA:HA	21:P:511:CLA:HMB3	1.92	0.51
2:B:212:ALA:HB2	21:B:609:CLA:HMC3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:315:ILE:HG22	2:N:426:PHE:HB3	1.93	0.51
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.92	0.51
3:C:240:ILE:HD11	30:C:515:BCR:H372	1.92	0.51
3:C:240:ILE:O	3:C:244:CYS:HB2	2.10	0.51
21:G:402:CLA:H202	21:G:403:CLA:H93	1.93	0.51
3:P:90:PRO:O	3:P:94:THR:HG23	2.11	0.51
34:V:201:HEM:HBC2	34:V:201:HEM:HHH	1.93	0.51
2:B:230:ARG:O	2:B:233:ASN:HB3	2.11	0.51
3:C:52:ALA:HA	21:C:511:CLA:HMB3	1.93	0.51
10:K:37:PHE:HB3	30:K:101:BCR:C40	2.41	0.51
1:A:78:ILE:O	1:A:176:ILE:HB	2.11	0.50
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.46	0.50
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.92	0.50
1:G:57:PRO:HG3	1:G:68:SER:HB3	1.93	0.50
3:P:240:ILE:HD11	30:P:516:BCR:H372	1.93	0.50
4:Q:250:ASN:HD22	4:Q:262:SER:HB3	1.76	0.50
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.93	0.50
21:A:405:CLA:HBC1	27:I:102:LMG:H341	1.92	0.50
21:P:506:CLA:HMC2	21:P:507:CLA:H102	1.92	0.50
26:F:101:SQD:H162	18:X:33:THR:HA	1.92	0.50
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.92	0.50
3:P:72:LEU:HD11	3:P:108:THR:HB	1.92	0.50
2:B:133:LEU:HB3	2:B:138:MET:CE	2.41	0.50
2:B:150:CYS:HB2	21:B:603:CLA:HMC3	1.94	0.50
24:B:628:DGD:HA21	31:B:630:LMT:H121	1.93	0.50
1:G:34:GLY:HA2	1:G:37:MET:HB3	1.92	0.50
13:O:87:GLN:O	13:O:88:GLU:HB3	2.12	0.50
4:Q:252:PHE:O	4:Q:256:ILE:HG22	2.11	0.50
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.46	0.50
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.93	0.50
1:G:188:ALA:HB2	1:G:328:MET:HB2	1.92	0.50
4:Q:261:PHE:HB2	23:Q:405:PL9:H522	1.94	0.50
23:G:407:PL9:H301	4:Q:42:TYR:HA	1.94	0.50
3:C:248:GLY:O	3:C:252:ILE:HG12	2.11	0.50
21:A:403:CLA:HAB	21:D:401:CLA:H72	1.93	0.50
2:N:271:THR:HB	2:N:274:GLN:HG3	1.93	0.50
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.92	0.50
2:B:133:LEU:HB3	2:B:138:MET:HE2	1.93	0.50
2:N:206:GLY:O	2:N:210:ILE:HG13	2.12	0.50
4:D:49:LEU:O	4:D:53:THR:HG23	2.11	0.50
1:A:224:ILE:O	4:D:265:ARG:NH2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:391:ARG:HB2	3:C:391:ARG:NH1	2.27	0.49
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.49
21:D:403:CLA:HMD2	31:D:409:LMT:H22	1.93	0.49
2:N:27:THR:HG22	2:N:107:LEU:HD13	1.94	0.49
4:Q:189:HIS:HA	4:Q:294:ARG:HD2	1.94	0.49
1:G:258:LEU:HD12	4:Q:128:ARG:HD3	1.94	0.49
2:B:222:PRO:HG3	7:H:27:THR:H	1.78	0.49
2:B:69:LEU:HD12	21:B:605:CLA:HBA1	1.93	0.49
3:C:425:TRP:CE2	21:C:504:CLA:HBA1	2.46	0.49
21:C:507:CLA:OBD	21:C:509:CLA:H122	2.13	0.49
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.77	0.49
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.78	0.49
2:N:486:LEU:O	2:N:486:LEU:HD13	2.12	0.49
13:O:218:LEU:HD22	15:U:119:THR:HG21	1.93	0.49
3:C:165:LEU:HD21	21:C:506:CLA:HHC	1.94	0.49
11:L:11:GLU:HG2	11:L:12:LEU:N	2.27	0.49
2:N:489:GLU:HB2	5:R:3:GLY:N	2.26	0.49
21:P:508:CLA:HAB	21:P:510:CLA:HMA1	1.94	0.49
21:P:507:CLA:OBD	21:P:509:CLA:H122	2.12	0.49
21:C:513:CLA:HAB	30:Z:101:BCR:H24C	1.93	0.49
21:B:608:CLA:H12	4:D:127:LEU:HD21	1.93	0.49
13:O:206:GLU:CD	13:O:206:GLU:H	2.16	0.49
4:Q:191:TRP:CE3	4:Q:289:LEU:HD11	2.48	0.49
4:Q:266:TRP:HD1	27:Q:407:LMG:HC3	1.76	0.49
5:R:27:ILE:HB	5:R:28:PRO:HD3	1.94	0.49
4:Q:56:THR:HG21	5:R:50:PRO:HD3	1.93	0.49
2:B:206:GLY:O	2:B:210:ILE:HG13	2.13	0.49
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.94	0.49
21:B:608:CLA:HBA2	26:B:624:SQD:H101	1.93	0.49
3:C:120:ILE:HD11	30:C:514:BCR:HC8	1.94	0.49
5:E:18:ARG:NH1	5:E:18:ARG:HB3	2.27	0.49
13:O:230:VAL:HG12	13:O:231:ASP:N	2.25	0.49
4:Q:54:PHE:HB3	5:R:47:PHE:CD2	2.48	0.49
20:Z:55:GLY:HA2	30:Z:101:BCR:H312	1.95	0.49
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.95	0.49
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.48	0.49
1:G:156:ALA:HA	1:G:160:ILE:HB	1.94	0.49
21:P:512:CLA:H143	21:P:513:CLA:H162	1.94	0.49
1:A:141:PRO:O	1:A:143:ILE:N	2.44	0.49
1:A:211:PHE:HA	1:A:214:MET:HB2	1.95	0.49
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:406:SER:O	3:C:418:ASN:ND2	2.43	0.49
21:C:503:CLA:H152	21:C:509:CLA:H2	1.95	0.49
1:G:78:ILE:O	1:G:176:ILE:HB	2.11	0.49
4:Q:201:VAL:HB	21:Q:402:CLA:HMB3	1.95	0.49
1:A:132:GLU:O	1:A:136:ARG:HG2	2.13	0.49
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.48	0.49
2:B:96:VAL:HG22	21:B:606:CLA:HBA1	1.94	0.49
21:N:606:CLA:H42	7:W:45:ILE:HD11	1.95	0.49
4:D:252:PHE:O	4:D:256:ILE:HG22	2.13	0.49
1:G:141:PRO:O	1:G:143:ILE:N	2.44	0.49
2:N:124:ARG:HH11	2:N:124:ARG:HG3	1.77	0.49
26:B:624:SQD:H301	26:B:624:SQD:H171	1.95	0.48
21:C:503:CLA:HBB1	27:C:520:LMG:C20	2.43	0.48
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.95	0.48
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.94	0.48
26:G:410:SQD:H241	25:G:412:LHG:HC81	1.95	0.48
2:N:280:PHE:O	2:N:284:ILE:HG13	2.12	0.48
13:O:190:LEU:HB2	13:O:214:LYS:HB2	1.95	0.48
30:B:618:BCR:HC32	27:Q:407:LMG:H392	1.95	0.48
1:A:238:LYS:HD2	14:T:32:LYS:HB3	1.96	0.48
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.48
1:A:40:THR:HG21	1:A:121:LEU:HD23	1.94	0.48
2:N:251:VAL:HA	24:W:102:DGD:HB51	1.95	0.48
4:Q:55:VAL:HG21	4:Q:110:LEU:HD12	1.94	0.48
31:N:625:LMT:H102	7:W:35:MET:SD	2.53	0.48
3:C:209:ILE:HG23	30:C:515:BCR:H382	1.94	0.48
1:G:126:TYR:O	1:G:130:GLN:HG3	2.14	0.48
27:M:101:LMG:H181	21:N:618:CLA:H61	1.96	0.48
21:N:609:CLA:HMC2	21:N:619:CLA:H2	1.96	0.48
2:B:486:LEU:O	2:B:486:LEU:HD13	2.13	0.48
21:B:607:CLA:H3A	21:B:607:CLA:HBA2	1.36	0.48
3:C:72:LEU:HD11	3:C:108:THR:HB	1.95	0.48
21:G:402:CLA:HAB	21:G:404:CLA:HMD2	1.95	0.48
26:N:601:SQD:H112	21:N:618:CLA:H2	1.96	0.48
21:N:606:CLA:H122	21:N:606:CLA:H162	1.55	0.48
3:P:391:ARG:NH1	3:P:391:ARG:HB2	2.28	0.48
4:Q:348:ARG:NH2	4:Q:352:LEU:O	2.41	0.48
21:A:401:CLA:H102	21:A:401:CLA:H62	1.61	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
2:B:191:ASN:HB2	7:H:58:VAL:CG2	2.44	0.48
21:C:509:CLA:CMB	21:C:511:CLA:HBB1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:512:CLA:H143	21:C:513:CLA:H162	1.96	0.48
21:B:606:CLA:H203	26:G:401:SQD:H332	1.94	0.48
2:N:191:ASN:HB2	7:W:58:VAL:CG2	2.42	0.48
2:N:230:ARG:O	2:N:233:ASN:HB3	2.12	0.48
15:U:38:GLU:HG2	15:U:39:LEU:N	2.28	0.48
23:A:406:PL9:H33	4:D:38:PHE:HD1	1.78	0.48
2:N:7:ARG:NH2	27:N:622:LMG:O3	2.47	0.48
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.95	0.48
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.44	0.48
10:K:31:LEU:HB3	30:K:101:BCR:C15	2.43	0.48
2:N:243:ALA:HA	2:N:246:PHE:CE2	2.48	0.48
4:Q:18:LEU:O	4:Q:22:LEU:HG	2.13	0.48
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.95	0.48
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.78	0.48
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.95	0.48
1:G:317:TRP:CD1	4:Q:177:ALA:HB2	2.49	0.48
20:Z:28:ALA:O	20:Z:30:PRO:HD3	2.14	0.48
21:B:606:CLA:H18	21:B:616:CLA:H121	1.96	0.48
3:C:240:ILE:HG13	21:C:501:CLA:HBB1	1.95	0.48
4:D:39:PRO:O	4:D:43:LEU:HD22	2.13	0.48
1:G:131:TRP:CH2	21:P:505:CLA:HAA2	2.48	0.48
11:L:6:ASN:O	11:L:8:GLN:NE2	2.47	0.48
21:N:607:CLA:HBA2	21:N:608:CLA:HED3	1.95	0.48
3:P:472:LEU:HD12	3:P:473:ASP:H	1.79	0.48
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.79	0.48
1:G:132:GLU:O	1:G:136:ARG:HG2	2.14	0.48
8:I:6:ILE:O	8:I:10:ILE:HG12	2.13	0.48
2:N:184:GLU:H	2:N:200:ALA:HB2	1.79	0.48
21:N:620:CLA:HBA2	21:N:620:CLA:CGD	2.44	0.48
13:O:36:ILE:HG23	13:O:41:LEU:HB3	1.96	0.48
4:Q:152:VAL:HG21	4:Q:279:LEU:HD12	1.96	0.48
2:B:198:VAL:O	2:B:202:HIS:ND1	2.43	0.47
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.96	0.47
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.48	0.47
3:P:223:TRP:CD2	3:P:224:ILE:HG13	2.49	0.47
4:Q:199:MET:HB3	23:Q:405:PL9:H28	1.96	0.47
16:V:98:LEU:O	16:V:102:MET:HG3	2.14	0.47
1:A:143:ILE:HD11	4:D:217:THR:HA	1.96	0.47
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.48	0.47
21:B:614:CLA:H51	30:B:617:BCR:H372	1.96	0.47
5:E:23:HIS:HA	5:E:26:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:GLU:OE2	1:G:334:ARG:NH2	2.48	0.47
10:K:24:VAL:O	10:K:27:VAL:HG12	2.14	0.47
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.49	0.47
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.96	0.47
20:Z:33:TRP:O	20:Z:33:TRP:HD1	1.97	0.47
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.96	0.47
4:D:134:ARG:HA	4:D:134:ARG:HE	1.79	0.47
2:N:329:PRO:HB3	21:N:611:CLA:HED1	1.95	0.47
21:B:605:CLA:HMB3	21:B:606:CLA:H11	1.97	0.47
3:C:275:SER:HB3	21:C:509:CLA:HED3	1.96	0.47
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.50	0.47
21:G:402:CLA:CAB	21:G:404:CLA:HMD2	2.44	0.47
22:G:405:PHO:H41	22:G:405:PHO:H62	1.49	0.47
7:H:19:GLY:O	7:H:21:VAL:HG13	2.14	0.47
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.50	0.47
3:P:275:SER:HB3	21:P:509:CLA:HED3	1.95	0.47
21:P:504:CLA:H121	24:P:518:DGD:HBE2	1.97	0.47
2:B:271:THR:HG22	2:B:273:TYR:N	2.29	0.47
21:B:610:CLA:H12	21:B:610:CLA:H112	1.95	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.14	0.47
3:C:472:LEU:HD12	3:C:473:ASP:H	1.80	0.47
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.15	0.47
5:E:7:GLU:H	5:E:7:GLU:CD	2.18	0.47
1:G:180:PHE:O	1:G:184:ILE:HG13	2.15	0.47
8:I:24:LEU:O	8:I:26:GLY:N	2.42	0.47
26:Q:408:SQD:H111	26:Q:408:SQD:H241	1.96	0.47
5:R:7:GLU:H	5:R:7:GLU:CD	2.18	0.47
1:A:126:TYR:O	1:A:130:GLN:HG3	2.14	0.47
3:C:75:PHE:CD1	3:C:86:LEU:HD21	2.47	0.47
4:D:18:LEU:O	4:D:22:LEU:HG	2.15	0.47
2:N:133:LEU:HB3	2:N:138:MET:CE	2.44	0.47
2:N:198:VAL:O	2:N:202:HIS:ND1	2.41	0.47
4:Q:161:PRO:HB3	4:Q:170:ALA:HB2	1.95	0.47
4:Q:210:LEU:HA	4:Q:213:ILE:HG22	1.96	0.47
1:A:176:ILE:HD12	21:A:402:CLA:HED3	1.97	0.47
2:B:12:LEU:HD22	2:B:18:ARG:HB2	1.97	0.47
3:C:276:LEU:HD11	3:C:444:HIS:HD2	1.79	0.47
31:B:626:LMT:H102	7:H:35:MET:SD	2.55	0.47
6:S:28:VAL:HB	6:S:29:PRO:HD3	1.97	0.47
21:A:402:CLA:CHA	21:A:402:CLA:HBA1	2.44	0.47
4:D:264:LYS:O	4:D:268:HIS:ND1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:21:VAL:O	6:F:25:THR:HG23	2.15	0.47
8:I:15:PHE:CE1	30:I:101:BCR:H312	2.49	0.47
11:L:5:PRO:HA	11:L:7:ARG:HH22	1.79	0.47
21:N:607:CLA:H141	21:N:607:CLA:H161	1.61	0.47
21:P:509:CLA:HMB3	21:P:510:CLA:HAA1	1.96	0.47
4:Q:129:GLN:HE22	4:Q:143:ALA:HA	1.80	0.47
21:A:401:CLA:HAB	21:A:403:CLA:HMD2	1.97	0.47
21:C:509:CLA:H92	21:C:509:CLA:H62	1.70	0.47
30:C:514:BCR:H321	30:C:514:BCR:H343	1.96	0.47
3:P:305:THR:HG22	3:P:308:GLU:HB2	1.97	0.47
4:Q:87:HIS:CD2	4:Q:162:LEU:HD23	2.46	0.47
1:A:119:PHE:HZ	21:A:401:CLA:H8	1.78	0.47
21:G:404:CLA:H202	27:Q:406:LMG:H401	1.96	0.47
22:G:405:PHO:H61	22:G:405:PHO:H92	1.62	0.47
30:T:101:BCR:H372	21:N:618:CLA:H51	1.96	0.47
26:G:410:SQD:H223	24:P:519:DGD:HAE1	1.96	0.47
3:P:75:PHE:CD1	3:P:86:LEU:HD21	2.48	0.47
5:R:23:HIS:HA	5:R:26:THR:OG1	2.14	0.47
7:W:19:GLY:O	7:W:21:VAL:HG13	2.14	0.47
2:B:286:ARG:HH11	2:B:286:ARG:HG2	1.80	0.46
2:B:474:LEU:O	4:D:134:ARG:NH1	2.48	0.46
21:C:501:CLA:C2D	21:C:503:CLA:H2	2.45	0.46
3:C:265:ILE:HG12	21:C:505:CLA:HED1	1.97	0.46
3:C:60:ILE:HG23	21:C:510:CLA:HMC2	1.97	0.46
5:E:8:ARG:HB2	6:F:13:TYR:CB	2.46	0.46
3:C:29:GLU:HB3	10:K:46:ARG:NH1	2.30	0.46
2:N:271:THR:HG22	2:N:273:TYR:N	2.29	0.46
2:N:286:ARG:HH11	2:N:286:ARG:HG2	1.80	0.46
21:P:505:CLA:HBA1	21:P:505:CLA:CBD	2.41	0.46
4:Q:244:TYR:OH	4:Q:264:LYS:HE3	2.14	0.46
14:T:22:PHE:HB3	30:T:103:BCR:H291	1.97	0.46
20:Z:30:PRO:C	20:Z:32:ASP:H	2.19	0.46
21:A:401:CLA:CAB	21:A:403:CLA:HMD2	2.45	0.46
21:C:504:CLA:H121	24:C:517:DGD:HBE2	1.97	0.46
21:C:509:CLA:HMB1	21:C:511:CLA:HBB1	1.97	0.46
1:G:182:PHE:O	1:G:186:PHE:HB2	2.16	0.46
2:N:483:ASP:CB	2:N:484:PRO:HD2	2.44	0.46
3:P:461:ARG:HG3	3:P:461:ARG:HH11	1.80	0.46
7:W:55:LEU:O	7:W:58:VAL:HG12	2.15	0.46
1:A:38:ILE:O	1:A:42:LEU:HG	2.16	0.46
2:B:251:VAL:HA	24:B:621:DGD:HB51	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.81	0.46
4:D:201:VAL:HB	21:D:401:CLA:HMB3	1.97	0.46
1:G:29:TYR:CG	1:G:133:LEU:HD13	2.50	0.46
1:G:27:ARG:NH1	4:Q:254:SER:O	2.48	0.46
21:G:404:CLA:H93	21:Q:402:CLA:H152	1.97	0.46
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.61	0.46
2:N:212:ALA:HB2	21:N:613:CLA:HMC3	1.97	0.46
3:P:197:ARG:NH2	3:P:231:GLU:OE2	2.48	0.46
4:Q:88:SER:HB2	5:R:69:ARG:NH2	2.30	0.46
6:S:11:VAL:HG12	6:S:12:SER:H	1.81	0.46
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.96	0.46
5:E:82:GLN:HG3	5:E:82:GLN:H	1.52	0.46
11:L:7:ARG:HD2	11:L:7:ARG:O	2.16	0.46
3:P:380:ILE:HA	3:P:384:ILE:HD11	1.97	0.46
3:P:60:ILE:HG23	21:P:510:CLA:HMC2	1.96	0.46
4:Q:67:TYR:CE1	4:Q:76:VAL:HG11	2.50	0.46
1:A:159:LEU:C	1:A:162:PRO:HD2	2.36	0.46
1:A:257:ARG:HH22	2:B:489:GLU:HA	1.81	0.46
2:B:462:PHE:CE1	21:B:613:CLA:HMB3	2.50	0.46
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.50	0.46
21:G:402:CLA:HBA1	21:G:402:CLA:H3A	1.55	0.46
30:J:102:BCR:H351	30:J:102:BCR:H15C	1.68	0.46
13:O:77:LEU:HD23	13:O:93:PRO:HA	1.97	0.46
22:Q:403:PHO:H151	21:Q:402:CLA:H172	1.98	0.46
3:C:28:GLN:HB2	21:C:511:CLA:HED3	1.97	0.46
21:G:403:CLA:CHA	21:G:403:CLA:HBA1	2.46	0.46
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.16	0.46
2:N:18:ARG:HD3	2:N:118:TRP:HB3	1.98	0.46
3:P:405:ASN:HB2	24:P:519:DGD:HG31	1.98	0.46
5:R:18:ARG:NH1	5:R:18:ARG:HB3	2.29	0.46
1:A:244:GLU:OE1	4:D:264:LYS:NZ	2.48	0.46
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.50	0.46
21:B:603:CLA:H141	21:B:603:CLA:H161	1.62	0.46
21:B:612:CLA:CMB	21:B:614:CLA:HBB1	2.46	0.46
30:B:618:BCR:H341	30:B:618:BCR:H11C	1.84	0.46
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.49	0.46
3:C:461:ARG:HG3	3:C:461:ARG:HH11	1.79	0.46
3:C:85:GLY:N	24:C:517:DGD:HE4	2.31	0.46
5:E:78:THR:O	5:E:81:GLU:HB2	2.15	0.46
2:N:256:MET:O	2:N:448:ARG:NH1	2.42	0.46
13:O:55:ALA:HA	13:O:230:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:165:LEU:HD21	21:P:506:CLA:HHC	1.98	0.46
3:P:245:ILE:O	3:P:249:ILE:HG12	2.15	0.46
3:P:38:GLY:HA3	21:P:511:CLA:HMD3	1.98	0.46
2:B:150:CYS:HA	21:B:603:CLA:HBC2	1.98	0.46
1:G:93:PHE:CD2	24:G:408:DGD:HD2	2.51	0.46
9:J:14:ALA:HB3	30:K:101:BCR:H393	1.97	0.46
9:J:9:PRO:HB2	9:J:12:ILE:HG13	1.98	0.46
10:K:18:PHE:O	10:K:22:VAL:HG23	2.16	0.46
2:N:462:PHE:CE1	21:N:617:CLA:HMB3	2.51	0.46
3:P:178:LYS:HA	3:P:182:PHE:HB2	1.97	0.46
4:Q:39:PRO:O	4:Q:43:LEU:HD22	2.16	0.46
1:G:262:TYR:O	27:R:102:LMG:H112	2.16	0.46
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.51	0.46
31:B:629:LMT:H3'	31:B:629:LMT:H1B	1.62	0.46
27:D:407:LMG:HC71	27:D:407:LMG:HC2	1.77	0.46
1:G:38:ILE:O	1:G:42:LEU:HG	2.15	0.46
4:Q:264:LYS:O	4:Q:268:HIS:ND1	2.32	0.46
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.51	0.46
1:A:180:PHE:O	1:A:184:ILE:HG13	2.16	0.46
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.81	0.46
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.98	0.46
23:A:406:PL9:H33	4:D:38:PHE:CD1	2.50	0.46
30:P:514:BCR:H321	30:P:514:BCR:H343	1.96	0.46
21:G:404:CLA:HAB	21:Q:402:CLA:H72	1.98	0.46
21:B:609:CLA:H62	21:B:609:CLA:H92	1.71	0.45
2:N:51:VAL:HG13	2:N:308:LYS:HB2	1.98	0.45
3:P:276:LEU:HD11	3:P:444:HIS:HD2	1.81	0.45
18:X:17:LYS:O	18:X:21:ILE:HG13	2.15	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.45
30:C:514:BCR:H312	20:Z:9:LEU:HD11	1.97	0.45
27:D:406:LMG:O4	9:J:31:GLY:O	2.34	0.45
1:G:329:GLU:O	1:G:332:HIS:ND1	2.40	0.45
4:Q:103:ARG:O	4:Q:107:LEU:HG	2.17	0.45
4:Q:239:GLN:HB3	4:Q:240:ALA:H	1.32	0.45
1:A:235:TYR:C	1:A:237:TYR:H	2.20	0.45
21:A:403:CLA:H202	27:D:406:LMG:H401	1.98	0.45
21:B:602:CLA:H61	7:H:46:LEU:HB2	1.97	0.45
3:C:155:ASN:HA	3:C:158:THR:HG22	1.98	0.45
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.98	0.45
24:B:621:DGD:HD2	4:D:87:HIS:ND1	2.32	0.45
2:B:192:PRO:HD2	7:H:60:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:601:SQD:H112	21:N:618:CLA:H51	1.98	0.45
13:O:33:TYR:O	13:O:37:VAL:HG23	2.17	0.45
3:P:120:ILE:CD1	30:P:514:BCR:HC8	2.46	0.45
14:T:7:VAL:HG12	31:N:603:LMT:H122	1.97	0.45
1:A:153:SER:HB3	21:A:401:CLA:HED1	1.99	0.45
1:A:249:VAL:HG11	2:B:486:LEU:HD23	1.99	0.45
3:C:305:THR:HG22	3:C:308:GLU:H	1.79	0.45
27:D:406:LMG:H171	30:D:405:BCR:H383	1.97	0.45
26:G:410:SQD:H202	24:P:519:DGD:HAH2	1.98	0.45
7:H:55:LEU:O	7:H:58:VAL:HG12	2.17	0.45
9:J:14:ALA:CB	30:K:101:BCR:H393	2.46	0.45
12:M:20:VAL:O	12:M:24:ILE:HG13	2.16	0.45
2:N:23:HIS:NE2	21:N:616:CLA:C4B	2.80	0.45
21:N:611:CLA:HBA2	21:N:611:CLA:H3A	1.34	0.45
18:X:12:ILE:HA	18:X:16:LEU:HD12	1.97	0.45
21:A:403:CLA:H93	21:D:401:CLA:H152	1.97	0.45
27:B:623:LMG:HC3	31:M:102:LMT:H2'	1.99	0.45
2:B:6:TYR:HA	21:B:611:CLA:H11	1.99	0.45
6:F:11:VAL:HG12	6:F:12:SER:H	1.81	0.45
30:B:617:BCR:H333	12:M:13:LEU:HD12	1.99	0.45
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.98	0.45
21:C:508:CLA:HAB	21:C:510:CLA:HMA1	1.99	0.45
3:C:38:GLY:HA3	21:C:511:CLA:HMD3	1.99	0.45
25:G:412:LHG:H271	25:G:412:LHG:H101	1.99	0.45
13:O:178:ARG:CG	13:O:178:ARG:HH11	2.26	0.45
3:P:80:PRO:HB3	3:P:82:TYR:CE1	2.52	0.45
4:Q:350:ASN:O	4:Q:352:LEU:N	2.45	0.45
5:R:78:THR:O	5:R:81:GLU:HB2	2.16	0.45
16:V:74:THR:O	16:V:75:ASN:HB2	2.17	0.45
21:A:405:CLA:H162	21:A:405:CLA:H141	1.60	0.45
21:B:606:CLA:H3A	21:B:606:CLA:HBA2	1.31	0.45
21:B:608:CLA:H92	26:B:624:SQD:H172	1.99	0.45
21:C:509:CLA:HMB3	21:C:510:CLA:HAA1	1.98	0.45
34:E:101:HEM:HBC2	6:F:31:ILE:HD13	1.99	0.45
1:G:272:HIS:CD2	4:Q:218:VAL:HG21	2.51	0.45
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.99	0.45
2:N:12:LEU:HB2	21:N:616:CLA:HMC2	1.99	0.45
21:N:616:CLA:CMB	21:N:618:CLA:HBB1	2.47	0.45
3:P:225:VAL:HG13	3:P:289:PHE:HA	1.98	0.45
3:P:415:ASN:O	3:P:416:SER:HB3	2.17	0.45
30:P:514:BCR:H311	30:P:514:BCR:H343	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:8:ARG:HB2	6:S:13:TYR:CB	2.47	0.45
3:C:135:ARG:HB2	20:Z:27:TYR:HB3	1.99	0.45
1:A:182:PHE:O	1:A:186:PHE:HB2	2.16	0.45
1:A:41:LEU:O	1:A:45:THR:HG22	2.16	0.45
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.99	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.97	0.45
2:B:349:LYS:HG2	2:B:395:GLN:O	2.17	0.45
21:B:603:CLA:CBB	21:B:605:CLA:H152	2.47	0.45
24:N:602:DGD:HB21	31:N:604:LMT:H72	1.99	0.45
4:Q:172:SER:HB2	4:Q:177:ALA:HB1	1.98	0.45
21:B:612:CLA:H162	21:B:612:CLA:H122	1.71	0.45
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.51	0.45
1:G:220:THR:O	1:G:223:LEU:HG	2.16	0.45
21:B:602:CLA:H42	7:H:45:ILE:HD11	1.99	0.45
9:J:18:GLY:HA3	30:K:101:BCR:H371	1.99	0.45
13:O:126:GLY:O	13:O:128:ASP:N	2.49	0.45
26:Q:408:SQD:H171	26:Q:408:SQD:H301	1.99	0.45
15:U:97:LEU:O	15:U:102:LYS:HE2	2.17	0.45
21:A:402:CLA:HMD2	21:D:401:CLA:CBB	2.46	0.45
1:A:49:VAL:O	1:A:53:ILE:HG13	2.17	0.45
2:B:122:LEU:O	7:H:15:ASN:ND2	2.49	0.45
26:B:624:SQD:H45	26:B:624:SQD:H81	1.79	0.45
3:C:53:HIS:HB3	21:C:512:CLA:OBD	2.16	0.45
1:G:69:GLY:O	1:G:81:ALA:N	2.40	0.45
21:A:401:CLA:H202	21:A:402:CLA:H93	1.98	0.44
1:G:235:TYR:C	1:G:237:TYR:H	2.20	0.44
21:G:403:CLA:HMD2	21:Q:402:CLA:CBB	2.47	0.44
26:G:410:SQD:H132	25:G:412:LHG:H132	1.98	0.44
1:G:49:VAL:O	1:G:53:ILE:HG13	2.16	0.44
10:K:16:ALA:O	10:K:19:ASP:HB2	2.17	0.44
21:N:612:CLA:H12	4:Q:127:LEU:HD21	1.98	0.44
3:P:305:THR:HG22	3:P:308:GLU:H	1.82	0.44
3:P:425:TRP:CE2	21:P:504:CLA:HBA1	2.52	0.44
21:A:402:CLA:H41	21:A:402:CLA:H62	1.82	0.44
2:B:184:GLU:H	2:B:200:ALA:HB2	1.81	0.44
21:B:609:CLA:HMD1	7:H:27:THR:HB	1.99	0.44
3:C:391:ARG:HB2	3:C:391:ARG:HH11	1.83	0.44
21:C:501:CLA:HMB3	30:C:515:BCR:C40	2.46	0.44
2:N:12:LEU:HD22	2:N:18:ARG:HB2	1.97	0.44
13:O:31:LEU:HB2	13:O:36:ILE:HD11	1.99	0.44
2:B:238:LEU:HB2	21:B:612:CLA:HMD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.32	0.44
3:C:245:ILE:O	3:C:249:ILE:HG12	2.17	0.44
3:C:425:TRP:HE1	24:C:517:DGD:HE62	1.82	0.44
1:G:255:PHE:CE2	23:G:407:PL9:H111	2.52	0.44
1:G:322:ASN:OD1	3:P:412:THR:HA	2.17	0.44
1:G:41:LEU:O	1:G:45:THR:HG22	2.17	0.44
30:I:101:BCR:H15C	30:I:101:BCR:H351	1.84	0.44
3:P:50:LEU:HD11	21:P:513:CLA:HBB1	1.98	0.44
6:S:11:VAL:HG12	6:S:12:SER:N	2.32	0.44
30:T:102:BCR:H19C	30:N:621:BCR:H363	1.99	0.44
1:A:220:THR:O	1:A:223:LEU:HG	2.17	0.44
2:N:134:ASP:OD2	2:N:137:LYS:HE3	2.16	0.44
21:N:616:CLA:H162	21:N:616:CLA:H122	1.66	0.44
13:O:118:SER:HA	13:O:159:VAL:HG12	2.00	0.44
3:P:363:GLY:O	3:P:367:GLU:HG2	2.17	0.44
5:R:79:PHE:HA	5:R:82:GLN:HE21	1.83	0.44
15:U:64:ALA:O	15:U:67:GLN:HG2	2.18	0.44
1:A:283:VAL:O	1:A:286:THR:HG22	2.16	0.44
21:A:401:CLA:H122	22:A:404:PHO:H3A	2.00	0.44
22:A:404:PHO:H92	22:A:404:PHO:H61	1.63	0.44
2:B:91:TRP:HE1	31:B:625:LMT:H12	1.81	0.44
3:C:284:PHE:HB3	24:C:516:DGD:HA51	2.00	0.44
3:C:80:PRO:HD2	16:V:129:LYS:HZ1	1.82	0.44
1:A:262:TYR:O	27:E:102:LMG:H112	2.18	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.99	0.44
21:B:616:CLA:H61	26:G:401:SQD:H301	1.99	0.44
11:L:5:PRO:HA	11:L:7:ARG:NH2	2.32	0.44
3:P:160:ILE:HA	3:P:163:PHE:CD2	2.52	0.44
30:P:514:BCR:H331	30:P:514:BCR:HC7	1.31	0.44
4:Q:294:ARG:H	4:Q:294:ARG:HG2	1.66	0.44
21:Q:402:CLA:H62	21:Q:402:CLA:H92	1.63	0.44
2:N:192:PRO:HD2	7:W:60:VAL:HG12	2.00	0.44
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.51	0.44
3:C:143:TYR:O	3:C:144:SER:HB2	2.18	0.44
21:C:501:CLA:C3D	21:C:503:CLA:H2	2.48	0.44
22:D:402:PHO:H143	22:D:402:PHO:H111	1.87	0.44
6:F:11:VAL:HG12	6:F:12:SER:N	2.33	0.44
1:G:265:PHE:CD1	1:G:271:LEU:HA	2.53	0.44
9:J:15:THR:O	9:J:19:MET:HG3	2.17	0.44
11:L:7:ARG:C	11:L:8:GLN:HE21	2.21	0.44
21:P:501:CLA:HMB3	30:P:516:BCR:C40	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:509:CLA:CMB	21:P:511:CLA:HBB1	2.48	0.44
30:P:515:BCR:H24C	30:P:515:BCR:H371	1.81	0.44
4:Q:346:LEU:O	4:Q:348:ARG:HG3	2.18	0.44
24:Q:409:DGD:HD2	24:Q:409:DGD:HG32	1.66	0.44
4:Q:49:LEU:HD13	30:S:101:BCR:C15	2.48	0.44
16:V:147:VAL:O	16:V:150:LYS:HB2	2.18	0.44
24:B:628:DGD:HB21	31:B:630:LMT:H72	1.99	0.44
3:C:126:GLY:O	3:C:130:VAL:HG23	2.18	0.44
3:C:141:GLU:CD	3:C:141:GLU:H	2.20	0.44
4:D:49:LEU:HD13	30:D:405:BCR:C15	2.47	0.44
10:K:18:PHE:HD2	10:K:18:PHE:N	2.15	0.44
21:N:609:CLA:H141	21:N:609:CLA:H161	1.77	0.44
3:P:53:HIS:HB3	21:P:512:CLA:OBD	2.17	0.44
16:V:135:GLU:O	16:V:139:VAL:HG23	2.18	0.44
21:A:401:CLA:H3A	21:A:401:CLA:HBA1	1.56	0.44
2:B:134:ASP:OD2	2:B:137:LYS:HE3	2.18	0.44
3:P:204:LEU:HD21	3:P:238:ILE:HG21	1.99	0.44
3:P:391:ARG:HD2	3:P:395:TYR:CE2	2.53	0.44
3:P:85:GLY:N	24:P:518:DGD:HE4	2.33	0.44
4:Q:222:LEU:HD23	4:Q:244:TYR:HB3	2.00	0.44
14:T:29:ILE:CD1	14:T:29:ILE:H	2.28	0.44
2:B:464:PHE:CZ	27:B:622:LMG:H141	2.52	0.44
24:C:517:DGD:HB62	30:J:102:BCR:H352	1.99	0.44
26:F:101:SQD:H131	18:X:36:VAL:HG11	2.00	0.44
6:F:19:ARG:O	6:F:23:VAL:HG23	2.18	0.44
13:O:83:LYS:HE2	2:N:338:GLN:HA	2.00	0.44
2:N:91:TRP:HE1	31:N:624:LMT:H12	1.82	0.44
13:O:69:LEU:HD12	13:O:70:CYS:N	2.28	0.44
21:P:502:CLA:HBD	21:P:503:CLA:H43	2.00	0.44
23:G:407:PL9:H33	4:Q:38:PHE:HD1	1.83	0.44
4:Q:93:TRP:HH2	21:Q:404:CLA:HBA2	1.83	0.44
21:N:606:CLA:H61	7:W:46:LEU:HB2	2.00	0.44
2:B:16:PRO:HB3	2:B:133:LEU:HD21	2.00	0.43
3:C:415:ASN:O	3:C:416:SER:HB3	2.17	0.43
21:C:507:CLA:H62	21:C:507:CLA:H92	1.75	0.43
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.83	0.43
10:K:19:ASP:N	10:K:20:PRO:HD2	2.33	0.43
21:N:608:CLA:H101	21:N:619:CLA:H42	2.01	0.43
21:B:616:CLA:CGD	21:B:616:CLA:HBA2	2.48	0.43
21:C:501:CLA:H141	21:C:501:CLA:H162	1.87	0.43
1:A:221:SER:HB2	4:D:139:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:235:GLU:OE1	2:N:472:ARG:NH1	2.50	0.43
13:O:94:THR:HB	13:O:135:GLN:O	2.18	0.43
1:G:92:HIS:CD2	3:P:219:GLY:HA3	2.53	0.43
21:P:504:CLA:H112	21:P:504:CLA:H142	1.82	0.43
1:G:129:ARG:NH2	4:Q:256:ILE:HA	2.34	0.43
21:B:608:CLA:HMA1	4:D:130:PHE:CE1	2.54	0.43
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.00	0.43
2:N:366:PHE:CD1	2:N:367:PRO:HD2	2.53	0.43
21:N:619:CLA:H62	21:N:619:CLA:H92	1.63	0.43
3:P:186:TYR:HE2	3:P:188:THR:HG22	1.83	0.43
21:P:503:CLA:H193	21:P:503:CLA:H161	1.68	0.43
30:S:101:BCR:H15C	30:S:101:BCR:H351	1.89	0.43
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.01	0.43
30:C:514:BCR:H311	30:C:514:BCR:H343	2.00	0.43
4:D:122:LEU:HD11	22:D:402:PHO:H92	2.00	0.43
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.99	0.43
5:E:42:LEU:O	5:E:46:VAL:HG23	2.19	0.43
21:G:406:CLA:H162	21:G:406:CLA:H141	1.63	0.43
12:M:19:SER:O	12:M:23:ILE:HG13	2.18	0.43
2:N:19:LEU:CD1	2:N:23:HIS:HE1	2.32	0.43
3:P:466:VAL:HA	3:P:469:MET:SD	2.59	0.43
3:P:240:ILE:HG13	21:P:501:CLA:HBB1	2.00	0.43
4:Q:153:PHE:HB2	21:Q:402:CLA:H41	2.00	0.43
34:R:101:HEM:HBC2	6:S:31:ILE:HD13	2.01	0.43
21:B:614:CLA:H2	26:B:627:SQD:C10	2.47	0.43
3:C:405:ASN:HB2	24:C:518:DGD:HG31	2.00	0.43
5:E:30:LEU:HG	34:E:101:HEM:HBB1	2.00	0.43
1:G:159:LEU:C	1:G:162:PRO:HD2	2.39	0.43
1:G:330:VAL:HG11	4:Q:328:TRP:CZ2	2.53	0.43
1:G:83:VAL:HA	1:G:84:PRO:HD3	1.91	0.43
2:N:464:PHE:CZ	27:N:622:LMG:H141	2.53	0.43
21:N:615:CLA:H141	21:N:615:CLA:H162	1.78	0.43
3:P:449:ARG:HE	21:P:505:CLA:CED	2.31	0.43
5:R:68:ASP:OD2	5:R:71:GLU:HB2	2.19	0.43
7:W:62:TRP:HD1	24:W:102:DGD:HE5	1.83	0.43
30:Z:101:BCR:H15C	30:Z:101:BCR:H351	1.78	0.43
2:B:256:MET:O	2:B:448:ARG:NH1	2.44	0.43
4:D:250:ASN:ND2	4:D:262:SER:HB3	2.34	0.43
7:H:35:MET:HE2	30:H:101:BCR:H322	2.01	0.43
10:K:18:PHE:CD2	10:K:18:PHE:N	2.85	0.43
9:J:11:TRP:CG	10:K:42:ALA:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:I:102:LMG:HC2	31:N:604:LMT:H11	1.99	0.43
3:P:141:GLU:CD	3:P:141:GLU:H	2.22	0.43
21:N:612:CLA:HMA1	4:Q:130:PHE:CE1	2.53	0.43
4:Q:134:ARG:HE	4:Q:134:ARG:HA	1.83	0.43
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.51	0.43
3:C:204:LEU:HD21	3:C:238:ILE:HG21	2.00	0.43
3:C:261:ARG:HA	3:C:266:TRP:CZ2	2.54	0.43
1:A:258:LEU:HD12	4:D:128:ARG:HD3	2.00	0.43
4:D:93:TRP:HH2	21:D:403:CLA:HBA2	1.83	0.43
4:D:103:ARG:NH1	5:E:77:GLU:OE2	2.50	0.43
1:G:81:ALA:HB2	1:G:175:GLY:HA3	2.00	0.43
2:N:306:PRO:HG2	2:N:309:LEU:HB2	2.00	0.43
21:N:614:CLA:H141	21:N:614:CLA:H162	1.71	0.43
30:P:514:BCR:H15C	30:P:514:BCR:H351	1.78	0.43
7:W:6:TRP:CE2	7:W:10:ILE:HD11	2.53	0.43
1:A:215:HIS:HA	23:A:406:PL9:O1	2.18	0.43
21:B:608:CLA:HBA1	21:B:608:CLA:CHA	2.48	0.43
3:C:269:GLU:O	3:C:272:LEU:HB3	2.19	0.43
1:G:215:HIS:HA	23:G:407:PL9:O1	2.19	0.43
1:G:61:ASP:HB2	1:G:63:ILE:HG12	2.00	0.43
2:N:103:LEU:HD22	21:N:610:CLA:H41	2.00	0.43
21:N:614:CLA:H12	21:N:614:CLA:H112	2.01	0.43
21:N:620:CLA:HBA2	21:N:620:CLA:HBD	2.00	0.43
13:O:123:GLU:HG2	13:O:124:GLU:N	2.34	0.43
4:Q:275:PRO:O	4:Q:279:LEU:HD23	2.18	0.43
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.00	0.43
2:B:174:LEU:HD23	2:B:308:LYS:HG2	2.01	0.43
21:B:605:CLA:HMA1	21:B:606:CLA:H3A	2.01	0.43
21:B:607:CLA:H193	11:L:27:LEU:HD11	2.00	0.43
3:C:291:TRP:O	3:C:305:THR:OG1	2.37	0.43
3:C:391:ARG:HD2	3:C:395:TYR:CE2	2.54	0.43
3:C:449:ARG:HE	21:C:505:CLA:CED	2.31	0.43
1:G:153:SER:HB2	21:G:402:CLA:H43	2.01	0.43
9:J:12:ILE:O	9:J:12:ILE:HG23	3.52	0.43
2:N:349:LYS:HG2	2:N:395:GLN:O	2.18	0.43
3:P:89:ILE:N	3:P:90:PRO:HD2	2.34	0.43
4:Q:176:ALA:HA	4:Q:179:PHE:CD2	2.54	0.43
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.01	0.43
1:A:228:THR:HG22	1:A:229:GLU:H	1.84	0.43
1:A:268:SER:O	1:A:272:HIS:ND1	2.48	0.43
1:A:51:ALA:HA	1:A:55:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:TRP:O	21:C:508:CLA:H11	2.19	0.43
21:C:508:CLA:H172	24:C:517:DGD:HBW2	1.99	0.43
4:D:263:ASN:O	4:D:266:TRP:N	2.50	0.43
3:P:155:ASN:HA	3:P:158:THR:HG22	2.00	0.43
3:P:310:SER:OG	3:P:355:THR:HG23	2.19	0.43
21:P:501:CLA:CHB	21:P:501:CLA:H2	2.49	0.43
3:C:161:LEU:HG	3:C:165:LEU:HD12	2.01	0.42
21:C:505:CLA:H193	21:C:505:CLA:H162	1.79	0.42
5:E:28:PRO:O	5:E:32:ILE:HG13	2.19	0.42
1:G:317:TRP:O	1:G:321:ILE:HG13	2.18	0.42
2:B:137:LYS:HD2	7:H:14:LEU:O	2.19	0.42
21:N:612:CLA:CHA	21:N:612:CLA:HBA1	2.47	0.42
13:O:97:VAL:HG21	13:O:135:GLN:HE21	1.84	0.42
4:Q:146:PHE:O	4:Q:150:ILE:HG12	2.19	0.42
20:Z:29:SER:HB2	20:Z:31:GLN:HG3	1.99	0.42
1:A:93:PHE:CD2	24:A:407:DGD:HD2	2.54	0.42
21:B:608:CLA:H161	21:B:608:CLA:H143	1.84	0.42
31:B:629:LMT:H31	1:G:72:LEU:HD21	2.01	0.42
3:C:435:PHE:O	3:C:438:LEU:N	2.51	0.42
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.00	0.42
4:D:41:ALA:HB1	22:D:402:PHO:H42	2.01	0.42
4:D:107:LEU:HD21	5:E:76:VAL:HG21	2.00	0.42
1:G:12:ASN:O	1:G:16:ARG:HG3	2.18	0.42
13:O:192:SER:OG	13:O:193:GLY:N	2.52	0.42
4:Q:43:LEU:HD23	4:Q:117:HIS:HE1	1.83	0.42
15:U:38:GLU:HG2	15:U:39:LEU:H	1.84	0.42
16:V:119:PRO:HG2	34:V:201:HEM:HMC2	2.02	0.42
1:A:183:MET:HE1	21:A:402:CLA:HMD3	2.01	0.42
22:A:404:PHO:H41	22:A:404:PHO:H62	1.46	0.42
2:B:103:LEU:HD22	21:B:606:CLA:H41	2.00	0.42
2:B:25:MET:CE	30:B:617:BCR:H23C	2.49	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.19	0.42
3:C:380:ILE:HA	3:C:384:ILE:HD11	2.00	0.42
3:C:50:LEU:HD11	21:C:513:CLA:HBB1	2.01	0.42
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.19	0.42
4:D:54:PHE:HB3	5:E:47:PHE:CD2	2.53	0.42
30:T:103:BCR:H393	2:N:112:CYS:HB3	2.01	0.42
21:P:509:CLA:HMB1	21:P:511:CLA:HBB1	2.01	0.42
27:Q:406:LMG:H171	30:S:101:BCR:H383	2.01	0.42
1:A:317:TRP:O	1:A:321:ILE:HG13	2.19	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:615:CLA:H92	21:B:615:CLA:H62	1.67	0.42
27:E:102:LMG:O9	27:E:102:LMG:HC71	2.18	0.42
5:E:26:THR:HB	34:E:101:HEM:CBB	2.50	0.42
2:N:137:LYS:HD2	7:W:14:LEU:O	2.19	0.42
2:N:341:LYS:HD2	2:N:429:ILE:HG22	2.02	0.42
21:N:609:CLA:HMA1	21:N:610:CLA:H3A	2.01	0.42
3:P:101:PRO:O	3:P:104:GLU:HB2	2.19	0.42
3:P:35:TRP:CG	3:P:36:TRP:N	2.88	0.42
4:Q:253:TRP:HA	4:Q:256:ILE:HG23	2.01	0.42
15:U:94:ILE:O	15:U:97:LEU:HG	2.20	0.42
5:E:61:ARG:NH2	16:V:153:GLY:HA3	2.34	0.42
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.02	0.42
30:B:619:BCR:H351	30:B:619:BCR:H15C	1.84	0.42
3:C:334:PRO:HA	13:O:179:THR:OG1	2.19	0.42
30:C:514:BCR:H391	10:K:36:ALA:HB2	2.00	0.42
1:G:190:HIS:HB3	1:G:293:MET:HE2	2.02	0.42
2:B:224:ARG:HG2	7:H:24:GLY:O	2.19	0.42
6:F:45:ARG:NH2	9:J:40:LEU:O	2.52	0.42
2:N:239:SER:O	2:N:466:HIS:ND1	2.47	0.42
2:N:36:SER:HB2	31:N:603:LMT:H91	2.01	0.42
2:N:54:PRO:HD2	2:N:57:ARG:HG3	2.02	0.42
21:N:607:CLA:CBB	21:N:609:CLA:H152	2.49	0.42
30:N:621:BCR:H15C	30:N:621:BCR:H351	1.82	0.42
3:P:240:ILE:HA	3:P:240:ILE:HD13	1.88	0.42
21:P:503:CLA:HBB1	27:P:521:LMG:C20	2.45	0.42
5:R:17:VAL:O	5:R:21:VAL:HG23	2.20	0.42
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.54	0.42
1:A:306:VAL:HG13	1:A:314:ILE:O	2.19	0.42
2:B:10:THR:O	2:B:13:ILE:HG13	2.20	0.42
30:C:514:BCR:H351	30:C:514:BCR:H15C	1.79	0.42
4:D:93:TRP:CH2	21:D:403:CLA:HBA2	2.54	0.42
1:G:161:TYR:HB3	1:G:162:PRO:HD3	2.00	0.42
3:P:143:TYR:O	3:P:144:SER:HB2	2.19	0.42
5:R:30:LEU:HG	34:R:101:HEM:HBB1	2.01	0.42
2:B:137:LYS:O	2:B:141:ILE:HG13	2.19	0.42
21:C:501:CLA:H2	21:C:501:CLA:CHB	2.49	0.42
5:E:26:THR:HB	34:E:101:HEM:CAB	2.50	0.42
21:B:616:CLA:H52	26:G:401:SQD:H261	2.02	0.42
1:G:76:ASN:OD1	1:G:79:THR:HG23	2.20	0.42
30:T:102:BCR:H341	30:N:621:BCR:H381	2.01	0.42
2:N:68:ARG:NH1	2:N:262:THR:HG23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:269:GLU:O	3:P:272:LEU:HB3	2.20	0.42
2:B:154:GLY:O	2:B:159:THR:HG23	2.20	0.42
2:B:262:THR:HG22	2:B:263:THR:HG23	2.02	0.42
1:G:177:SER:HA	1:G:180:PHE:CD2	2.54	0.42
1:G:228:THR:HG22	1:G:229:GLU:H	1.84	0.42
1:G:306:VAL:HG13	1:G:314:ILE:O	2.19	0.42
30:N:621:BCR:H341	30:N:621:BCR:H11C	1.91	0.42
13:O:147:THR:OG1	13:O:148:VAL:N	2.52	0.42
13:O:154:SER:N	13:O:169:LYS:O	2.50	0.42
3:P:269:GLU:OE1	21:P:508:CLA:HED1	2.19	0.42
1:G:296:ASN:HB2	3:P:400:PRO:O	2.20	0.42
18:X:12:ILE:O	18:X:12:ILE:HG23	2.19	0.42
1:A:20:TRP:NE1	26:A:414:SQD:O3	2.51	0.42
1:A:153:SER:HB2	21:A:401:CLA:H43	2.00	0.42
5:E:22:ILE:O	5:E:26:THR:HG23	2.20	0.42
2:N:348:ASN:OD1	2:N:352:GLU:HB2	2.20	0.42
2:N:474:LEU:O	4:Q:134:ARG:NH1	2.53	0.42
13:O:59:ASP:C	13:O:61:SER:H	2.23	0.42
13:O:59:ASP:HB3	13:O:62:GLN:HB3	2.02	0.42
3:P:391:ARG:HH11	3:P:391:ARG:HB2	1.84	0.42
21:P:507:CLA:H62	21:P:507:CLA:H92	1.73	0.42
30:P:515:BCR:H15C	30:P:515:BCR:H351	1.79	0.42
20:Z:29:SER:C	20:Z:31:GLN:H	2.22	0.42
20:Z:32:ASP:HB3	20:Z:35:ARG:NH1	2.35	0.42
2:B:331:ASN:HB3	2:B:437:LEU:HD12	2.01	0.42
21:B:610:CLA:H141	21:B:610:CLA:H162	1.71	0.42
3:C:303:GLY:O	3:C:423:ARG:NE	2.44	0.42
3:C:120:ILE:CD1	30:C:514:BCR:HC8	2.50	0.42
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.83	0.42
1:G:249:VAL:HG11	2:N:486:LEU:HD23	2.02	0.42
2:N:270:PRO:HG3	2:N:312:TYR:CD2	2.51	0.42
2:N:483:ASP:OD2	2:N:484:PRO:HD2	2.20	0.42
4:Q:157:PHE:CE1	4:Q:171:PRO:HG2	2.55	0.42
5:R:22:ILE:O	5:R:26:THR:HG23	2.20	0.42
2:B:278:SER:HB3	2:B:281:GLN:HB3	2.02	0.41
3:C:162:GLY:O	3:C:166:ILE:HG13	2.20	0.41
3:C:160:ILE:HA	3:C:163:PHE:CD2	2.55	0.41
3:C:418:ASN:HB2	24:C:518:DGD:HE2	2.00	0.41
3:C:466:VAL:HA	3:C:469:MET:SD	2.60	0.41
4:D:275:PRO:O	4:D:279:LEU:HD23	2.20	0.41
4:D:334:GLN:N	4:D:335:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:403:CLA:HMA1	21:G:403:CLA:H122	2.02	0.41
27:M:101:LMG:H292	21:N:618:CLA:CMD	2.50	0.41
26:N:601:SQD:C10	21:N:618:CLA:H2	2.46	0.41
3:P:161:LEU:HG	3:P:165:LEU:HD12	2.02	0.41
3:P:229:ASN:HD22	3:P:231:GLU:HB2	1.85	0.41
3:P:28:GLN:HB2	21:P:511:CLA:HED3	2.02	0.41
4:Q:250:ASN:ND2	4:Q:262:SER:HB3	2.35	0.41
4:Q:26:ARG:CD	6:S:18:VAL:HG11	2.39	0.41
1:A:20:TRP:O	1:A:23:SER:HB3	2.20	0.41
2:B:10:THR:C	2:B:12:LEU:H	2.23	0.41
2:B:124:ARG:NE	2:B:131:PRO:HD3	2.34	0.41
2:B:483:ASP:OD2	2:B:484:PRO:HD2	2.19	0.41
30:C:515:BCR:H15C	30:C:515:BCR:H351	1.84	0.41
3:C:89:ILE:N	3:C:90:PRO:HD2	2.35	0.41
21:G:402:CLA:H191	27:Q:407:LMG:H352	2.02	0.41
2:N:10:THR:O	2:N:13:ILE:HG13	2.19	0.41
1:A:72:LEU:HD21	31:N:603:LMT:H31	2.02	0.41
5:R:26:THR:HB	34:R:101:HEM:CAB	2.50	0.41
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.41
16:V:143:GLY:O	16:V:147:VAL:HG23	2.19	0.41
30:B:617:BCR:H351	30:B:617:BCR:H15C	1.84	0.41
30:B:617:BCR:H371	30:B:617:BCR:H24C	1.87	0.41
3:C:310:SER:OG	3:C:355:THR:HG23	2.19	0.41
3:C:375:LEU:HB3	3:C:380:ILE:HD11	2.03	0.41
30:C:514:BCR:HC7	30:C:514:BCR:H331	1.34	0.41
4:D:101:PHE:O	4:D:104:TRP:HB3	2.21	0.41
1:G:143:ILE:HD11	4:Q:217:THR:HA	2.01	0.41
2:N:201:HIS:CE1	21:N:607:CLA:HMB3	2.55	0.41
2:N:224:ARG:HG2	7:W:24:GLY:O	2.20	0.41
13:O:215:ARG:NH1	13:O:252:GLY:O	2.53	0.41
15:U:73:PRO:HG2	16:V:107:THR:HB	2.02	0.41
7:W:12:ARG:N	7:W:13:PRO:HD2	2.35	0.41
2:B:25:MET:HG2	30:B:617:BCR:H23C	2.01	0.41
3:C:250:TRP:O	3:C:254:THR:OG1	2.22	0.41
3:C:35:TRP:CG	3:C:36:TRP:N	2.88	0.41
21:C:509:CLA:H203	21:C:509:CLA:H161	1.81	0.41
4:D:201:VAL:O	4:D:205:LEU:HB2	2.21	0.41
4:D:253:TRP:HA	4:D:256:ILE:HG23	2.02	0.41
30:J:102:BCR:H20C	30:J:102:BCR:H361	1.87	0.41
21:N:605:CLA:HMB3	30:W:101:BCR:H281	2.02	0.41
2:N:23:HIS:CD2	21:N:616:CLA:C1B	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:68:VAL:O	16:V:71:ILE:HG12	2.20	0.41
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.41
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.55	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.73	0.41
21:C:504:CLA:H112	21:C:504:CLA:H142	1.80	0.41
4:D:320:LEU:HD23	4:D:323:GLU:OE1	2.21	0.41
22:G:405:PHO:H102	22:G:405:PHO:H13	1.81	0.41
1:G:93:PHE:HD2	24:G:408:DGD:HD2	1.86	0.41
30:J:102:BCR:C8	30:J:102:BCR:H331	2.51	0.41
9:J:14:ALA:O	9:J:18:GLY:N	2.50	0.41
30:T:101:BCR:H23C	2:N:25:MET:HG2	2.01	0.41
3:P:279:LEU:HD12	3:P:437:PHE:HE1	1.86	0.41
15:U:68:TYR:HB2	15:U:71:LEU:HD12	2.02	0.41
2:N:188:ASP:OD1	7:W:58:VAL:HA	2.20	0.41
1:A:234:ASN:HA	1:A:234:ASN:HD22	1.63	0.41
2:B:130:GLU:HB2	2:B:131:PRO:HD2	2.02	0.41
21:B:610:CLA:H62	21:B:610:CLA:H41	1.88	0.41
21:B:612:CLA:HMB3	21:B:613:CLA:HAA1	2.03	0.41
2:B:112:CYS:HB3	30:B:620:BCR:H393	2.02	0.41
3:C:404:LEU:HD12	3:C:404:LEU:HA	1.92	0.41
4:D:103:ARG:O	4:D:107:LEU:HG	2.19	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.82	0.41
27:I:102:LMG:H221	31:I:103:LMT:H81	2.02	0.41
9:J:15:THR:HG23	30:K:101:BCR:H392	2.03	0.41
2:N:201:HIS:HD2	2:N:202:HIS:ND1	2.18	0.41
2:N:262:THR:HG22	2:N:263:THR:HG23	2.01	0.41
2:N:475:PHE:CD1	4:Q:140:PRO:HD3	2.56	0.41
30:W:101:BCR:H351	30:W:101:BCR:H15C	1.95	0.41
1:A:12:ASN:O	1:A:16:ARG:HG3	2.21	0.41
21:A:402:CLA:HMA1	21:A:402:CLA:H122	2.03	0.41
21:A:403:CLA:H143	21:A:403:CLA:H161	1.95	0.41
2:B:153:PHE:O	2:B:157:HIS:HB3	2.21	0.41
1:A:296:ASN:HB2	3:C:400:PRO:O	2.20	0.41
1:G:214:MET:CE	1:G:214:MET:HA	2.49	0.41
23:G:407:PL9:H222	22:Q:403:PHO:HMA2	2.03	0.41
1:G:51:ALA:HA	1:G:55:ALA:HB2	2.03	0.41
30:I:101:BCR:H371	30:I:101:BCR:H24C	1.91	0.41
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.85	0.41
2:N:18:ARG:HD2	2:N:115:TRP:CE3	2.56	0.41
1:G:191:ASN:HB2	3:P:411:ALA:HB1	2.03	0.41
3:P:418:ASN:HB2	24:P:519:DGD:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:G:407:PL9:H33	4:Q:38:PHE:CD1	2.55	0.41
4:Q:43:LEU:HD12	4:Q:43:LEU:HA	1.94	0.41
14:T:18:PHE:HB2	30:T:102:BCR:H10C	2.02	0.41
20:Z:35:ARG:O	20:Z:38:GLN:HB3	2.20	0.41
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.02	0.41
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.56	0.41
1:G:238:LYS:HA	1:G:238:LYS:HD3	1.83	0.41
1:G:283:VAL:O	1:G:286:THR:HG22	2.20	0.41
21:G:403:CLA:H41	21:G:403:CLA:H62	1.84	0.41
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.55	0.41
8:I:8:VAL:O	8:I:12:VAL:HG23	2.21	0.41
3:P:455:PHE:C	3:P:457:LYS:H	2.24	0.41
21:P:502:CLA:H111	21:P:503:CLA:HMB2	2.03	0.41
21:P:512:CLA:H112	21:P:512:CLA:H72	1.77	0.41
26:Q:408:SQD:H81	26:Q:408:SQD:H45	1.85	0.41
5:R:82:GLN:H	5:R:82:GLN:HG3	1.52	0.41
1:A:328:MET:HE1	4:D:183:LEU:HD22	2.02	0.41
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.56	0.41
2:B:49:ASP:HA	2:B:50:PRO:HD2	1.98	0.41
21:B:605:CLA:HMC2	21:B:615:CLA:H2	2.03	0.41
3:C:256:PRO:HA	21:C:506:CLA:HED3	2.02	0.41
21:A:403:CLA:HMD3	4:D:182:LEU:HD11	2.02	0.41
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.56	0.41
3:P:296:VAL:HG23	3:P:297:TYR:CD2	2.56	0.41
1:A:172:MET:SD	1:A:179:THR:HG23	2.60	0.41
1:A:330:VAL:HG11	4:D:328:TRP:CZ2	2.55	0.41
2:B:112:CYS:HA	30:B:617:BCR:H282	2.03	0.41
3:C:425:TRP:CZ2	21:C:504:CLA:HBA1	2.56	0.41
4:D:308:ASP:HA	4:D:309:PRO:HD3	1.87	0.41
1:G:142:TRP:HB2	4:Q:220:ASN:OD1	2.20	0.41
1:G:221:SER:HB2	4:Q:139:ARG:O	2.20	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.56	0.41
30:P:514:BCR:H11C	30:P:514:BCR:H341	1.92	0.41
27:R:102:LMG:HC71	27:R:102:LMG:O9	2.21	0.41
15:U:80:VAL:HG22	15:U:127:ARG:NH2	2.35	0.41
20:Z:32:ASP:CB	20:Z:35:ARG:HG2	2.50	0.41
21:A:402:CLA:H51	22:A:404:PHO:HMB3	2.02	0.41
3:C:29:GLU:HB2	3:C:30:SER:H	1.73	0.41
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.41
1:G:93:PHE:HZ	21:G:406:CLA:HAA1	1.85	0.41
7:H:18:TYR:CG	7:H:19:GLY:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:55:LEU:HB2	7:H:58:VAL:CG1	2.51	0.41
2:N:155:ALA:O	2:N:159:THR:OG1	2.26	0.41
3:P:107:ASP:OD2	3:P:110:PRO:HD3	2.20	0.41
3:P:116:VAL:CG2	30:P:515:BCR:H323	2.51	0.41
3:P:362:ARG:H	24:P:517:DGD:HE4	1.86	0.41
6:S:18:VAL:HG13	6:S:19:ARG:N	2.36	0.41
14:T:9:ILE:O	14:T:13:ILE:HG13	2.21	0.41
21:N:606:CLA:H12	7:W:49:TYR:HD2	1.85	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.37	0.40
21:A:401:CLA:H191	27:D:407:LMG:H352	2.03	0.40
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.90	0.40
2:B:3:LEU:HA	2:B:4:PRO:HD3	1.97	0.40
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.40
5:E:17:VAL:O	5:E:21:VAL:HG23	2.21	0.40
1:G:192:ILE:HA	1:G:293:MET:HE3	2.03	0.40
13:O:240:THR:HG22	13:O:264:VAL:HG12	2.02	0.40
1:G:300:PHE:CZ	3:P:404:LEU:HD23	2.56	0.40
3:P:421:SER:HA	3:P:422:PRO:HD3	1.90	0.40
4:Q:47:GLY:HA2	30:S:101:BCR:H332	2.03	0.40
16:V:63:CYS:SG	34:V:201:HEM:CAB	3.10	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.40
1:A:265:PHE:CD1	1:A:271:LEU:HA	2.57	0.40
1:A:76:ASN:OD1	1:A:79:THR:HG23	2.20	0.40
1:G:268:SER:O	1:G:272:HIS:ND1	2.53	0.40
1:G:308:ASP:O	6:S:45:ARG:NE	2.54	0.40
21:G:402:CLA:HBD	21:G:403:CLA:HAC2	2.03	0.40
7:H:12:ARG:HD3	7:H:12:ARG:C	2.42	0.40
2:N:153:PHE:O	2:N:157:HIS:HB3	2.22	0.40
2:N:154:GLY:O	2:N:159:THR:HG23	2.21	0.40
21:N:612:CLA:HMD1	21:N:614:CLA:HAB	2.03	0.40
21:G:402:CLA:HBB1	21:Q:402:CLA:NC	2.36	0.40
5:R:42:LEU:O	5:R:46:VAL:HG23	2.20	0.40
21:B:602:CLA:H122	21:B:602:CLA:H162	1.58	0.40
21:B:613:CLA:H62	21:B:613:CLA:H41	1.88	0.40
4:D:346:LEU:O	4:D:348:ARG:HG3	2.20	0.40
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.36	0.40
1:G:219:VAL:HG11	4:Q:268:HIS:CD2	2.57	0.40
12:M:16:LEU:HD21	21:N:618:CLA:H202	2.02	0.40
21:N:609:CLA:HMB3	21:N:610:CLA:H11	2.04	0.40
3:P:319:ILE:HG21	3:P:389:GLU:HG3	2.04	0.40
4:Q:194:ASN:HA	4:Q:195:PRO:HD2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:TYR:OH	4:Q:246:MET:HG2	2.20	0.40
4:Q:334:GLN:N	4:Q:335:PRO:HD3	2.35	0.40
1:A:140:ARG:NH2	25:A:408:LHG:O5	2.45	0.40
2:B:483:ASP:CG	2:B:484:PRO:HD2	2.41	0.40
3:C:321:ASP:HA	3:C:324:LEU:HD23	2.03	0.40
4:D:146:PHE:O	4:D:150:ILE:HG12	2.22	0.40
21:A:401:CLA:HBB1	21:D:401:CLA:NC	2.36	0.40
5:E:68:ASP:OD2	5:E:71:GLU:HB2	2.21	0.40
5:E:7:GLU:HB3	6:F:19:ARG:CZ	2.52	0.40
10:K:20:PRO:O	10:K:23:ASP:HB2	2.21	0.40
13:O:31:LEU:HB2	13:O:36:ILE:CD1	2.51	0.40
21:P:509:CLA:H203	21:P:509:CLA:H161	1.87	0.40
4:Q:93:TRP:CH2	21:Q:404:CLA:HBA2	2.56	0.40
30:T:102:BCR:H341	30:T:102:BCR:H11C	1.85	0.40
30:T:102:BCR:H331	30:T:102:BCR:C8	2.52	0.40
18:X:11:THR:HG23	18:X:12:ILE:HG22	2.03	0.40
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.57	0.40
3:C:307:PRO:HG3	3:C:358:PHE:CD1	2.57	0.40
3:C:42:LEU:HD13	21:C:511:CLA:HMA3	2.03	0.40
26:A:409:SQD:H202	24:C:518:DGD:HAH2	2.03	0.40
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.52	0.40
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.57	0.40
1:A:269:ARG:NH1	4:D:231:THR:HB	2.37	0.40
4:D:350:ASN:O	4:D:352:LEU:N	2.45	0.40
1:G:211:PHE:HA	1:G:214:MET:HB2	2.04	0.40
3:P:257:PHE:HB3	3:P:258:GLY:H	1.59	0.40
3:P:261:ARG:HA	3:P:266:TRP:CZ2	2.57	0.40
3:P:261:ARG:HA	3:P:266:TRP:HZ2	1.87	0.40
26:G:410:SQD:H5	4:Q:232:PHE:HB3	2.04	0.40
22:Q:403:PHO:H111	22:Q:403:PHO:H143	1.89	0.40
1:G:214:MET:HE1	22:Q:403:PHO:OBD	2.22	0.40
5:R:49:THR:HA	5:R:50:PRO:HD3	1.85	0.40
30:T:102:BCR:H24C	30:T:102:BCR:H371	1.92	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:60:PHE:O	13:f:115:SER:OG[3_755]	2.16	0.04

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%)	297 (89%)	31 (9%)	5 (2%)	12	53
1	G	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	12	53
2	B	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	6	41
2	N	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	6	41
3	C	445/461 (96%)	375 (84%)	55 (12%)	15 (3%)	4	35
3	P	445/461 (96%)	376 (84%)	53 (12%)	16 (4%)	4	33
4	D	338/352 (96%)	292 (86%)	40 (12%)	6 (2%)	10	49
4	Q	338/352 (96%)	291 (86%)	41 (12%)	6 (2%)	10	49
5	E	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	4	32
5	R	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	4	32
6	F	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
6	S	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
7	H	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	17
7	W	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	17
8	I	33/38 (87%)	24 (73%)	7 (21%)	2 (6%)	2	22
8	a	33/38 (87%)	25 (76%)	6 (18%)	2 (6%)	2	22
9	J	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	22
9	b	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	22
10	K	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	2	24
10	c	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	2	24
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	d	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	e	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	203 (84%)	27 (11%)	11 (5%)	3	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	f	241/246 (98%)	203 (84%)	29 (12%)	9 (4%)	4	33
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	35
14	g	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	35
15	U	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	30
15	h	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	30
16	V	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	25	68
16	i	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	25	68
17	m	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	18
17	y	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	18
18	X	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	8
18	j	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	8
20	Z	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	2	27
20	l	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	2	27
All	All	5138/5426 (95%)	4357 (85%)	626 (12%)	155 (3%)	5	37

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO
2	B	488	PRO
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
4	D	240	ALA
4	D	262	SER
7	H	18	TYR
8	I	25	SER
9	J	35	GLY
13	O	52	ALA
14	T	30	THR
15	U	72	TYR
15	U	83	ALA

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Mol	Chain	Res	Type
16	V	75	ASN
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
1	G	12	ASN
1	G	142	TRP
2	N	176	GLY
2	N	230	ARG
2	N	484	PRO
2	N	488	PRO
3	P	144	SER
3	P	257	PHE
3	P	416	SER
3	P	452	ALA
4	Q	239	GLN
4	Q	240	ALA
4	Q	262	SER
7	W	18	TYR
8	a	25	SER
9	b	35	GLY
13	f	52	ALA
14	g	30	THR
15	h	72	TYR
15	h	83	ALA
16	i	75	ASN
17	m	43	ARG
18	j	45	LYS
20	l	32	ASP
1	A	141	PRO
2	B	349	LYS
3	C	46	SER
3	C	136	GLY
3	C	194	GLY
3	C	452	ALA
4	D	234	ALA
4	D	264	LYS
5	E	82	GLN
7	H	26	GLY
9	J	38	SER
13	O	231	ASP
15	U	73	PRO
1	G	141	PRO

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Mol	Chain	Res	Type
2	N	349	LYS
3	P	46	SER
3	P	136	GLY
3	P	194	GLY
4	Q	234	ALA
4	Q	264	LYS
5	R	82	GLN
7	W	26	GLY
9	b	38	SER
13	f	231	ASP
15	h	73	PRO
17	m	25	ILE
2	B	436	THR
3	C	32	GLY
3	C	141	GLU
3	C	209	ILE
3	C	375	LEU
3	C	456	GLU
4	D	263	ASN
5	E	9	PRO
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
13	O	158	ASN
13	O	165	SER
17	y	25	ILE
18	X	43	ILE
2	N	436	THR
3	P	32	GLY
3	P	141	GLU
3	P	209	ILE
3	P	375	LEU
3	P	456	GLU
4	Q	263	ASN
5	R	9	PRO
7	W	16	SER
10	c	13	GLU
10	c	45	PHE
13	f	158	ASN
13	f	165	SER
18	j	43	ILE
20	l	28	ALA

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Mol	Chain	Res	Type
2	B	127	ARG
2	B	183	PRO
2	B	414	PRO
13	O	60	SER
13	O	82	PRO
20	Z	24	PRO
20	Z	28	ALA
2	N	127	ARG
2	N	183	PRO
2	N	414	PRO
13	f	60	SER
13	f	82	PRO
20	l	24	PRO
1	A	334	ARG
2	B	13	ILE
2	B	173	GLY
3	C	154	LYS
3	C	462	GLU
5	E	10	PHE
7	H	6	TRP
13	O	51	THR
13	O	88	GLU
1	G	334	ARG
2	N	13	ILE
2	N	173	GLY
3	P	154	LYS
3	P	411	ALA
3	P	462	GLU
5	R	10	PHE
7	W	6	TRP
13	f	51	THR
13	f	88	GLU
15	U	42	VAL
18	X	12	ILE
18	X	44	ASP
18	j	12	ILE
18	j	44	ASP
15	h	42	VAL
8	I	32	PRO
8	a	32	PRO
1	A	176	ILE
2	B	16	PRO

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Mol	Chain	Res	Type
3	C	201	ASN
7	H	60	VAL
13	O	127	ILE
13	O	159	VAL
1	G	176	ILE
2	N	16	PRO
3	P	201	ASN
13	f	159	VAL
13	O	271	PRO
7	W	60	VAL

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%)	260 (96%)	11 (4%)	35	65
1	G	271/280 (97%)	260 (96%)	11 (4%)	35	65
2	B	390/407 (96%)	377 (97%)	13 (3%)	43	70
2	N	390/407 (96%)	376 (96%)	14 (4%)	40	68
3	C	347/362 (96%)	327 (94%)	20 (6%)	23	56
3	P	347/362 (96%)	327 (94%)	20 (6%)	23	56
4	D	275/283 (97%)	259 (94%)	16 (6%)	23	56
4	Q	275/283 (97%)	258 (94%)	17 (6%)	21	54
5	E	72/72 (100%)	66 (92%)	6 (8%)	13	43
5	R	72/72 (100%)	66 (92%)	6 (8%)	13	43
6	F	29/38 (76%)	29 (100%)	0	100	100
6	S	29/38 (76%)	29 (100%)	0	100	100
7	H	53/54 (98%)	50 (94%)	3 (6%)	24	56
7	W	53/54 (98%)	50 (94%)	3 (6%)	24	56
8	I	32/35 (91%)	31 (97%)	1 (3%)	45	71
8	a	32/35 (91%)	31 (97%)	1 (3%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/27 (89%)	23 (96%)	1 (4%)	34	64
9	b	24/27 (89%)	23 (96%)	1 (4%)	34	64
10	K	30/30 (100%)	28 (93%)	2 (7%)	19	51
10	c	30/30 (100%)	28 (93%)	2 (7%)	19	51
11	L	35/35 (100%)	32 (91%)	3 (9%)	12	42
11	d	35/35 (100%)	32 (91%)	3 (9%)	12	42
12	M	31/33 (94%)	31 (100%)	0	100	100
12	e	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	196 (97%)	6 (3%)	46	72
13	f	202/208 (97%)	196 (97%)	6 (3%)	46	72
14	T	29/29 (100%)	28 (97%)	1 (3%)	42	69
14	g	29/29 (100%)	28 (97%)	1 (3%)	42	69
15	U	84/89 (94%)	80 (95%)	4 (5%)	30	61
15	h	84/89 (94%)	80 (95%)	4 (5%)	30	61
16	V	116/117 (99%)	111 (96%)	5 (4%)	33	64
16	i	116/117 (99%)	111 (96%)	5 (4%)	33	64
17	m	20/37 (54%)	18 (90%)	2 (10%)	9	33
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	33
18	X	30/33 (91%)	27 (90%)	3 (10%)	9	33
18	j	30/33 (91%)	27 (90%)	3 (10%)	9	33
20	Z	52/52 (100%)	47 (90%)	5 (10%)	10	35
20	l	52/52 (100%)	47 (90%)	5 (10%)	10	35
All	All	4244/4442 (96%)	4038 (95%)	206 (5%)	29	61

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	32	TRP
1	A	157	VAL
1	A	202	VAL
1	A	206	PHE
1	A	234	ASN
1	A	243	GLU

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	286	THR
1	A	292	THR
1	A	308	ASP
2	B	11	VAL
2	B	18	ARG
2	B	84	THR
2	B	223	GLN
2	B	246	PHE
2	B	262	THR
2	B	308	LYS
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	486	LEU
2	B	488	PRO
2	B	490	GLN
3	C	29	GLU
3	C	78	GLU
3	C	86	LEU
3	C	104	GLU
3	C	165	LEU
3	C	174	LEU
3	C	201	ASN
3	C	207	ARG
3	C	232	ASP
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	401	LEU
3	C	447	ARG
3	C	469	MET
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	53	THR
4	D	84	SER
4	D	91	LEU

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Mol	Chain	Res	Type
4	D	130	PHE
4	D	180	ARG
4	D	201	VAL
4	D	241	GLU
4	D	256	ILE
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	346	LEU
5	E	5	THR
5	E	9	PRO
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
10	K	18	PHE
10	K	19	ASP
11	L	7	ARG
11	L	8	GLN
11	L	11	GLU
13	O	31	LEU
13	O	86	ARG
13	O	97	VAL
13	O	141	ARG
13	O	178	ARG
13	O	219	THR
14	T	29	ILE
15	U	61	ASN
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	35	THR
16	V	63	CYS
16	V	92	ARG
16	V	116	GLU

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Mol	Chain	Res	Type
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	45	LYS
20	Z	14	ILE
20	Z	25	VAL
20	Z	33	TRP
20	Z	58	ASN
20	Z	62	VAL
1	G	30	VAL
1	G	32	TRP
1	G	157	VAL
1	G	202	VAL
1	G	206	PHE
1	G	234	ASN
1	G	243	GLU
1	G	271	LEU
1	G	286	THR
1	G	292	THR
1	G	308	ASP
2	N	11	VAL
2	N	18	ARG
2	N	84	THR
2	N	223	GLN
2	N	246	PHE
2	N	262	THR
2	N	308	LYS
2	N	309	LEU
2	N	362	PHE
2	N	414	PRO
2	N	422	ARG
2	N	486	LEU
2	N	488	PRO
2	N	490	GLN
3	P	29	GLU
3	P	78	GLU
3	P	86	LEU
3	P	104	GLU
3	P	165	LEU
3	P	174	LEU

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Mol	Chain	Res	Type
3	P	201	ASN
3	P	207	ARG
3	P	232	ASP
3	P	244	CYS
3	P	254	THR
3	P	289	PHE
3	P	305	THR
3	P	355	THR
3	P	382	ASN
3	P	391	ARG
3	P	401	LEU
3	P	447	ARG
3	P	469	MET
3	P	472	LEU
4	Q	20	ASP
4	Q	43	LEU
4	Q	53	THR
4	Q	84	SER
4	Q	91	LEU
4	Q	130	PHE
4	Q	180	ARG
4	Q	201	VAL
4	Q	221	THR
4	Q	241	GLU
4	Q	256	ILE
4	Q	259	ILE
4	Q	279	LEU
4	Q	291	LEU
4	Q	294	ARG
4	Q	323	GLU
4	Q	346	LEU
5	R	5	THR
5	R	9	PRO
5	R	18	ARG
5	R	77	GLU
5	R	82	GLN
5	R	84	LYS
7	W	27	THR
7	W	49	TYR
7	W	60	VAL
8	a	33	LYS
9	b	7	ARG

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Mol	Chain	Res	Type
10	c	18	PHE
10	c	19	ASP
11	d	7	ARG
11	d	8	GLN
11	d	11	GLU
13	f	31	LEU
13	f	86	ARG
13	f	97	VAL
13	f	141	ARG
13	f	178	ARG
13	f	219	THR
14	g	29	ILE
15	h	61	ASN
15	h	88	VAL
15	h	114	VAL
15	h	132	LEU
16	i	35	THR
16	i	63	CYS
16	i	92	ARG
16	i	116	GLU
16	i	122	ARG
17	m	28	ILE
17	m	46	LEU
18	j	11	THR
18	j	12	ILE
18	j	45	LYS
20	l	14	ILE
20	l	25	VAL
20	l	33	TRP
20	l	58	ASN
20	l	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	241	GLN
2	B	201	HIS
3	C	118	HIS
11	L	8	GLN
1	G	234	ASN
1	G	241	GLN

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Mol	Chain	Res	Type
2	N	201	HIS
4	Q	129	GLN
4	Q	250	ASN
11	d	8	GLN
13	f	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 182 ligands modelled in this entry, 6 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	$\# Z > 2$
21	CLA	A	401	-	56,73,73	1.39	12 (21%)	65,113,113	1.50	11 (16%)
21	CLA	A	402	-	56,73,73	1.39	12 (21%)	65,113,113	1.55	10 (15%)
21	CLA	A	403	-	56,73,73	1.39	10 (17%)	65,113,113	1.50	8 (12%)
22	PHO	A	404	-	67,69,69	2.12	17 (25%)	87,99,99	1.94	22 (25%)
21	CLA	A	405	-	56,73,73	1.38	12 (21%)	65,113,113	1.53	10 (15%)
23	PL9	A	406	-	45,45,55	1.19	7 (15%)	57,57,69	1.66	17 (29%)
24	DGD	A	407	-	57,57,67	0.97	3 (5%)	71,71,81	1.51	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	A	408	-	38,38,48	1.05	2 (5%)	39,44,54	0.99	3 (7%)
26	SQD	A	409	-	50,51,54	1.21	4 (8%)	60,62,65	1.57	9 (15%)
27	LMG	A	410	-	51,51,55	0.94	2 (3%)	59,59,63	1.30	4 (6%)
25	LHG	A	411	-	36,36,48	1.06	2 (5%)	37,42,54	1.14	2 (5%)
28	OEC	A	412	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	SQD	A	414	-	53,54,54	1.17	4 (7%)	63,65,65	1.25	5 (7%)
21	CLA	B	601	-	56,73,73	1.38	12 (21%)	65,113,113	1.54	9 (13%)
21	CLA	B	602	-	56,73,73	1.39	10 (17%)	65,113,113	1.48	12 (18%)
21	CLA	B	603	-	56,73,73	1.40	12 (21%)	65,113,113	1.52	11 (16%)
21	CLA	B	604	-	56,73,73	1.39	11 (19%)	65,113,113	1.48	9 (13%)
21	CLA	B	605	-	56,73,73	1.38	11 (19%)	65,113,113	1.51	11 (16%)
21	CLA	B	606	-	56,73,73	1.38	11 (19%)	65,113,113	1.53	12 (18%)
21	CLA	B	607	-	56,73,73	1.40	10 (17%)	65,113,113	1.51	8 (12%)
21	CLA	B	608	-	56,73,73	1.40	10 (17%)	65,113,113	1.44	8 (12%)
21	CLA	B	609	-	56,73,73	1.40	11 (19%)	65,113,113	1.45	8 (12%)
21	CLA	B	610	-	56,73,73	1.39	12 (21%)	65,113,113	1.49	8 (12%)
21	CLA	B	611	-	56,73,73	1.39	12 (21%)	65,113,113	1.53	12 (18%)
21	CLA	B	612	-	56,73,73	1.39	11 (19%)	65,113,113	1.52	8 (12%)
21	CLA	B	613	-	56,73,73	1.39	12 (21%)	65,113,113	1.46	8 (12%)
21	CLA	B	614	-	56,73,73	1.39	10 (17%)	65,113,113	1.46	9 (13%)
21	CLA	B	615	-	56,73,73	1.38	10 (17%)	65,113,113	1.52	11 (16%)
21	CLA	B	616	-	56,73,73	1.37	12 (21%)	65,113,113	1.52	9 (13%)
30	BCR	B	617	-	41,41,41	0.69	0	56,56,56	1.60	10 (17%)
30	BCR	B	618	-	41,41,41	0.68	0	56,56,56	1.88	16 (28%)
30	BCR	B	619	-	41,41,41	0.72	0	56,56,56	1.52	10 (17%)
30	BCR	B	620	-	41,41,41	0.69	0	56,56,56	1.61	10 (17%)
24	DGD	B	621	-	59,59,67	0.94	3 (5%)	73,73,81	1.42	9 (12%)
27	LMG	B	622	-	49,49,55	0.92	2 (4%)	57,57,63	1.31	8 (14%)
27	LMG	B	623	-	49,49,55	0.94	2 (4%)	57,57,63	1.28	8 (14%)
26	SQD	B	624	-	42,43,54	1.34	5 (11%)	52,54,65	1.56	8 (15%)
31	LMT	B	625	-	36,36,36	0.41	0	47,47,47	0.71	0
31	LMT	B	626	-	36,36,36	0.44	0	47,47,47	0.70	1 (2%)
26	SQD	B	627	-	46,47,54	1.28	5 (10%)	56,58,65	1.70	9 (16%)
24	DGD	B	628	-	53,53,67	1.01	3 (5%)	67,67,81	1.58	12 (17%)
31	LMT	B	629	-	36,36,36	0.45	0	47,47,47	0.80	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	B	630	-	36,36,36	0.39	0	47,47,47	0.65	0
21	CLA	C	501	-	56,73,73	1.39	11 (19%)	65,113,113	1.46	8 (12%)
21	CLA	C	502	-	56,73,73	1.37	12 (21%)	65,113,113	1.48	7 (10%)
21	CLA	C	503	-	56,73,73	1.37	11 (19%)	65,113,113	1.49	10 (15%)
21	CLA	C	504	-	56,73,73	1.40	10 (17%)	65,113,113	1.45	9 (13%)
21	CLA	C	505	-	56,73,73	1.38	11 (19%)	65,113,113	1.50	10 (15%)
21	CLA	C	506	-	56,73,73	1.40	12 (21%)	65,113,113	1.50	11 (16%)
21	CLA	C	507	-	56,73,73	1.37	12 (21%)	65,113,113	1.48	8 (12%)
21	CLA	C	508	-	56,73,73	1.38	10 (17%)	65,113,113	1.54	11 (16%)
21	CLA	C	509	-	56,73,73	1.40	11 (19%)	65,113,113	1.45	9 (13%)
21	CLA	C	510	-	56,73,73	1.39	10 (17%)	65,113,113	1.48	9 (13%)
21	CLA	C	511	3	56,73,73	1.38	12 (21%)	65,113,113	1.52	7 (10%)
21	CLA	C	512	-	56,73,73	1.38	10 (17%)	65,113,113	1.56	9 (13%)
21	CLA	C	513	-	56,73,73	1.39	11 (19%)	65,113,113	1.47	9 (13%)
30	BCR	C	514	-	41,41,41	0.70	0	56,56,56	2.34	19 (33%)
30	BCR	C	515	-	41,41,41	0.73	0	56,56,56	1.69	13 (23%)
24	DGD	C	516	-	54,54,67	0.97	3 (5%)	68,68,81	1.55	10 (14%)
24	DGD	C	517	-	63,63,67	0.91	3 (4%)	77,77,81	1.54	13 (16%)
24	DGD	C	518	-	67,67,67	0.91	4 (5%)	81,81,81	1.37	8 (9%)
27	LMG	C	519	-	48,48,55	0.95	2 (4%)	56,56,63	1.32	6 (10%)
27	LMG	C	520	-	45,45,55	1.02	2 (4%)	53,53,63	1.30	7 (13%)
21	CLA	D	401	-	56,73,73	1.40	9 (16%)	65,113,113	1.49	9 (13%)
22	PHO	D	402	-	67,69,69	2.14	16 (23%)	87,99,99	1.86	22 (25%)
21	CLA	D	403	-	56,73,73	1.38	10 (17%)	65,113,113	1.54	9 (13%)
23	PL9	D	404	-	55,55,55	1.19	8 (14%)	69,69,69	1.59	17 (24%)
30	BCR	D	405	-	41,41,41	0.69	0	56,56,56	1.72	10 (17%)
27	LMG	D	406	-	46,46,55	0.97	2 (4%)	54,54,63	1.39	7 (12%)
27	LMG	D	407	-	48,48,55	0.94	2 (4%)	56,56,63	1.32	4 (7%)
24	DGD	D	408	-	64,64,67	0.90	2 (3%)	78,78,81	1.35	8 (10%)
31	LMT	D	409	-	32,32,36	0.47	0	43,43,47	0.67	1 (2%)
32	BCT	D	410	29	0,3,3	0.00	-	0,3,3	0.00	-
27	LMG	D	412	-	42,42,55	1.02	2 (4%)	50,50,63	1.30	5 (10%)
34	HEM	E	101	5,6	28,50,50	2.20	6 (21%)	17,82,82	2.00	4 (23%)
27	LMG	E	102	-	44,44,55	1.01	2 (4%)	52,52,63	1.15	5 (9%)
26	SQD	F	101	-	44,45,54	1.30	4 (9%)	54,56,65	1.38	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	G	401	-	53,54,54	1.17	4 (7%)	63,65,65	1.21	4 (6%)
21	CLA	G	402	-	56,73,73	1.40	12 (21%)	65,113,113	1.52	10 (15%)
21	CLA	G	403	-	56,73,73	1.38	12 (21%)	65,113,113	1.54	9 (13%)
21	CLA	G	404	-	56,73,73	1.37	11 (19%)	65,113,113	1.54	8 (12%)
22	PHO	G	405	-	67,69,69	2.11	17 (25%)	87,99,99	1.96	24 (27%)
21	CLA	G	406	-	56,73,73	1.36	11 (19%)	65,113,113	1.52	10 (15%)
23	PL9	G	407	-	45,45,55	1.19	7 (15%)	57,57,69	1.66	17 (29%)
24	DGD	G	408	-	57,57,67	0.96	3 (5%)	71,71,81	1.51	9 (12%)
25	LHG	G	409	-	38,38,48	1.05	2 (5%)	39,44,54	0.99	3 (7%)
26	SQD	G	410	-	50,51,54	1.21	4 (8%)	60,62,65	1.60	10 (16%)
27	LMG	G	411	-	51,51,55	0.94	2 (3%)	59,59,63	1.26	4 (6%)
25	LHG	G	412	-	36,36,48	1.07	2 (5%)	37,42,54	1.11	2 (5%)
28	OEC	G	413	1	0,0,13	0.00	-	0,0,27	0.00	-
30	BCR	H	101	-	41,41,41	0.74	0	56,56,56	1.46	10 (17%)
30	BCR	I	101	-	41,41,41	0.67	0	56,56,56	1.57	12 (21%)
27	LMG	I	102	-	43,43,55	0.99	2 (4%)	51,51,63	1.33	5 (9%)
31	LMT	I	103	-	36,36,36	0.47	0	47,47,47	0.72	1 (2%)
23	PL9	J	101	-	35,35,55	1.14	5 (14%)	45,45,69	1.52	8 (17%)
30	BCR	J	102	-	41,41,41	0.77	0	56,56,56	3.06	21 (37%)
30	BCR	K	101	-	41,41,41	0.77	0	56,56,56	1.61	11 (19%)
27	LMG	M	101	-	42,42,55	1.01	2 (4%)	50,50,63	1.34	6 (12%)
31	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
26	SQD	N	601	-	46,47,54	1.28	4 (8%)	56,58,65	1.75	10 (17%)
24	DGD	N	602	-	53,53,67	1.01	3 (5%)	67,67,81	1.57	10 (14%)
31	LMT	N	603	-	36,36,36	0.45	0	47,47,47	0.83	1 (2%)
31	LMT	N	604	-	36,36,36	0.42	0	47,47,47	0.65	1 (2%)
21	CLA	N	605	-	56,73,73	1.37	12 (21%)	65,113,113	1.53	9 (13%)
21	CLA	N	606	-	56,73,73	1.40	13 (23%)	65,113,113	1.51	10 (15%)
21	CLA	N	607	-	56,73,73	1.41	11 (19%)	65,113,113	1.51	12 (18%)
21	CLA	N	608	-	56,73,73	1.39	11 (19%)	65,113,113	1.50	9 (13%)
21	CLA	N	609	-	56,73,73	1.38	12 (21%)	65,113,113	1.53	11 (16%)
21	CLA	N	610	-	56,73,73	1.40	12 (21%)	65,113,113	1.54	11 (16%)
21	CLA	N	611	-	56,73,73	1.41	9 (16%)	65,113,113	1.50	8 (12%)
21	CLA	N	612	-	56,73,73	1.40	10 (17%)	65,113,113	1.44	8 (12%)
21	CLA	N	613	-	56,73,73	1.37	11 (19%)	65,113,113	1.46	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	N	614	-	56,73,73	1.39	11 (19%)	65,113,113	1.47	9 (13%)
21	CLA	N	615	-	56,73,73	1.39	12 (21%)	65,113,113	1.53	11 (16%)
21	CLA	N	616	-	56,73,73	1.41	11 (19%)	65,113,113	1.54	9 (13%)
21	CLA	N	617	-	56,73,73	1.41	12 (21%)	65,113,113	1.46	8 (12%)
21	CLA	N	618	-	56,73,73	1.40	10 (17%)	65,113,113	1.48	9 (13%)
21	CLA	N	619	-	56,73,73	1.36	10 (17%)	65,113,113	1.53	11 (16%)
21	CLA	N	620	-	56,73,73	1.38	11 (19%)	65,113,113	1.52	8 (12%)
30	BCR	N	621	-	41,41,41	0.72	0	56,56,56	1.54	13 (23%)
27	LMG	N	622	-	49,49,55	0.92	2 (4%)	57,57,63	1.39	8 (14%)
27	LMG	N	623	-	49,49,55	0.93	2 (4%)	57,57,63	1.27	8 (14%)
31	LMT	N	624	-	36,36,36	0.41	0	47,47,47	0.68	0
31	LMT	N	625	-	36,36,36	0.42	0	47,47,47	0.70	1 (2%)
21	CLA	P	501	-	56,73,73	1.40	11 (19%)	65,113,113	1.47	9 (13%)
21	CLA	P	502	-	56,73,73	1.39	11 (19%)	65,113,113	1.48	8 (12%)
21	CLA	P	503	-	56,73,73	1.38	11 (19%)	65,113,113	1.48	10 (15%)
21	CLA	P	504	-	56,73,73	1.41	10 (17%)	65,113,113	1.43	8 (12%)
21	CLA	P	505	-	56,73,73	1.37	10 (17%)	65,113,113	1.49	8 (12%)
21	CLA	P	506	-	56,73,73	1.40	12 (21%)	65,113,113	1.49	11 (16%)
21	CLA	P	507	-	56,73,73	1.37	11 (19%)	65,113,113	1.47	8 (12%)
21	CLA	P	508	-	56,73,73	1.38	11 (19%)	65,113,113	1.57	11 (16%)
21	CLA	P	509	-	56,73,73	1.39	12 (21%)	65,113,113	1.46	10 (15%)
21	CLA	P	510	-	56,73,73	1.38	12 (21%)	65,113,113	1.51	9 (13%)
21	CLA	P	511	3	56,73,73	1.38	10 (17%)	65,113,113	1.51	8 (12%)
21	CLA	P	512	-	56,73,73	1.39	10 (17%)	65,113,113	1.54	8 (12%)
21	CLA	P	513	-	56,73,73	1.40	11 (19%)	65,113,113	1.47	9 (13%)
30	BCR	P	514	-	41,41,41	0.68	0	56,56,56	2.37	18 (32%)
30	BCR	P	515	-	41,41,41	0.66	0	56,56,56	1.57	12 (21%)
30	BCR	P	516	-	41,41,41	0.73	0	56,56,56	1.69	15 (26%)
24	DGD	P	517	-	54,54,67	0.98	3 (5%)	68,68,81	1.59	10 (14%)
24	DGD	P	518	-	63,63,67	0.91	3 (4%)	77,77,81	1.55	13 (16%)
24	DGD	P	519	-	67,67,67	0.89	4 (5%)	81,81,81	1.31	8 (9%)
27	LMG	P	520	-	48,48,55	0.94	2 (4%)	56,56,63	1.32	7 (12%)
27	LMG	P	521	-	45,45,55	1.02	2 (4%)	53,53,63	1.27	6 (11%)
27	LMG	Q	401	-	42,42,55	1.02	2 (4%)	50,50,63	1.28	5 (10%)
21	CLA	Q	402	-	56,73,73	1.40	9 (16%)	65,113,113	1.49	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PHO	Q	403	-	67,69,69	2.13	17 (25%)	87,99,99	1.84	22 (25%)
21	CLA	Q	404	-	56,73,73	1.40	10 (17%)	65,113,113	1.54	9 (13%)
23	PL9	Q	405	-	55,55,55	1.20	8 (14%)	69,69,69	1.61	19 (27%)
27	LMG	Q	406	-	46,46,55	0.98	2 (4%)	54,54,63	1.36	6 (11%)
27	LMG	Q	407	-	48,48,55	0.94	2 (4%)	56,56,63	1.33	4 (7%)
26	SQD	Q	408	-	42,43,54	1.35	5 (11%)	52,54,65	1.57	8 (15%)
24	DGD	Q	409	-	64,64,67	0.90	2 (3%)	78,78,81	1.35	10 (12%)
31	LMT	Q	410	-	32,32,36	0.47	0	43,43,47	0.67	1 (2%)
32	BCT	Q	411	29	0,3,3	0.00	-	0,3,3	0.00	-
34	HEM	R	101	5,6	28,50,50	2.20	5 (17%)	17,82,82	2.19	3 (17%)
27	LMG	R	102	-	44,44,55	0.99	2 (4%)	52,52,63	1.16	5 (9%)
30	BCR	S	101	-	41,41,41	0.70	0	56,56,56	1.74	11 (19%)
26	SQD	S	102	-	44,45,54	1.31	5 (11%)	54,56,65	1.38	8 (14%)
30	BCR	T	101	-	41,41,41	0.69	0	56,56,56	1.58	11 (19%)
30	BCR	T	102	-	41,41,41	0.67	0	56,56,56	1.86	15 (26%)
30	BCR	T	103	-	41,41,41	0.67	0	56,56,56	1.63	11 (19%)
34	HEM	V	201	16	28,50,50	2.23	6 (21%)	17,82,82	1.92	3 (17%)
30	BCR	W	101	-	41,41,41	0.73	0	56,56,56	1.45	9 (16%)
24	DGD	W	102	-	59,59,67	0.94	3 (5%)	73,73,81	1.44	10 (13%)
30	BCR	Z	101	-	41,41,41	0.65	0	56,56,56	1.62	12 (21%)
30	BCR	a	101	-	41,41,41	0.67	0	56,56,56	1.59	11 (19%)
27	LMG	a	102	-	43,43,55	0.99	2 (4%)	51,51,63	1.35	7 (13%)
31	LMT	a	103	-	36,36,36	0.46	0	47,47,47	0.71	1 (2%)
23	PL9	b	101	-	35,35,55	1.14	5 (14%)	45,45,69	1.54	10 (22%)
30	BCR	b	102	-	41,41,41	0.76	0	56,56,56	3.10	20 (35%)
30	BCR	c	101	-	41,41,41	0.76	0	56,56,56	1.56	10 (17%)
31	LMT	e	101	-	36,36,36	0.41	0	47,47,47	0.68	1 (2%)
27	LMG	e	102	-	42,42,55	1.02	2 (4%)	50,50,63	1.36	6 (12%)
34	HEM	i	201	16	28,50,50	2.23	6 (21%)	17,82,82	1.91	4 (23%)

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
21	CLA	A	401	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	402	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	A	404	-	-	0/53/103/103	0/1/6/6
21	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	DGD	A	407	-	3/3/13/13	0/45/85/95	0/2/2/2
25	LHG	A	408	-	-	0/43/43/53	0/0/0/0
26	SQD	A	409	-	-	0/46/66/69	0/1/1/1
27	LMG	A	410	-	2/2/8/8	0/46/66/70	0/1/1/1
25	LHG	A	411	-	-	0/41/41/53	0/0/0/0
28	OEC	A	412	1,3	-	0/0/0/54	0/0/0/5
26	SQD	A	414	-	-	0/49/69/69	0/1/1/1
21	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
30	BCR	B	617	-	-	0/29/63/63	0/2/2/2
30	BCR	B	618	-	-	0/29/63/63	0/2/2/2
30	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	DGD	B	621	-	3/3/13/13	0/47/87/95	0/2/2/2
27	LMG	B	622	-	2/2/8/8	0/44/64/70	0/1/1/1
27	LMG	B	623	-	2/2/8/8	0/44/64/70	0/1/1/1
26	SQD	B	624	-	-	1/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	B	625	-	-	0/21/61/61	0/2/2/2
31	LMT	B	626	-	-	0/21/61/61	0/2/2/2
26	SQD	B	627	-	-	0/42/62/69	0/1/1/1
24	DGD	B	628	-	3/3/13/13	0/41/81/95	0/2/2/2
31	LMT	B	629	-	-	0/21/61/61	0/2/2/2
31	LMT	B	630	-	-	0/21/61/61	0/2/2/2
21	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	505	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	509	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	C	510	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	C	513	-	3/3/20/25	1/37/135/135	0/0/9/9
30	BCR	C	514	-	-	0/29/63/63	0/2/2/2
30	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	DGD	C	516	-	3/3/13/13	0/42/82/95	0/2/2/2
24	DGD	C	517	-	3/3/13/13	0/51/91/95	0/2/2/2
24	DGD	C	518	-	3/3/13/13	0/55/95/95	0/2/2/2
27	LMG	C	519	-	2/2/8/8	0/43/63/70	0/1/1/1
27	LMG	C	520	-	2/2/8/8	0/40/60/70	0/1/1/1
21	CLA	D	401	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	D	402	-	-	0/53/103/103	0/1/6/6
21	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	D	404	-	-	0/53/73/73	0/1/1/1
30	BCR	D	405	-	-	0/29/63/63	0/2/2/2
27	LMG	D	406	-	2/2/8/8	0/41/61/70	0/1/1/1
27	LMG	D	407	-	2/2/8/8	1/43/63/70	0/1/1/1
24	DGD	D	408	-	3/3/13/13	0/52/92/95	0/2/2/2
31	LMT	D	409	-	-	0/17/57/61	0/2/2/2
32	BCT	D	410	29	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	D	412	-	2/2/8/8	0/37/57/70	0/1/1/1
34	HEM	E	101	5,6	-	0/6/54/54	0/0/8/8
27	LMG	E	102	-	2/2/8/8	0/39/59/70	0/1/1/1
26	SQD	F	101	-	-	0/40/60/69	0/1/1/1
26	SQD	G	401	-	-	0/49/69/69	0/1/1/1
21	CLA	G	402	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	G	403	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	G	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	G	405	-	-	0/53/103/103	0/1/6/6
21	CLA	G	406	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	G	407	-	-	0/41/61/73	0/1/1/1
24	DGD	G	408	-	3/3/13/13	0/45/85/95	0/2/2/2
25	LHG	G	409	-	-	0/43/43/53	0/0/0/0
26	SQD	G	410	-	-	0/46/66/69	0/1/1/1
27	LMG	G	411	-	2/2/8/8	0/46/66/70	0/1/1/1
25	LHG	G	412	-	-	0/41/41/53	0/0/0/0
28	OEC	G	413	1	-	0/0/0/54	0/0/0/5
30	BCR	H	101	-	-	0/29/63/63	0/2/2/2
30	BCR	I	101	-	-	0/29/63/63	0/2/2/2
27	LMG	I	102	-	2/2/8/8	0/38/58/70	0/1/1/1
31	LMT	I	103	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
30	BCR	J	102	-	-	0/29/63/63	0/2/2/2
30	BCR	K	101	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	2/2/8/8	0/37/57/70	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
26	SQD	N	601	-	-	0/42/62/69	0/1/1/1
24	DGD	N	602	-	3/3/13/13	0/41/81/95	0/2/2/2
31	LMT	N	603	-	-	0/21/61/61	0/2/2/2
31	LMT	N	604	-	-	0/21/61/61	0/2/2/2
21	CLA	N	605	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	606	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	607	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	608	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	609	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	610	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	N	611	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	612	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	N	613	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	614	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	615	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	616	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	617	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	618	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	619	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	N	620	-	3/3/20/25	0/37/135/135	0/0/9/9
30	BCR	N	621	-	-	0/29/63/63	0/2/2/2
27	LMG	N	622	-	2/2/8/8	0/44/64/70	0/1/1/1
27	LMG	N	623	-	2/2/8/8	0/44/64/70	0/1/1/1
31	LMT	N	624	-	-	0/21/61/61	0/2/2/2
31	LMT	N	625	-	-	0/21/61/61	0/2/2/2
21	CLA	P	501	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	502	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	503	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	504	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	505	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	506	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	507	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	508	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	509	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	510	-	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	P	511	3	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	512	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	P	513	-	3/3/20/25	1/37/135/135	0/0/9/9
30	BCR	P	514	-	-	0/29/63/63	0/2/2/2
30	BCR	P	515	-	-	0/29/63/63	0/2/2/2
30	BCR	P	516	-	-	0/29/63/63	0/2/2/2
24	DGD	P	517	-	3/3/13/13	0/42/82/95	0/2/2/2
24	DGD	P	518	-	3/3/13/13	0/51/91/95	0/2/2/2
24	DGD	P	519	-	3/3/13/13	0/55/95/95	0/2/2/2
27	LMG	P	520	-	2/2/8/8	0/43/63/70	0/1/1/1
27	LMG	P	521	-	2/2/8/8	0/40/60/70	0/1/1/1
27	LMG	Q	401	-	2/2/8/8	0/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	Q	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	PHO	Q	403	-	-	0/53/103/103	0/1/6/6
21	CLA	Q	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	Q	405	-	-	0/53/73/73	0/1/1/1
27	LMG	Q	406	-	2/2/8/8	0/41/61/70	0/1/1/1
27	LMG	Q	407	-	2/2/8/8	1/43/63/70	0/1/1/1
26	SQD	Q	408	-	-	1/38/58/69	0/1/1/1
24	DGD	Q	409	-	3/3/13/13	0/52/92/95	0/2/2/2
31	LMT	Q	410	-	-	0/17/57/61	0/2/2/2
32	BCT	Q	411	29	-	0/0/0/0	0/0/0/0
34	HEM	R	101	5,6	-	0/6/54/54	0/0/8/8
27	LMG	R	102	-	2/2/8/8	0/39/59/70	0/1/1/1
30	BCR	S	101	-	-	0/29/63/63	0/2/2/2
26	SQD	S	102	-	-	0/40/60/69	0/1/1/1
30	BCR	T	101	-	-	0/29/63/63	0/2/2/2
30	BCR	T	102	-	-	0/29/63/63	0/2/2/2
30	BCR	T	103	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
30	BCR	W	101	-	-	0/29/63/63	0/2/2/2
24	DGD	W	102	-	3/3/13/13	0/47/87/95	0/2/2/2
30	BCR	Z	101	-	-	0/29/63/63	0/2/2/2
30	BCR	a	101	-	-	0/29/63/63	0/2/2/2
27	LMG	a	102	-	2/2/8/8	0/38/58/70	0/1/1/1
31	LMT	a	103	-	-	0/21/61/61	0/2/2/2
23	PL9	b	101	-	-	0/29/49/73	0/1/1/1
30	BCR	b	102	-	-	0/29/63/63	0/2/2/2
30	BCR	c	101	-	-	0/29/63/63	0/2/2/2
31	LMT	e	101	-	-	0/21/61/61	0/2/2/2
27	LMG	e	102	-	2/2/8/8	0/37/57/70	0/1/1/1
34	HEM	i	201	16	-	0/6/54/54	0/0/8/8

All (1038) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	R	101	HEM	C3B-C2B	-5.30	1.33	1.40
34	E	101	HEM	C3B-C2B	-5.30	1.33	1.40
34	i	201	HEM	C3C-C2C	-4.91	1.33	1.40
34	V	201	HEM	C3C-C2C	-4.90	1.33	1.40
34	i	201	HEM	C3B-C2B	-4.49	1.34	1.40
34	V	201	HEM	C3B-C2B	-4.47	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	R	101	HEM	C3C-C2C	-3.92	1.35	1.40
22	Q	403	PHO	C4A-NA	-3.80	1.26	1.35
22	D	402	PHO	C4A-NA	-3.79	1.26	1.35
34	E	101	HEM	C3C-C2C	-3.77	1.35	1.40
22	A	404	PHO	C4A-NA	-3.76	1.26	1.35
22	G	405	PHO	C4A-NA	-3.74	1.26	1.35
22	A	404	PHO	C3D-C4D	-2.90	1.34	1.43
22	D	402	PHO	C3D-C4D	-2.85	1.34	1.43
22	G	405	PHO	C3D-C4D	-2.81	1.34	1.43
22	Q	403	PHO	C3D-C4D	-2.81	1.34	1.43
26	N	601	SQD	C6-S	-2.80	1.66	1.77
26	B	627	SQD	C6-S	-2.80	1.66	1.77
26	A	414	SQD	C6-S	-2.78	1.66	1.77
26	Q	408	SQD	C6-S	-2.71	1.66	1.77
26	G	401	SQD	C6-S	-2.71	1.66	1.77
26	B	624	SQD	C6-S	-2.69	1.66	1.77
26	A	409	SQD	C6-S	-2.66	1.66	1.77
26	G	410	SQD	C6-S	-2.65	1.66	1.77
26	S	102	SQD	C6-S	-2.60	1.66	1.77
26	F	101	SQD	C6-S	-2.60	1.66	1.77
21	Q	402	CLA	O2D-CED	-2.58	1.39	1.45
21	D	401	CLA	O2D-CED	-2.58	1.39	1.45
21	B	611	CLA	C3B-C2B	-2.54	1.37	1.40
21	C	506	CLA	C3B-C2B	-2.53	1.37	1.40
21	A	401	CLA	C1A-CHA	-2.51	1.32	1.43
21	N	617	CLA	C3B-C2B	-2.50	1.37	1.40
21	G	403	CLA	C3B-C2B	-2.49	1.37	1.40
21	A	402	CLA	C3B-C2B	-2.48	1.37	1.40
21	P	504	CLA	O2D-CED	-2.47	1.39	1.45
21	N	616	CLA	C3B-C2B	-2.47	1.37	1.40
21	N	615	CLA	C3B-C2B	-2.47	1.37	1.40
21	B	613	CLA	C3B-C2B	-2.47	1.37	1.40
21	C	509	CLA	O2D-CED	-2.46	1.39	1.45
21	C	504	CLA	O2D-CED	-2.46	1.39	1.45
21	G	402	CLA	C1A-CHA	-2.45	1.32	1.43
21	C	507	CLA	C3B-C2B	-2.45	1.37	1.40
21	C	510	CLA	O2D-CED	-2.45	1.39	1.45
21	N	607	CLA	C3B-C2B	-2.45	1.37	1.40
21	C	508	CLA	O2D-CED	-2.44	1.39	1.45
21	C	507	CLA	O2D-CED	-2.44	1.39	1.45
21	N	613	CLA	O2D-CED	-2.44	1.39	1.45
21	N	611	CLA	O2D-CED	-2.44	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	602	CLA	O2D-CED	-2.43	1.39	1.45
21	G	402	CLA	C3B-C2B	-2.43	1.37	1.40
21	B	608	CLA	O2D-CED	-2.43	1.39	1.45
21	B	607	CLA	O2D-CED	-2.43	1.39	1.45
21	P	509	CLA	O2D-CED	-2.43	1.39	1.45
21	G	403	CLA	O2D-CED	-2.43	1.39	1.45
21	P	513	CLA	O2D-CED	-2.43	1.39	1.45
21	B	613	CLA	O2D-CED	-2.43	1.39	1.45
21	A	402	CLA	O2D-CED	-2.43	1.39	1.45
21	C	511	CLA	C3B-C2B	-2.42	1.37	1.40
21	P	501	CLA	O2D-CED	-2.42	1.39	1.45
21	A	403	CLA	O2D-CED	-2.42	1.39	1.45
21	N	617	CLA	O2D-CED	-2.42	1.39	1.45
21	P	501	CLA	C3B-C2B	-2.42	1.37	1.40
21	P	506	CLA	O2D-CED	-2.42	1.39	1.45
21	C	509	CLA	C3B-C2B	-2.42	1.37	1.40
21	B	601	CLA	O2D-CED	-2.42	1.39	1.45
21	N	618	CLA	O2D-CED	-2.42	1.39	1.45
21	B	603	CLA	C3B-C2B	-2.42	1.37	1.40
21	A	401	CLA	C3B-C2B	-2.42	1.37	1.40
21	N	616	CLA	O2D-CED	-2.42	1.39	1.45
21	B	606	CLA	C1A-CHA	-2.41	1.33	1.43
21	N	608	CLA	C3B-C2B	-2.41	1.37	1.40
21	B	609	CLA	O2D-CED	-2.41	1.39	1.45
21	B	615	CLA	O2D-CED	-2.41	1.39	1.45
21	P	502	CLA	C3B-C2B	-2.41	1.37	1.40
21	B	612	CLA	O2D-CED	-2.41	1.39	1.45
21	B	604	CLA	O2D-CED	-2.41	1.39	1.45
21	B	614	CLA	O2D-CED	-2.41	1.39	1.45
21	N	608	CLA	O2D-CED	-2.41	1.39	1.45
21	P	511	CLA	O2D-CED	-2.41	1.39	1.45
21	P	507	CLA	O2D-CED	-2.41	1.39	1.45
21	C	510	CLA	C3B-C2B	-2.40	1.37	1.40
21	C	506	CLA	O2D-CED	-2.40	1.39	1.45
21	C	512	CLA	O2D-CED	-2.40	1.39	1.45
21	P	506	CLA	C3B-C2B	-2.40	1.37	1.40
21	C	502	CLA	O2D-CED	-2.40	1.39	1.45
21	D	401	CLA	C1A-CHA	-2.40	1.33	1.43
21	Q	404	CLA	O2D-CED	-2.40	1.39	1.45
21	C	503	CLA	O2D-CED	-2.40	1.39	1.45
21	P	508	CLA	O2D-CED	-2.40	1.39	1.45
21	G	402	CLA	O2D-CED	-2.40	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	510	CLA	O2D-CED	-2.40	1.39	1.45
21	D	403	CLA	O2D-CED	-2.39	1.39	1.45
21	N	619	CLA	O2D-CED	-2.39	1.39	1.45
21	N	612	CLA	O2D-CED	-2.39	1.39	1.45
21	C	501	CLA	O2D-CED	-2.39	1.39	1.45
21	N	605	CLA	O2D-CED	-2.39	1.39	1.45
21	N	614	CLA	O2D-CED	-2.39	1.39	1.45
21	B	612	CLA	C1A-CHA	-2.38	1.33	1.43
21	P	504	CLA	C1A-CHA	-2.38	1.33	1.43
21	C	511	CLA	O2D-CED	-2.38	1.39	1.45
21	B	616	CLA	O2D-CED	-2.38	1.39	1.45
21	P	503	CLA	O2D-CED	-2.37	1.39	1.45
21	N	615	CLA	O2D-CED	-2.37	1.39	1.45
21	G	406	CLA	O2D-CED	-2.37	1.39	1.45
21	N	607	CLA	O2D-CED	-2.37	1.39	1.45
21	Q	402	CLA	C1A-CHA	-2.37	1.33	1.43
21	B	605	CLA	O2D-CED	-2.37	1.39	1.45
21	N	616	CLA	C1A-CHA	-2.37	1.33	1.43
21	P	512	CLA	O2D-CED	-2.37	1.39	1.45
21	P	505	CLA	O2D-CED	-2.37	1.39	1.45
21	B	611	CLA	O2D-CED	-2.36	1.39	1.45
21	C	501	CLA	C3B-C2B	-2.36	1.37	1.40
21	G	404	CLA	O2D-CED	-2.36	1.39	1.45
21	N	615	CLA	CMB-C2B	-2.36	1.46	1.51
21	B	606	CLA	O2D-CED	-2.36	1.39	1.45
21	A	405	CLA	O2D-CED	-2.36	1.39	1.45
21	B	604	CLA	C3B-C2B	-2.36	1.37	1.40
21	B	603	CLA	O2D-CED	-2.36	1.39	1.45
21	N	612	CLA	C3B-C2B	-2.36	1.37	1.40
21	C	504	CLA	C1A-CHA	-2.35	1.33	1.43
21	N	606	CLA	O2D-CED	-2.35	1.39	1.45
21	C	505	CLA	O2D-CED	-2.35	1.39	1.45
21	C	509	CLA	C1A-CHA	-2.35	1.33	1.43
21	B	608	CLA	C1A-CHA	-2.35	1.33	1.43
21	C	513	CLA	O2D-CED	-2.35	1.39	1.45
21	N	611	CLA	C3B-C2B	-2.35	1.37	1.40
21	N	612	CLA	C1A-CHA	-2.35	1.33	1.43
21	Q	404	CLA	C3B-C2B	-2.35	1.37	1.40
21	P	513	CLA	C1A-CHA	-2.34	1.33	1.43
21	B	614	CLA	C1A-CHA	-2.34	1.33	1.43
21	C	510	CLA	C1A-CHA	-2.34	1.33	1.43
21	B	610	CLA	O2D-CED	-2.34	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	510	CLA	C3B-C2B	-2.34	1.37	1.40
21	N	620	CLA	O2D-CED	-2.33	1.39	1.45
21	A	401	CLA	O2D-CED	-2.33	1.39	1.45
21	B	616	CLA	C3B-C2B	-2.33	1.37	1.40
21	N	618	CLA	C1A-CHA	-2.33	1.33	1.43
21	N	609	CLA	O2D-CED	-2.33	1.39	1.45
21	G	403	CLA	C1A-CHA	-2.33	1.33	1.43
21	N	606	CLA	C3B-C2B	-2.33	1.37	1.40
21	P	502	CLA	O2D-CED	-2.33	1.39	1.45
21	B	605	CLA	C1A-CHA	-2.33	1.33	1.43
21	B	612	CLA	C3B-C2B	-2.33	1.37	1.40
21	B	615	CLA	C3B-C2B	-2.32	1.37	1.40
21	P	507	CLA	C3B-C2B	-2.32	1.37	1.40
21	A	403	CLA	C1A-CHA	-2.32	1.33	1.43
21	P	503	CLA	C1A-CHA	-2.32	1.33	1.43
21	P	510	CLA	C1A-CHA	-2.32	1.33	1.43
21	P	509	CLA	C3B-C2B	-2.32	1.37	1.40
21	P	505	CLA	C1A-CHA	-2.32	1.33	1.43
21	B	607	CLA	C3B-C2B	-2.32	1.37	1.40
21	C	513	CLA	C1A-CHA	-2.31	1.33	1.43
21	G	402	CLA	O2A-C1	-2.31	1.39	1.46
21	N	614	CLA	C1A-CHA	-2.31	1.33	1.43
21	N	610	CLA	O2D-CED	-2.31	1.39	1.45
21	P	506	CLA	C1A-CHA	-2.31	1.33	1.43
21	C	502	CLA	C1A-CHA	-2.30	1.33	1.43
21	N	611	CLA	C1A-CHA	-2.30	1.33	1.43
21	N	620	CLA	C3B-C2B	-2.30	1.37	1.40
21	C	504	CLA	C3B-C2B	-2.30	1.37	1.40
21	C	503	CLA	C1A-CHA	-2.30	1.33	1.43
21	N	608	CLA	C1A-CHA	-2.30	1.33	1.43
21	B	602	CLA	C3B-C2B	-2.29	1.37	1.40
21	Q	404	CLA	C1A-CHA	-2.29	1.33	1.43
21	C	506	CLA	C1A-CHA	-2.29	1.33	1.43
21	B	607	CLA	C1A-CHA	-2.29	1.33	1.43
21	D	403	CLA	C1A-CHA	-2.29	1.33	1.43
21	N	615	CLA	C1A-CHA	-2.29	1.33	1.43
21	N	605	CLA	C3B-C2B	-2.29	1.37	1.40
21	B	611	CLA	CMB-C2B	-2.28	1.47	1.51
21	B	604	CLA	C1A-CHA	-2.28	1.33	1.43
21	A	403	CLA	C3B-C2B	-2.28	1.37	1.40
21	P	513	CLA	C3B-C2B	-2.28	1.37	1.40
21	N	609	CLA	C1A-CHA	-2.28	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	513	CLA	C3B-C2B	-2.28	1.37	1.40
21	B	602	CLA	C1A-CHA	-2.27	1.33	1.43
21	A	401	CLA	O2A-C1	-2.27	1.39	1.46
21	P	512	CLA	C1A-CHA	-2.27	1.33	1.43
21	A	402	CLA	C1A-CHA	-2.27	1.33	1.43
21	B	613	CLA	C1A-CHA	-2.27	1.33	1.43
21	C	508	CLA	C1A-CHA	-2.27	1.33	1.43
21	G	404	CLA	C3B-C2B	-2.27	1.37	1.40
21	N	605	CLA	C1A-CHA	-2.27	1.33	1.43
21	P	509	CLA	C1A-CHA	-2.27	1.33	1.43
21	C	507	CLA	C1A-CHA	-2.26	1.33	1.43
21	N	609	CLA	C3B-C2B	-2.26	1.37	1.40
21	N	610	CLA	C1A-CHA	-2.26	1.33	1.43
21	P	508	CLA	C1A-CHA	-2.26	1.33	1.43
21	N	613	CLA	C1A-CHA	-2.26	1.33	1.43
21	C	502	CLA	C3B-C2B	-2.26	1.37	1.40
21	B	601	CLA	C3B-C2B	-2.26	1.37	1.40
21	B	610	CLA	C1A-CHA	-2.26	1.33	1.43
21	B	608	CLA	C3B-C2B	-2.25	1.37	1.40
21	B	609	CLA	C1A-CHA	-2.25	1.33	1.43
21	P	502	CLA	C1A-CHA	-2.25	1.33	1.43
21	B	615	CLA	C1A-CHA	-2.25	1.33	1.43
21	P	508	CLA	C3B-C2B	-2.25	1.37	1.40
21	G	406	CLA	C1A-CHA	-2.24	1.33	1.43
21	A	405	CLA	C1A-CHA	-2.24	1.33	1.43
21	P	505	CLA	O2A-C1	-2.24	1.39	1.46
21	B	601	CLA	C1A-CHA	-2.23	1.33	1.43
21	G	404	CLA	C1A-CHA	-2.23	1.33	1.43
21	C	505	CLA	C1A-CHA	-2.23	1.33	1.43
21	P	504	CLA	C3B-C2B	-2.23	1.37	1.40
21	N	617	CLA	C1A-CHA	-2.23	1.33	1.43
21	C	511	CLA	C1A-CHA	-2.23	1.33	1.43
21	C	505	CLA	C3B-C2B	-2.22	1.37	1.40
21	N	615	CLA	O2A-C1	-2.22	1.39	1.46
21	C	510	CLA	O2A-C1	-2.22	1.39	1.46
21	C	501	CLA	C1A-CHA	-2.22	1.33	1.43
21	B	611	CLA	O2A-C1	-2.21	1.39	1.46
21	G	406	CLA	O2A-C1	-2.21	1.39	1.46
21	P	505	CLA	C3B-C2B	-2.21	1.37	1.40
21	C	505	CLA	O2A-C1	-2.21	1.39	1.46
21	N	606	CLA	C1A-CHA	-2.21	1.33	1.43
21	C	508	CLA	C3B-C2B	-2.21	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	616	CLA	O2A-C1	-2.20	1.39	1.46
21	C	512	CLA	C1A-CHA	-2.20	1.33	1.43
21	B	616	CLA	C1A-CHA	-2.20	1.33	1.43
21	D	403	CLA	C3B-C2B	-2.20	1.37	1.40
21	N	617	CLA	O2A-C1	-2.20	1.39	1.46
21	B	615	CLA	O2A-C1	-2.20	1.39	1.46
21	P	507	CLA	C1A-CHA	-2.20	1.34	1.43
21	B	603	CLA	C1A-CHA	-2.19	1.34	1.43
21	G	406	CLA	C3B-C2B	-2.19	1.37	1.40
21	B	613	CLA	O2A-C1	-2.19	1.39	1.46
21	N	619	CLA	O2A-C1	-2.19	1.39	1.46
21	N	614	CLA	C3B-C2B	-2.19	1.37	1.40
21	N	616	CLA	CMB-C2B	-2.19	1.47	1.51
21	P	501	CLA	C1A-CHA	-2.18	1.34	1.43
21	P	511	CLA	C1A-CHA	-2.18	1.34	1.43
21	N	619	CLA	C1A-CHA	-2.18	1.34	1.43
21	P	512	CLA	C3B-C2B	-2.18	1.37	1.40
21	N	613	CLA	O2A-C1	-2.18	1.39	1.46
21	C	508	CLA	O2A-C1	-2.18	1.39	1.46
21	B	606	CLA	O2A-C1	-2.18	1.39	1.46
21	N	607	CLA	C1A-CHA	-2.18	1.34	1.43
21	P	508	CLA	O2A-C1	-2.18	1.39	1.46
21	B	611	CLA	C1A-CHA	-2.18	1.34	1.43
21	P	511	CLA	C3B-C2B	-2.17	1.37	1.40
21	N	614	CLA	O2A-C1	-2.17	1.39	1.46
21	B	605	CLA	C3B-C2B	-2.17	1.37	1.40
21	P	510	CLA	O2A-C1	-2.17	1.39	1.46
21	B	610	CLA	C3B-C2B	-2.17	1.37	1.40
21	C	511	CLA	O2A-C1	-2.16	1.39	1.46
21	B	609	CLA	C3B-C2B	-2.16	1.37	1.40
21	N	613	CLA	C3B-C2B	-2.16	1.37	1.40
21	N	620	CLA	C1A-CHA	-2.15	1.34	1.43
21	A	405	CLA	O2A-C1	-2.15	1.39	1.46
21	C	512	CLA	C3B-C2B	-2.15	1.37	1.40
21	N	619	CLA	C3B-C2B	-2.15	1.37	1.40
21	G	404	CLA	O2A-C1	-2.15	1.39	1.46
21	C	507	CLA	O2A-C1	-2.14	1.39	1.46
21	B	612	CLA	O2A-C1	-2.14	1.39	1.46
21	P	513	CLA	O2A-C1	-2.14	1.39	1.46
21	N	610	CLA	C3B-C2B	-2.14	1.37	1.40
21	P	509	CLA	O2A-C1	-2.14	1.39	1.46
21	B	609	CLA	O2A-C1	-2.14	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	509	CLA	CMB-C2B	-2.14	1.47	1.51
21	P	507	CLA	O2A-C1	-2.14	1.39	1.46
21	N	606	CLA	O2A-C1	-2.14	1.39	1.46
21	N	620	CLA	O2A-C1	-2.13	1.39	1.46
21	B	606	CLA	C3B-C2B	-2.13	1.37	1.40
21	A	405	CLA	C3B-C2B	-2.13	1.37	1.40
21	B	602	CLA	O2A-C1	-2.13	1.39	1.46
21	C	509	CLA	O2A-C1	-2.13	1.39	1.46
21	B	601	CLA	O2A-C1	-2.13	1.39	1.46
21	A	403	CLA	O2A-C1	-2.13	1.39	1.46
21	P	506	CLA	O2A-C1	-2.13	1.39	1.46
21	A	402	CLA	C1B-CHB	-2.12	1.34	1.40
21	A	402	CLA	O2A-C1	-2.12	1.39	1.46
21	N	605	CLA	O2A-C1	-2.12	1.39	1.46
21	B	610	CLA	O2A-C1	-2.12	1.39	1.46
21	N	610	CLA	O2A-C1	-2.12	1.39	1.46
21	B	605	CLA	O2A-C1	-2.12	1.39	1.46
21	N	618	CLA	C3B-C2B	-2.12	1.37	1.40
21	G	403	CLA	O2A-C1	-2.12	1.39	1.46
21	N	617	CLA	CMB-C2B	-2.11	1.47	1.51
21	C	506	CLA	O2A-C1	-2.11	1.39	1.46
21	B	614	CLA	C3B-C2B	-2.11	1.37	1.40
21	C	506	CLA	CMB-C2B	-2.10	1.47	1.51
21	N	608	CLA	O2A-C1	-2.10	1.39	1.46
21	B	604	CLA	O2A-C1	-2.10	1.39	1.46
21	D	403	CLA	O2A-C1	-2.10	1.39	1.46
21	P	509	CLA	CMB-C2B	-2.10	1.47	1.51
21	B	612	CLA	CMB-C2B	-2.09	1.47	1.51
21	P	511	CLA	O2A-C1	-2.09	1.39	1.46
21	B	613	CLA	CMB-C2B	-2.09	1.47	1.51
21	N	609	CLA	O2A-C1	-2.09	1.39	1.46
21	C	501	CLA	O2A-C1	-2.09	1.39	1.46
21	C	503	CLA	O2A-C1	-2.09	1.39	1.46
21	P	503	CLA	O2A-C1	-2.08	1.39	1.46
21	C	510	CLA	CMB-C2B	-2.08	1.47	1.51
21	N	605	CLA	CMB-C2B	-2.08	1.47	1.51
21	C	513	CLA	O2A-C1	-2.08	1.40	1.46
21	C	502	CLA	O2A-C1	-2.08	1.40	1.46
21	P	506	CLA	CMB-C2B	-2.08	1.47	1.51
21	N	607	CLA	C1B-CHB	-2.07	1.34	1.40
21	N	608	CLA	CMB-C2B	-2.07	1.47	1.51
21	G	403	CLA	CMB-C2B	-2.07	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	606	CLA	C1B-CHB	-2.07	1.34	1.40
21	B	608	CLA	CMB-C2B	-2.06	1.47	1.51
21	P	502	CLA	O2A-C1	-2.06	1.40	1.46
21	B	603	CLA	CMB-C2B	-2.06	1.47	1.51
21	B	604	CLA	CMB-C2B	-2.05	1.47	1.51
21	B	601	CLA	CMB-C2B	-2.05	1.47	1.51
21	C	504	CLA	O2A-C1	-2.05	1.40	1.46
21	G	403	CLA	C1B-CHB	-2.05	1.34	1.40
21	A	402	CLA	CMB-C2B	-2.05	1.47	1.51
21	Q	402	CLA	O2A-C1	-2.04	1.40	1.46
21	C	511	CLA	CMB-C2B	-2.04	1.47	1.51
21	B	610	CLA	CMB-C2B	-2.04	1.47	1.51
21	Q	404	CLA	O2A-C1	-2.04	1.40	1.46
21	A	405	CLA	C1B-CHB	-2.04	1.34	1.40
21	N	616	CLA	O2A-C1	-2.03	1.40	1.46
21	N	618	CLA	O2A-C1	-2.03	1.40	1.46
21	P	501	CLA	O2A-C1	-2.03	1.40	1.46
21	P	503	CLA	C3B-C2B	-2.03	1.37	1.40
21	C	507	CLA	C1B-CHB	-2.03	1.34	1.40
21	B	606	CLA	CMB-C2B	-2.02	1.47	1.51
21	C	507	CLA	CMB-C2B	-2.02	1.47	1.51
21	C	503	CLA	C3B-C2B	-2.02	1.37	1.40
21	B	616	CLA	CMB-C2B	-2.02	1.47	1.51
21	N	610	CLA	C1B-CHB	-2.02	1.34	1.40
21	N	606	CLA	CMB-C2B	-2.02	1.47	1.51
21	D	401	CLA	O2A-C1	-2.01	1.40	1.46
21	C	502	CLA	CMB-C2B	-2.01	1.47	1.51
21	B	603	CLA	C1B-CHB	-2.01	1.34	1.40
21	B	607	CLA	C1B-CHB	-2.01	1.34	1.40
21	P	504	CLA	O2A-C1	-2.01	1.40	1.46
22	Q	403	PHO	C1A-NA	-2.01	1.33	1.37
21	N	609	CLA	C1B-CHB	-2.01	1.34	1.40
21	G	402	CLA	C1B-CHB	-2.01	1.34	1.40
21	A	401	CLA	C1B-CHB	-2.00	1.34	1.40
21	P	510	CLA	CMB-C2B	-2.00	1.47	1.51
21	B	614	CLA	O2A-C1	-2.00	1.40	1.46
21	P	508	CLA	C1B-CHB	-2.00	1.34	1.40
21	B	613	CLA	O2D-CGD	2.00	1.38	1.33
22	G	405	PHO	C4C-C3C	2.00	1.49	1.45
21	C	502	CLA	O2D-CGD	2.00	1.38	1.33
21	N	607	CLA	O2D-CGD	2.01	1.38	1.33
26	B	627	SQD	O6-C1	2.01	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	503	CLA	O2D-CGD	2.01	1.38	1.33
21	P	501	CLA	O2D-CGD	2.01	1.38	1.33
21	N	610	CLA	O2D-CGD	2.01	1.38	1.33
21	B	616	CLA	O2D-CGD	2.01	1.38	1.33
21	C	506	CLA	C5-C3	2.02	1.55	1.51
21	G	406	CLA	O2D-CGD	2.02	1.38	1.33
21	P	510	CLA	O2D-CGD	2.02	1.38	1.33
21	P	507	CLA	O2D-CGD	2.02	1.38	1.33
21	B	601	CLA	O2D-CGD	2.02	1.38	1.33
21	N	619	CLA	C5-C3	2.02	1.55	1.51
21	C	511	CLA	C5-C3	2.02	1.55	1.51
21	P	512	CLA	O2D-CGD	2.02	1.38	1.33
21	C	511	CLA	O2D-CGD	2.02	1.38	1.33
21	P	509	CLA	O2D-CGD	2.02	1.38	1.33
21	N	614	CLA	O2D-CGD	2.03	1.38	1.33
21	G	402	CLA	O2A-CGA	2.03	1.39	1.33
21	N	605	CLA	O2D-CGD	2.03	1.38	1.33
21	C	501	CLA	O2D-CGD	2.03	1.38	1.33
21	B	606	CLA	C5-C3	2.03	1.55	1.51
21	G	404	CLA	O2D-CGD	2.04	1.38	1.33
21	N	615	CLA	O2D-CGD	2.04	1.38	1.33
21	P	503	CLA	O2D-CGD	2.04	1.38	1.33
21	P	510	CLA	C5-C3	2.04	1.55	1.51
21	B	605	CLA	C5-C3	2.04	1.55	1.51
21	P	511	CLA	C5-C3	2.04	1.55	1.51
21	C	512	CLA	O2D-CGD	2.04	1.38	1.33
21	G	406	CLA	O2A-CGA	2.04	1.39	1.33
21	P	508	CLA	C5-C3	2.04	1.55	1.51
21	B	602	CLA	C5-C3	2.04	1.55	1.51
21	G	402	CLA	O2D-CGD	2.04	1.38	1.33
21	C	505	CLA	O2D-CGD	2.05	1.38	1.33
21	B	613	CLA	C5-C3	2.05	1.55	1.51
26	B	624	SQD	O6-C1	2.05	1.43	1.40
21	C	513	CLA	O2D-CGD	2.05	1.38	1.33
21	P	513	CLA	O2D-CGD	2.05	1.38	1.33
24	P	519	DGD	O3G-C1D	2.05	1.43	1.40
21	C	507	CLA	C5-C3	2.05	1.55	1.51
21	P	506	CLA	C5-C3	2.06	1.55	1.51
21	C	505	CLA	C5-C3	2.06	1.55	1.51
21	N	617	CLA	C5-C3	2.06	1.55	1.51
21	P	505	CLA	O2D-CGD	2.06	1.38	1.33
21	B	610	CLA	O2D-CGD	2.06	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	612	CLA	O2D-CGD	2.06	1.38	1.33
21	N	609	CLA	C5-C3	2.06	1.55	1.51
21	B	603	CLA	O2D-CGD	2.06	1.38	1.33
21	B	611	CLA	O2D-CGD	2.06	1.38	1.33
21	N	620	CLA	O2D-CGD	2.06	1.38	1.33
21	A	405	CLA	O2D-CGD	2.07	1.38	1.33
21	B	611	CLA	O2A-CGA	2.07	1.39	1.33
21	G	404	CLA	C5-C3	2.07	1.55	1.51
21	A	401	CLA	O2A-CGA	2.07	1.39	1.33
21	C	503	CLA	C5-C3	2.07	1.55	1.51
21	B	609	CLA	C5-C3	2.08	1.55	1.51
21	N	619	CLA	O2A-CGA	2.08	1.39	1.33
21	B	606	CLA	O2A-CGA	2.08	1.39	1.33
21	C	512	CLA	C5-C3	2.08	1.55	1.51
21	P	507	CLA	C5-C3	2.09	1.55	1.51
21	G	406	CLA	C5-C3	2.09	1.55	1.51
21	C	506	CLA	O2D-CGD	2.09	1.38	1.33
21	C	511	CLA	O2A-CGA	2.09	1.39	1.33
21	C	509	CLA	C5-C3	2.09	1.55	1.51
21	N	606	CLA	C5-C3	2.09	1.55	1.51
21	N	605	CLA	O2A-CGA	2.09	1.39	1.33
21	N	613	CLA	O2D-CGD	2.09	1.38	1.33
26	S	102	SQD	O6-C1	2.09	1.43	1.40
21	B	610	CLA	C5-C3	2.09	1.55	1.51
21	B	611	CLA	C5-C3	2.09	1.55	1.51
21	B	615	CLA	C5-C3	2.10	1.55	1.51
21	B	615	CLA	O2A-CGA	2.10	1.39	1.33
21	N	615	CLA	O2A-CGA	2.10	1.39	1.33
21	B	613	CLA	O2A-CGA	2.10	1.39	1.33
21	N	615	CLA	C5-C3	2.10	1.55	1.51
21	P	505	CLA	O2A-CGA	2.10	1.39	1.33
21	G	403	CLA	C5-C3	2.10	1.55	1.51
34	E	101	HEM	C4D-ND	2.10	1.39	1.36
21	N	613	CLA	C5-C3	2.10	1.55	1.51
21	N	617	CLA	O2D-CGD	2.10	1.38	1.33
21	C	507	CLA	O2A-CGA	2.10	1.39	1.33
21	C	513	CLA	C5-C3	2.10	1.55	1.51
21	P	506	CLA	O2D-CGD	2.11	1.38	1.33
26	Q	408	SQD	O6-C1	2.11	1.43	1.40
21	P	503	CLA	C5-C3	2.11	1.55	1.51
21	G	402	CLA	C5-C3	2.11	1.55	1.51
21	A	405	CLA	C5-C3	2.11	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	510	CLA	O2A-CGA	2.11	1.39	1.33
21	N	614	CLA	C5-C3	2.11	1.55	1.51
22	A	404	PHO	C4C-C3C	2.11	1.49	1.45
21	C	505	CLA	O2A-CGA	2.11	1.39	1.33
21	N	617	CLA	O2A-CGA	2.11	1.39	1.33
21	B	605	CLA	O2D-CGD	2.12	1.38	1.33
21	B	604	CLA	C5-C3	2.12	1.55	1.51
21	P	513	CLA	C5-C3	2.12	1.55	1.51
21	N	606	CLA	O2D-CGD	2.12	1.38	1.33
21	A	405	CLA	O2A-CGA	2.12	1.39	1.33
21	P	507	CLA	O2A-CGA	2.12	1.39	1.33
21	C	504	CLA	C5-C3	2.13	1.56	1.51
21	C	506	CLA	O2A-CGA	2.13	1.39	1.33
21	A	401	CLA	C5-C3	2.13	1.56	1.51
21	A	403	CLA	C5-C3	2.13	1.56	1.51
24	B	621	DGD	O5D-C1E	2.13	1.43	1.40
21	P	510	CLA	O2A-CGA	2.13	1.39	1.33
21	N	608	CLA	C5-C3	2.13	1.56	1.51
21	P	508	CLA	O2A-CGA	2.13	1.39	1.33
21	B	601	CLA	O2A-CGA	2.14	1.39	1.33
21	D	403	CLA	C5-C3	2.14	1.56	1.51
21	B	612	CLA	C5-C3	2.14	1.56	1.51
21	B	601	CLA	C5-C3	2.14	1.56	1.51
21	Q	404	CLA	C5-C3	2.14	1.56	1.51
21	P	509	CLA	C5-C3	2.14	1.56	1.51
21	A	402	CLA	C5-C3	2.14	1.56	1.51
23	G	407	PL9	C28-C29	2.14	1.38	1.33
21	B	609	CLA	O2D-CGD	2.14	1.38	1.33
21	P	511	CLA	O2A-CGA	2.14	1.39	1.33
21	N	609	CLA	O2D-CGD	2.14	1.38	1.33
21	B	616	CLA	O2A-CGA	2.14	1.39	1.33
21	B	612	CLA	O2A-CGA	2.14	1.39	1.33
21	A	401	CLA	O2D-CGD	2.15	1.38	1.33
21	N	605	CLA	C5-C3	2.15	1.56	1.51
21	N	613	CLA	O2A-CGA	2.15	1.39	1.33
21	N	614	CLA	O2A-CGA	2.15	1.39	1.33
21	P	512	CLA	C5-C3	2.15	1.56	1.51
21	C	508	CLA	C5-C3	2.16	1.56	1.51
21	P	509	CLA	O2A-CGA	2.16	1.39	1.33
23	A	406	PL9	C28-C29	2.16	1.38	1.33
21	B	616	CLA	C5-C3	2.16	1.56	1.51
21	C	508	CLA	O2A-CGA	2.16	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	PHO	C1D-C2D	2.16	1.50	1.45
21	G	403	CLA	O2A-CGA	2.16	1.39	1.33
21	N	610	CLA	C5-C3	2.16	1.56	1.51
21	N	610	CLA	O2A-CGA	2.16	1.39	1.33
21	P	506	CLA	O2A-CGA	2.17	1.39	1.33
21	C	501	CLA	C5-C3	2.17	1.56	1.51
21	A	402	CLA	O2A-CGA	2.17	1.39	1.33
21	B	608	CLA	C5-C3	2.17	1.56	1.51
21	Q	402	CLA	C5-C3	2.17	1.56	1.51
21	P	502	CLA	O2D-CGD	2.18	1.38	1.33
21	B	610	CLA	O2A-CGA	2.18	1.39	1.33
21	N	616	CLA	C3B-CAB	2.18	1.52	1.47
21	C	502	CLA	C5-C3	2.18	1.56	1.51
21	Q	402	CLA	O2A-CGA	2.18	1.39	1.33
21	G	404	CLA	O2A-CGA	2.18	1.39	1.33
21	B	609	CLA	O2A-CGA	2.19	1.39	1.33
21	P	502	CLA	C5-C3	2.19	1.56	1.51
21	C	509	CLA	O2A-CGA	2.19	1.39	1.33
21	P	501	CLA	C5-C3	2.19	1.56	1.51
22	Q	403	PHO	C1D-C2D	2.19	1.50	1.45
21	N	606	CLA	O2A-CGA	2.20	1.39	1.33
21	B	602	CLA	O2A-CGA	2.20	1.39	1.33
21	N	608	CLA	O2A-CGA	2.20	1.39	1.33
21	N	620	CLA	O2A-CGA	2.20	1.39	1.33
21	P	513	CLA	O2A-CGA	2.21	1.39	1.33
21	N	616	CLA	C5-C3	2.21	1.56	1.51
21	D	401	CLA	C5-C3	2.21	1.56	1.51
21	D	403	CLA	O2A-CGA	2.21	1.39	1.33
24	C	518	DGD	O3G-C1D	2.21	1.44	1.40
21	N	612	CLA	C5-C3	2.21	1.56	1.51
21	A	403	CLA	O2A-CGA	2.21	1.39	1.33
21	N	620	CLA	C5-C3	2.22	1.56	1.51
21	C	513	CLA	O2A-CGA	2.22	1.39	1.33
24	C	517	DGD	O5D-C1E	2.22	1.44	1.40
24	B	628	DGD	O5D-C1E	2.22	1.44	1.40
22	G	405	PHO	C1D-C2D	2.22	1.50	1.45
21	P	503	CLA	O2A-CGA	2.22	1.39	1.33
21	B	604	CLA	O2A-CGA	2.22	1.39	1.33
21	C	502	CLA	O2A-CGA	2.22	1.39	1.33
21	N	609	CLA	O2A-CGA	2.23	1.39	1.33
21	P	507	CLA	C3B-CAB	2.24	1.52	1.47
21	P	502	CLA	O2A-CGA	2.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	607	CLA	C5-C3	2.24	1.56	1.51
24	N	602	DGD	O5D-C1E	2.24	1.44	1.40
21	B	605	CLA	O2A-CGA	2.24	1.39	1.33
21	N	618	CLA	C5-C3	2.24	1.56	1.51
22	A	404	PHO	C3B-C4B	2.24	1.48	1.43
21	B	614	CLA	C5-C3	2.24	1.56	1.51
21	C	503	CLA	O2A-CGA	2.24	1.39	1.33
21	P	504	CLA	C5-C3	2.24	1.56	1.51
24	W	102	DGD	O5D-C1E	2.24	1.44	1.40
21	B	607	CLA	C5-C3	2.25	1.56	1.51
21	C	501	CLA	O2A-CGA	2.25	1.39	1.33
21	P	501	CLA	O2A-CGA	2.26	1.40	1.33
24	P	518	DGD	O5D-C1E	2.26	1.44	1.40
21	C	507	CLA	C3B-CAB	2.26	1.52	1.47
21	P	512	CLA	O2A-CGA	2.26	1.40	1.33
21	N	611	CLA	C5-C3	2.26	1.56	1.51
21	N	616	CLA	O2A-CGA	2.27	1.40	1.33
21	D	401	CLA	O2A-CGA	2.27	1.40	1.33
21	C	512	CLA	O2A-CGA	2.27	1.40	1.33
21	B	603	CLA	C5-C3	2.27	1.56	1.51
23	b	101	PL9	C28-C29	2.27	1.39	1.32
22	D	402	PHO	C1D-C2D	2.28	1.50	1.45
22	G	405	PHO	C3B-C4B	2.29	1.48	1.43
23	J	101	PL9	C28-C29	2.29	1.39	1.32
21	N	618	CLA	O2A-CGA	2.29	1.40	1.33
21	Q	404	CLA	O2A-CGA	2.30	1.40	1.33
21	B	614	CLA	O2A-CGA	2.30	1.40	1.33
21	N	612	CLA	O2A-CGA	2.31	1.40	1.33
21	B	608	CLA	O2A-CGA	2.32	1.40	1.33
24	P	519	DGD	O5D-C1E	2.33	1.44	1.40
23	Q	405	PL9	C28-C29	2.33	1.38	1.33
24	C	516	DGD	O5D-C1E	2.33	1.44	1.40
21	B	603	CLA	O2A-CGA	2.33	1.40	1.33
23	D	404	PL9	C28-C29	2.35	1.38	1.33
21	C	504	CLA	O2A-CGA	2.36	1.40	1.33
21	P	504	CLA	O2A-CGA	2.38	1.40	1.33
21	B	607	CLA	O2A-CGA	2.40	1.40	1.33
21	N	607	CLA	O2A-CGA	2.42	1.40	1.33
24	C	518	DGD	O5D-C1E	2.42	1.44	1.40
23	A	406	PL9	C8-C9	2.43	1.39	1.33
24	G	408	DGD	O5D-C1E	2.43	1.44	1.40
23	G	407	PL9	C18-C19	2.44	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	DGD	O5D-C1E	2.44	1.44	1.40
24	P	517	DGD	O5D-C1E	2.44	1.44	1.40
23	A	406	PL9	C18-C19	2.45	1.39	1.33
21	N	611	CLA	O2A-CGA	2.45	1.40	1.33
21	B	610	CLA	C3B-CAB	2.45	1.52	1.47
21	N	614	CLA	C3B-CAB	2.45	1.52	1.47
21	P	501	CLA	C3B-CAB	2.46	1.52	1.47
21	B	616	CLA	C3B-CAB	2.46	1.52	1.47
21	B	603	CLA	C3B-CAB	2.46	1.52	1.47
21	N	611	CLA	C3B-CAB	2.46	1.52	1.47
23	G	407	PL9	C8-C9	2.46	1.39	1.33
23	Q	405	PL9	C18-C19	2.46	1.39	1.33
21	C	505	CLA	C3B-CAB	2.46	1.52	1.47
21	C	501	CLA	C3B-CAB	2.46	1.52	1.47
21	G	404	CLA	C3B-CAB	2.47	1.52	1.47
21	G	402	CLA	C3B-CAB	2.48	1.52	1.47
21	B	609	CLA	C3B-CAB	2.48	1.52	1.47
23	G	407	PL9	C13-C14	2.48	1.39	1.33
21	C	509	CLA	C3B-CAB	2.48	1.52	1.47
21	N	620	CLA	C3B-CAB	2.49	1.52	1.47
21	B	608	CLA	C3B-CAB	2.49	1.52	1.47
23	A	406	PL9	C13-C14	2.49	1.39	1.33
21	N	609	CLA	C3B-CAB	2.49	1.52	1.47
22	D	402	PHO	C3B-C4B	2.50	1.48	1.43
22	Q	403	PHO	C3B-C4B	2.50	1.48	1.43
21	A	403	CLA	C3B-CAB	2.50	1.52	1.47
21	A	401	CLA	C3B-CAB	2.50	1.52	1.47
21	B	607	CLA	C3B-CAB	2.51	1.52	1.47
21	B	605	CLA	C3B-CAB	2.51	1.52	1.47
21	B	604	CLA	C3B-CAB	2.51	1.52	1.47
21	N	613	CLA	C3B-CAB	2.51	1.52	1.47
21	C	513	CLA	C3B-CAB	2.52	1.52	1.47
21	C	504	CLA	C3B-CAB	2.52	1.52	1.47
21	C	502	CLA	C3B-CAB	2.52	1.52	1.47
21	Q	404	CLA	C3B-CAB	2.52	1.52	1.47
21	N	617	CLA	C3B-CAB	2.53	1.52	1.47
23	D	404	PL9	C8-C9	2.53	1.39	1.33
21	C	512	CLA	C3B-CAB	2.53	1.52	1.47
21	P	502	CLA	C3B-CAB	2.53	1.52	1.47
21	B	611	CLA	C3B-CAB	2.54	1.52	1.47
21	N	605	CLA	C3B-CAB	2.54	1.52	1.47
21	B	606	CLA	C3B-CAB	2.54	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	607	CLA	C3B-CAB	2.54	1.52	1.47
21	D	403	CLA	C3B-CAB	2.54	1.52	1.47
21	P	506	CLA	C3B-CAB	2.55	1.52	1.47
23	D	404	PL9	C18-C19	2.55	1.39	1.33
21	C	511	CLA	C3B-CAB	2.55	1.52	1.47
21	P	509	CLA	C3B-CAB	2.55	1.53	1.47
21	B	613	CLA	C3B-CAB	2.55	1.53	1.47
23	G	407	PL9	C23-C24	2.55	1.39	1.33
21	N	612	CLA	C3B-CAB	2.56	1.53	1.47
23	D	404	PL9	C13-C14	2.56	1.39	1.33
21	N	608	CLA	C3B-CAB	2.56	1.53	1.47
21	C	506	CLA	C3B-CAB	2.56	1.53	1.47
21	P	513	CLA	C3B-CAB	2.56	1.53	1.47
23	Q	405	PL9	C13-C14	2.56	1.39	1.33
23	Q	405	PL9	C8-C9	2.57	1.39	1.33
23	A	406	PL9	C23-C24	2.57	1.39	1.33
21	P	512	CLA	C3B-CAB	2.57	1.53	1.47
21	C	510	CLA	C3B-CAB	2.57	1.53	1.47
23	b	101	PL9	C18-C19	2.57	1.39	1.33
23	J	101	PL9	C18-C19	2.58	1.39	1.33
21	P	505	CLA	C3B-CAB	2.58	1.53	1.47
21	P	511	CLA	C3B-CAB	2.58	1.53	1.47
21	B	612	CLA	C3B-CAB	2.58	1.53	1.47
21	A	405	CLA	C3B-CAB	2.59	1.53	1.47
21	G	406	CLA	C3B-CAB	2.59	1.53	1.47
21	P	504	CLA	C3B-CAB	2.60	1.53	1.47
21	N	619	CLA	C3B-CAB	2.60	1.53	1.47
23	J	101	PL9	C8-C9	2.61	1.39	1.33
21	N	615	CLA	C3B-CAB	2.61	1.53	1.47
21	P	510	CLA	C3B-CAB	2.61	1.53	1.47
34	V	201	HEM	C4D-ND	2.61	1.39	1.36
21	C	508	CLA	C3B-CAB	2.61	1.53	1.47
23	J	101	PL9	C13-C14	2.62	1.39	1.33
21	B	601	CLA	C3B-CAB	2.62	1.53	1.47
21	N	606	CLA	C3B-CAB	2.62	1.53	1.47
21	P	508	CLA	C3B-CAB	2.62	1.53	1.47
21	B	614	CLA	C3B-CAB	2.63	1.53	1.47
21	B	602	CLA	C3B-CAB	2.64	1.53	1.47
23	b	101	PL9	C13-C14	2.64	1.39	1.33
23	b	101	PL9	C8-C9	2.64	1.39	1.33
34	i	201	HEM	C4D-ND	2.64	1.39	1.36
23	Q	405	PL9	C23-C24	2.64	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	615	CLA	C3B-CAB	2.65	1.53	1.47
21	N	610	CLA	C3B-CAB	2.65	1.53	1.47
23	D	404	PL9	C23-C24	2.66	1.39	1.33
23	b	101	PL9	C23-C24	2.67	1.39	1.33
21	A	402	CLA	C3B-CAB	2.68	1.53	1.47
21	G	403	CLA	C3B-CAB	2.68	1.53	1.47
21	P	503	CLA	C3B-CAB	2.70	1.53	1.47
21	C	503	CLA	C3B-CAB	2.72	1.53	1.47
21	N	618	CLA	C3B-CAB	2.72	1.53	1.47
23	J	101	PL9	C23-C24	2.75	1.39	1.33
22	A	404	PHO	C3D-C2D	2.77	1.46	1.38
22	G	405	PHO	C3D-C2D	2.81	1.46	1.38
21	Q	402	CLA	C3B-CAB	2.81	1.53	1.47
21	N	613	CLA	C4C-C3C	2.83	1.50	1.45
21	D	401	CLA	C3B-CAB	2.85	1.53	1.47
21	B	612	CLA	C4C-C3C	2.85	1.50	1.45
21	N	609	CLA	C4C-C3C	2.86	1.50	1.45
21	B	611	CLA	C2-C3	2.87	1.40	1.33
23	D	404	PL9	C43-C44	2.87	1.40	1.33
22	D	402	PHO	C3D-C2D	2.88	1.46	1.38
21	C	502	CLA	C4C-C3C	2.89	1.50	1.45
21	N	615	CLA	C2-C3	2.90	1.40	1.33
21	B	613	CLA	C2-C3	2.90	1.40	1.33
23	Q	405	PL9	C43-C44	2.91	1.40	1.33
21	P	505	CLA	C2-C3	2.91	1.40	1.33
21	C	507	CLA	C2-C3	2.91	1.40	1.33
21	G	406	CLA	C2-C3	2.92	1.40	1.33
21	B	603	CLA	C4C-C3C	2.92	1.50	1.45
21	C	505	CLA	C2-C3	2.93	1.40	1.33
21	B	605	CLA	C4C-C3C	2.94	1.50	1.45
21	P	510	CLA	C2-C3	2.94	1.40	1.33
21	N	607	CLA	C4C-C3C	2.94	1.50	1.45
21	B	606	CLA	C2-C3	2.94	1.40	1.33
21	G	406	CLA	C4C-C3C	2.95	1.50	1.45
21	N	619	CLA	C2-C3	2.95	1.40	1.33
21	G	404	CLA	C2-C3	2.95	1.40	1.33
21	C	506	CLA	C4C-C3C	2.95	1.50	1.45
21	C	507	CLA	C4C-C3C	2.95	1.50	1.45
21	C	508	CLA	C4C-C3C	2.96	1.50	1.45
21	P	507	CLA	C2-C3	2.96	1.40	1.33
21	G	402	CLA	C2-C3	2.96	1.40	1.33
21	N	617	CLA	C2-C3	2.96	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	508	CLA	C4C-C3C	2.97	1.50	1.45
21	P	508	CLA	C2-C3	2.97	1.40	1.33
21	N	613	CLA	C2-C3	2.97	1.40	1.33
21	C	510	CLA	C4C-C3C	2.97	1.50	1.45
21	C	511	CLA	C2-C3	2.97	1.40	1.33
23	A	406	PL9	C38-C39	2.97	1.41	1.32
21	N	616	CLA	C4C-C3C	2.97	1.50	1.45
21	B	616	CLA	C4C-C3C	2.97	1.50	1.45
21	B	615	CLA	C2-C3	2.98	1.40	1.33
21	B	608	CLA	C4C-C3C	2.98	1.50	1.45
21	P	502	CLA	C4C-C3C	2.98	1.50	1.45
21	B	602	CLA	C2-C3	2.98	1.40	1.33
21	B	613	CLA	C4C-C3C	2.98	1.50	1.45
22	Q	403	PHO	C3D-C2D	2.98	1.46	1.38
21	G	403	CLA	C2-C3	2.99	1.40	1.33
21	C	510	CLA	C2-C3	2.99	1.40	1.33
21	P	506	CLA	C4C-C3C	2.99	1.50	1.45
21	A	405	CLA	C4C-C3C	2.99	1.50	1.45
21	A	401	CLA	C2-C3	3.00	1.40	1.33
21	B	609	CLA	C4C-C3C	3.00	1.50	1.45
21	A	401	CLA	C4C-C3C	3.00	1.50	1.45
21	A	402	CLA	C2-C3	3.01	1.40	1.33
21	P	510	CLA	C4C-C3C	3.01	1.50	1.45
21	C	508	CLA	C2-C3	3.01	1.40	1.33
21	C	512	CLA	C4C-C3C	3.01	1.50	1.45
21	N	606	CLA	C4C-C3C	3.01	1.50	1.45
21	N	615	CLA	C4C-C3C	3.01	1.50	1.45
21	P	513	CLA	C2-C3	3.02	1.40	1.33
21	C	503	CLA	C4C-C3C	3.02	1.50	1.45
21	D	403	CLA	C4C-C3C	3.02	1.50	1.45
21	N	612	CLA	C4C-C3C	3.02	1.50	1.45
21	P	506	CLA	C2-C3	3.02	1.40	1.33
21	A	405	CLA	C2-C3	3.02	1.40	1.33
21	N	617	CLA	C4C-C3C	3.02	1.50	1.45
21	A	403	CLA	C2-C3	3.02	1.40	1.33
23	G	407	PL9	C38-C39	3.02	1.41	1.32
21	B	612	CLA	C2-C3	3.02	1.40	1.33
21	C	502	CLA	C2-C3	3.03	1.40	1.33
21	B	609	CLA	C2-C3	3.03	1.40	1.33
21	N	619	CLA	C4C-C3C	3.03	1.50	1.45
21	N	606	CLA	C2-C3	3.03	1.40	1.33
21	P	503	CLA	C2-C3	3.03	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	503	CLA	C4C-C3C	3.03	1.50	1.45
21	C	513	CLA	C4C-C3C	3.03	1.50	1.45
21	C	503	CLA	C2-C3	3.03	1.40	1.33
21	P	507	CLA	C4C-C3C	3.04	1.50	1.45
21	Q	404	CLA	C4C-C3C	3.04	1.50	1.45
21	C	511	CLA	C4C-C3C	3.04	1.50	1.45
23	Q	405	PL9	C33-C34	3.04	1.40	1.33
21	Q	402	CLA	C4C-C3C	3.04	1.50	1.45
21	B	611	CLA	C4C-C3C	3.04	1.50	1.45
23	D	404	PL9	C33-C34	3.04	1.40	1.33
21	C	506	CLA	C2-C3	3.05	1.40	1.33
21	P	511	CLA	C2-C3	3.05	1.40	1.33
21	N	609	CLA	C2-C3	3.05	1.40	1.33
21	N	620	CLA	C4C-C3C	3.05	1.50	1.45
21	B	601	CLA	C2-C3	3.05	1.40	1.33
21	N	605	CLA	C2-C3	3.05	1.40	1.33
21	B	610	CLA	C2-C3	3.05	1.40	1.33
21	D	401	CLA	C4C-C3C	3.05	1.50	1.45
21	B	616	CLA	C2-C3	3.05	1.40	1.33
21	N	610	CLA	C2-C3	3.05	1.40	1.33
21	C	509	CLA	C2-C3	3.05	1.40	1.33
21	N	614	CLA	C2-C3	3.05	1.40	1.33
21	C	501	CLA	C2-C3	3.06	1.40	1.33
21	B	605	CLA	C2-C3	3.06	1.40	1.33
21	B	607	CLA	C4C-C3C	3.06	1.50	1.45
21	Q	404	CLA	C2-C3	3.06	1.40	1.33
21	P	512	CLA	C2-C3	3.06	1.40	1.33
21	C	512	CLA	C2-C3	3.06	1.40	1.33
21	D	403	CLA	C2-C3	3.06	1.40	1.33
21	B	602	CLA	C4C-C3C	3.06	1.50	1.45
21	P	511	CLA	C4C-C3C	3.07	1.50	1.45
21	Q	402	CLA	C2-C3	3.07	1.40	1.33
21	N	618	CLA	C2-C3	3.07	1.40	1.33
21	B	614	CLA	C2-C3	3.08	1.40	1.33
23	D	404	PL9	C38-C39	3.08	1.40	1.33
21	N	608	CLA	C2-C3	3.08	1.40	1.33
21	P	509	CLA	C2-C3	3.08	1.40	1.33
21	P	501	CLA	C2-C3	3.09	1.40	1.33
21	P	512	CLA	C4C-C3C	3.09	1.50	1.45
21	C	513	CLA	C2-C3	3.10	1.40	1.33
21	C	504	CLA	C4C-C3C	3.10	1.50	1.45
21	N	620	CLA	C2-C3	3.10	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	502	CLA	C2-C3	3.10	1.40	1.33
21	P	504	CLA	C4C-C3C	3.10	1.50	1.45
21	G	402	CLA	C4C-C3C	3.12	1.50	1.45
21	C	504	CLA	C2-C3	3.12	1.40	1.33
21	P	509	CLA	C4C-C3C	3.12	1.50	1.45
21	D	401	CLA	C2-C3	3.13	1.40	1.33
21	B	604	CLA	C2-C3	3.13	1.40	1.33
21	P	513	CLA	C4C-C3C	3.13	1.50	1.45
21	N	616	CLA	C2-C3	3.13	1.40	1.33
21	B	606	CLA	C4C-C3C	3.13	1.50	1.45
23	Q	405	PL9	C38-C39	3.13	1.40	1.33
21	P	505	CLA	C4C-C3C	3.14	1.50	1.45
21	P	501	CLA	C4C-C3C	3.14	1.50	1.45
21	N	608	CLA	C4C-C3C	3.14	1.50	1.45
21	G	403	CLA	C1C-C2C	3.15	1.50	1.44
21	B	610	CLA	C4C-C3C	3.15	1.50	1.45
21	N	614	CLA	C4C-C3C	3.15	1.50	1.45
21	C	501	CLA	C4C-C3C	3.15	1.50	1.45
23	G	407	PL9	C33-C34	3.16	1.40	1.33
21	N	612	CLA	C2-C3	3.17	1.40	1.33
21	B	615	CLA	C4C-C3C	3.17	1.50	1.45
21	C	509	CLA	C4C-C3C	3.17	1.50	1.45
21	C	505	CLA	C4C-C3C	3.18	1.50	1.45
21	B	604	CLA	C4C-C3C	3.18	1.50	1.45
21	N	618	CLA	C4C-C3C	3.18	1.50	1.45
21	N	611	CLA	C4C-C3C	3.18	1.50	1.45
21	N	611	CLA	C2-C3	3.19	1.40	1.33
23	A	406	PL9	C33-C34	3.19	1.41	1.33
21	N	605	CLA	C1C-C2C	3.20	1.50	1.44
21	B	608	CLA	C2-C3	3.20	1.41	1.33
21	G	404	CLA	C4C-C3C	3.20	1.50	1.45
34	V	201	HEM	C3B-CAB	3.20	1.54	1.47
21	N	610	CLA	C4C-C3C	3.21	1.50	1.45
21	A	403	CLA	C4C-C3C	3.21	1.50	1.45
21	P	504	CLA	C2-C3	3.21	1.41	1.33
21	N	607	CLA	C2-C3	3.23	1.41	1.33
21	B	607	CLA	C2-C3	3.23	1.41	1.33
21	B	603	CLA	C2-C3	3.23	1.41	1.33
21	B	614	CLA	C4C-C3C	3.25	1.50	1.45
21	B	601	CLA	C1C-C2C	3.25	1.50	1.44
21	N	605	CLA	C4C-C3C	3.25	1.50	1.45
22	Q	403	PHO	CHB-C4A	3.25	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	601	CLA	C4C-C3C	3.27	1.50	1.45
34	i	201	HEM	C3B-CAB	3.29	1.54	1.47
21	A	402	CLA	C1C-C2C	3.30	1.50	1.44
21	G	403	CLA	C4C-C3C	3.31	1.50	1.45
21	A	402	CLA	C4C-C3C	3.32	1.50	1.45
22	D	402	PHO	CHB-C4A	3.35	1.48	1.40
21	B	616	CLA	C1C-C2C	3.35	1.51	1.44
22	G	405	PHO	CHB-C4A	3.38	1.48	1.40
21	N	620	CLA	C1C-C2C	3.39	1.51	1.44
22	A	404	PHO	CHB-C4A	3.42	1.48	1.40
22	Q	403	PHO	CHD-C4C	3.43	1.48	1.40
22	A	404	PHO	OBD-CAD	3.44	1.28	1.22
21	P	504	CLA	C1C-C2C	3.46	1.51	1.44
22	A	404	PHO	CHD-C4C	3.46	1.48	1.40
22	G	405	PHO	CHD-C4C	3.46	1.48	1.40
34	E	101	HEM	C3B-CAB	3.48	1.54	1.47
21	N	608	CLA	C1C-C2C	3.48	1.51	1.44
22	D	402	PHO	CHD-C4C	3.49	1.48	1.40
21	G	404	CLA	C1C-C2C	3.49	1.51	1.44
21	C	502	CLA	C1C-C2C	3.49	1.51	1.44
21	C	504	CLA	C1C-C2C	3.50	1.51	1.44
21	G	406	CLA	C1C-C2C	3.50	1.51	1.44
34	R	101	HEM	C3B-CAB	3.51	1.54	1.47
22	G	405	PHO	OBD-CAD	3.51	1.28	1.22
21	N	615	CLA	C1C-C2C	3.52	1.51	1.44
21	B	607	CLA	C1C-C2C	3.52	1.51	1.44
22	Q	403	PHO	OBD-CAD	3.52	1.28	1.22
21	C	506	CLA	C1C-C2C	3.53	1.51	1.44
21	A	403	CLA	C1C-C2C	3.54	1.51	1.44
22	D	402	PHO	OBD-CAD	3.54	1.28	1.22
21	P	507	CLA	C1C-C2C	3.54	1.51	1.44
21	P	502	CLA	C1C-C2C	3.54	1.51	1.44
22	G	405	PHO	CHC-C4B	3.54	1.48	1.40
21	B	605	CLA	C1C-C2C	3.55	1.51	1.44
21	C	501	CLA	C1C-C2C	3.55	1.51	1.44
21	N	619	CLA	C1C-C2C	3.56	1.51	1.44
21	C	507	CLA	C1C-C2C	3.56	1.51	1.44
21	N	611	CLA	C1C-C2C	3.57	1.51	1.44
21	A	405	CLA	C1C-C2C	3.58	1.51	1.44
22	A	404	PHO	CHC-C4B	3.58	1.49	1.40
21	A	401	CLA	C1C-C2C	3.58	1.51	1.44
21	B	611	CLA	C1C-C2C	3.58	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	604	CLA	C1C-C2C	3.58	1.51	1.44
21	P	509	CLA	C1C-C2C	3.59	1.51	1.44
21	P	501	CLA	C1C-C2C	3.59	1.51	1.44
21	C	511	CLA	C1C-C2C	3.59	1.51	1.44
21	N	609	CLA	C1C-C2C	3.60	1.51	1.44
21	B	613	CLA	C1C-C2C	3.60	1.51	1.44
21	C	503	CLA	C1C-C2C	3.60	1.51	1.44
21	B	615	CLA	C1C-C2C	3.61	1.51	1.44
21	C	509	CLA	C1C-C2C	3.61	1.51	1.44
21	B	614	CLA	C1C-C2C	3.62	1.51	1.44
21	N	612	CLA	C1C-C2C	3.62	1.51	1.44
21	P	510	CLA	C1C-C2C	3.63	1.51	1.44
21	P	512	CLA	C1C-C2C	3.63	1.51	1.44
21	C	510	CLA	C1C-C2C	3.64	1.51	1.44
21	D	403	CLA	C1C-C2C	3.64	1.51	1.44
22	D	402	PHO	CHC-C4B	3.64	1.49	1.40
21	P	503	CLA	C1C-C2C	3.64	1.51	1.44
22	Q	403	PHO	CHC-C4B	3.64	1.49	1.40
21	B	606	CLA	C1C-C2C	3.65	1.51	1.44
21	C	508	CLA	C1C-C2C	3.65	1.51	1.44
21	B	608	CLA	C1C-C2C	3.65	1.51	1.44
21	N	618	CLA	C1C-C2C	3.65	1.51	1.44
21	P	508	CLA	C1C-C2C	3.66	1.51	1.44
21	N	614	CLA	C1C-C2C	3.67	1.51	1.44
21	C	512	CLA	C1C-C2C	3.67	1.51	1.44
21	B	612	CLA	C1C-C2C	3.68	1.51	1.44
21	N	610	CLA	C1C-C2C	3.68	1.51	1.44
21	N	613	CLA	C1C-C2C	3.68	1.51	1.44
21	B	602	CLA	C1C-C2C	3.69	1.51	1.44
21	N	607	CLA	C1C-C2C	3.70	1.51	1.44
21	P	513	CLA	C1C-C2C	3.70	1.51	1.44
21	P	506	CLA	C1C-C2C	3.70	1.51	1.44
21	N	606	CLA	C1C-C2C	3.70	1.51	1.44
21	B	603	CLA	C1C-C2C	3.70	1.51	1.44
21	C	513	CLA	C1C-C2C	3.71	1.51	1.44
21	D	401	CLA	C1C-C2C	3.71	1.51	1.44
21	P	511	CLA	C1C-C2C	3.72	1.51	1.44
21	B	610	CLA	C1C-C2C	3.73	1.51	1.44
21	Q	404	CLA	C1C-C2C	3.73	1.51	1.44
34	i	201	HEM	C3C-CAC	3.74	1.55	1.47
21	N	617	CLA	C1C-C2C	3.75	1.51	1.44
21	P	505	CLA	C1C-C2C	3.76	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	402	CLA	C1C-C2C	3.77	1.51	1.44
21	Q	402	CLA	C1C-C2C	3.79	1.51	1.44
34	V	201	HEM	C3C-CAC	3.80	1.55	1.47
27	P	520	LMG	O7-C10	3.82	1.45	1.34
34	R	101	HEM	C3C-CAC	3.82	1.55	1.47
27	C	519	LMG	O7-C10	3.82	1.45	1.34
21	B	609	CLA	C1C-C2C	3.83	1.51	1.44
21	C	505	CLA	C1C-C2C	3.84	1.51	1.44
21	N	616	CLA	C1C-C2C	3.85	1.52	1.44
34	E	101	HEM	C3C-CAC	3.87	1.55	1.47
26	A	409	SQD	O47-C7	3.91	1.45	1.34
26	G	410	SQD	O47-C7	3.93	1.45	1.34
27	D	407	LMG	O7-C10	3.93	1.45	1.34
26	B	627	SQD	O47-C7	3.94	1.45	1.34
24	W	102	DGD	O2G-C1B	3.95	1.45	1.34
26	N	601	SQD	O47-C7	3.95	1.45	1.34
27	Q	407	LMG	O7-C10	3.96	1.45	1.34
27	N	622	LMG	O7-C10	3.96	1.45	1.34
24	B	621	DGD	O2G-C1B	3.98	1.45	1.34
27	a	102	LMG	O7-C10	3.98	1.45	1.34
24	P	518	DGD	O2G-C1B	3.98	1.45	1.34
27	B	622	LMG	O7-C10	3.98	1.45	1.34
26	B	624	SQD	O47-C7	4.00	1.45	1.34
27	I	102	LMG	O7-C10	4.01	1.45	1.34
26	G	401	SQD	O47-C7	4.01	1.45	1.34
25	A	411	LHG	O7-C7	4.01	1.45	1.34
26	F	101	SQD	O47-C7	4.01	1.45	1.34
26	Q	408	SQD	O47-C7	4.02	1.46	1.34
27	D	406	LMG	O7-C10	4.02	1.46	1.34
24	C	516	DGD	O2G-C1B	4.03	1.46	1.34
26	A	414	SQD	O47-C7	4.03	1.46	1.34
25	G	412	LHG	O7-C7	4.05	1.46	1.34
27	N	623	LMG	O7-C10	4.05	1.46	1.34
27	N	622	LMG	O8-C28	4.05	1.45	1.33
27	Q	406	LMG	O7-C10	4.05	1.46	1.34
25	G	409	LHG	O7-C7	4.06	1.46	1.34
27	B	623	LMG	O7-C10	4.06	1.46	1.34
24	C	517	DGD	O2G-C1B	4.06	1.46	1.34
22	Q	403	PHO	O2A-CGA	4.07	1.45	1.33
27	B	622	LMG	O8-C28	4.08	1.45	1.33
27	D	412	LMG	O7-C10	4.08	1.46	1.34
27	Q	401	LMG	O7-C10	4.09	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	102	SQD	O47-C7	4.11	1.46	1.34
25	A	408	LHG	O7-C7	4.12	1.46	1.34
24	P	517	DGD	O2G-C1B	4.12	1.46	1.34
27	M	101	LMG	O8-C28	4.12	1.45	1.33
24	N	602	DGD	O2G-C1B	4.12	1.46	1.34
24	P	519	DGD	O2G-C1B	4.12	1.46	1.34
24	B	628	DGD	O2G-C1B	4.12	1.46	1.34
27	R	102	LMG	O8-C28	4.12	1.45	1.33
24	A	407	DGD	O1G-C1A	4.12	1.45	1.33
27	e	102	LMG	O7-C10	4.13	1.46	1.34
24	G	408	DGD	O1G-C1A	4.13	1.45	1.33
22	G	405	PHO	O2A-CGA	4.13	1.45	1.33
22	D	402	PHO	O2A-CGA	4.13	1.45	1.33
27	D	412	LMG	O8-C28	4.14	1.45	1.33
24	C	518	DGD	O2G-C1B	4.15	1.46	1.34
26	F	101	SQD	O48-C23	4.15	1.45	1.33
27	Q	401	LMG	O8-C28	4.16	1.45	1.33
27	D	407	LMG	O8-C28	4.17	1.45	1.33
24	P	517	DGD	O1G-C1A	4.18	1.45	1.33
25	A	411	LHG	O8-C23	4.18	1.45	1.33
24	C	516	DGD	O1G-C1A	4.18	1.45	1.33
26	S	102	SQD	O48-C23	4.19	1.45	1.33
27	e	102	LMG	O8-C28	4.19	1.45	1.33
27	M	101	LMG	O7-C10	4.19	1.46	1.34
24	P	519	DGD	O1G-C1A	4.20	1.45	1.33
27	R	102	LMG	O7-C10	4.20	1.46	1.34
24	G	408	DGD	O2G-C1B	4.20	1.46	1.34
27	Q	407	LMG	O8-C28	4.20	1.45	1.33
27	D	406	LMG	O8-C28	4.21	1.45	1.33
27	G	411	LMG	O8-C28	4.21	1.45	1.33
25	G	412	LHG	O8-C23	4.21	1.45	1.33
26	G	401	SQD	O48-C23	4.22	1.45	1.33
27	P	521	LMG	O7-C10	4.22	1.46	1.34
27	A	410	LMG	O8-C28	4.23	1.45	1.33
27	B	623	LMG	O8-C28	4.23	1.45	1.33
26	A	414	SQD	O48-C23	4.24	1.45	1.33
22	A	404	PHO	O2A-CGA	4.24	1.45	1.33
24	B	621	DGD	O1G-C1A	4.24	1.45	1.33
27	Q	406	LMG	O8-C28	4.24	1.45	1.33
27	N	623	LMG	O8-C28	4.24	1.45	1.33
27	I	102	LMG	O8-C28	4.24	1.45	1.33
27	A	410	LMG	O7-C10	4.24	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	E	102	LMG	O8-C28	4.25	1.45	1.33
24	C	518	DGD	O1G-C1A	4.25	1.45	1.33
27	a	102	LMG	O8-C28	4.26	1.45	1.33
27	E	102	LMG	O7-C10	4.27	1.46	1.34
24	A	407	DGD	O2G-C1B	4.28	1.46	1.34
25	A	408	LHG	O8-C23	4.28	1.45	1.33
26	G	410	SQD	O48-C23	4.28	1.45	1.33
24	D	408	DGD	O2G-C1B	4.28	1.46	1.34
27	G	411	LMG	O7-C10	4.29	1.46	1.34
26	B	624	SQD	O48-C23	4.29	1.46	1.33
26	B	627	SQD	O48-C23	4.29	1.46	1.33
26	N	601	SQD	O48-C23	4.29	1.46	1.33
27	C	520	LMG	O7-C10	4.29	1.46	1.34
25	G	409	LHG	O8-C23	4.30	1.46	1.33
26	Q	408	SQD	O48-C23	4.31	1.46	1.33
24	Q	409	DGD	O2G-C1B	4.31	1.46	1.34
24	W	102	DGD	O1G-C1A	4.31	1.46	1.33
26	A	409	SQD	O48-C23	4.31	1.46	1.33
24	P	518	DGD	O1G-C1A	4.32	1.46	1.33
24	B	628	DGD	O1G-C1A	4.32	1.46	1.33
24	C	517	DGD	O1G-C1A	4.33	1.46	1.33
24	Q	409	DGD	O1G-C1A	4.35	1.46	1.33
24	D	408	DGD	O1G-C1A	4.35	1.46	1.33
27	P	520	LMG	O8-C28	4.37	1.46	1.33
24	N	602	DGD	O1G-C1A	4.38	1.46	1.33
27	C	520	LMG	O8-C28	4.43	1.46	1.33
27	P	521	LMG	O8-C28	4.44	1.46	1.33
27	C	519	LMG	O8-C28	4.45	1.46	1.33
22	A	404	PHO	O2D-CGD	4.70	1.45	1.33
26	N	601	SQD	O8-S	4.70	1.63	1.47
26	B	627	SQD	O8-S	4.72	1.63	1.47
26	A	409	SQD	O8-S	4.74	1.63	1.47
26	A	414	SQD	O8-S	4.75	1.63	1.47
26	S	102	SQD	O8-S	4.76	1.63	1.47
26	B	624	SQD	O8-S	4.79	1.63	1.47
26	F	101	SQD	O8-S	4.79	1.63	1.47
22	G	405	PHO	O2D-CGD	4.79	1.45	1.33
26	Q	408	SQD	O8-S	4.79	1.63	1.47
26	G	410	SQD	O8-S	4.79	1.63	1.47
26	G	401	SQD	O8-S	4.80	1.63	1.47
22	Q	403	PHO	CHD-C1D	4.84	1.48	1.38
22	G	405	PHO	CHD-C1D	4.84	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	PHO	CHD-C1D	4.84	1.48	1.38
22	D	402	PHO	CHD-C1D	4.96	1.48	1.38
22	Q	403	PHO	O2D-CGD	4.96	1.45	1.33
22	D	402	PHO	O2D-CGD	4.98	1.45	1.33
22	G	405	PHO	CHC-C1C	5.13	1.48	1.38
22	A	404	PHO	CHC-C1C	5.21	1.48	1.38
22	D	402	PHO	C3C-C2C	5.21	1.47	1.36
22	Q	403	PHO	C3C-C2C	5.24	1.48	1.36
22	D	402	PHO	CHC-C1C	5.25	1.49	1.38
22	A	404	PHO	C3C-C2C	5.27	1.48	1.36
22	Q	403	PHO	CHC-C1C	5.31	1.49	1.38
22	G	405	PHO	C3C-C2C	5.31	1.48	1.36
34	R	101	HEM	C3D-C2D	5.34	1.53	1.37
34	E	101	HEM	C3D-C2D	5.39	1.53	1.37
34	V	201	HEM	C3D-C2D	5.45	1.53	1.37
34	i	201	HEM	C3D-C2D	5.46	1.53	1.37
22	A	404	PHO	C3B-C2B	5.50	1.47	1.37
22	G	405	PHO	C3B-C2B	5.50	1.47	1.37
22	D	402	PHO	C3B-C2B	5.51	1.47	1.37
22	Q	403	PHO	CHB-C1B	5.58	1.49	1.38
22	Q	403	PHO	C3B-C2B	5.59	1.47	1.37
22	D	402	PHO	CHB-C1B	5.59	1.49	1.38
22	G	405	PHO	CHB-C1B	5.63	1.49	1.38
22	A	404	PHO	CHB-C1B	5.73	1.49	1.38

All (1524) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	102	BCR	C32-C1-C6	-13.48	88.45	110.31
30	J	102	BCR	C32-C1-C6	-13.41	88.56	110.31
30	b	102	BCR	C32-C1-C31	-8.53	82.38	108.50
30	J	102	BCR	C32-C1-C31	-8.51	82.42	108.50
30	T	102	BCR	C7-C8-C9	-6.87	115.89	126.21
30	B	618	BCR	C7-C8-C9	-6.81	115.99	126.21
34	R	101	HEM	CBD-CAD-C3D	-6.46	100.15	112.47
30	S	101	BCR	C7-C8-C9	-5.96	117.26	126.21
30	D	405	BCR	C7-C8-C9	-5.81	117.48	126.21
34	V	201	HEM	CBD-CAD-C3D	-5.51	101.96	112.47
34	i	201	HEM	CBD-CAD-C3D	-5.47	102.03	112.47
34	E	101	HEM	CBD-CAD-C3D	-5.39	102.19	112.47
30	J	102	BCR	C32-C1-C2	-5.28	87.99	108.80
30	b	102	BCR	C32-C1-C2	-5.26	88.04	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	P	514	BCR	C33-C5-C6	-4.70	119.25	124.51
30	b	102	BCR	C15-C14-C13	-4.68	120.63	127.31
30	b	102	BCR	C24-C23-C22	-4.63	119.26	126.21
30	J	102	BCR	C15-C14-C13	-4.60	120.74	127.31
30	b	102	BCR	C20-C21-C22	-4.59	120.75	127.31
30	J	102	BCR	C24-C23-C22	-4.46	119.51	126.21
30	J	102	BCR	C20-C21-C22	-4.40	121.03	127.31
30	C	514	BCR	C33-C5-C6	-4.38	119.60	124.51
30	T	102	BCR	C28-C27-C26	-4.15	106.64	113.78
30	T	103	BCR	C24-C23-C22	-4.14	119.99	126.21
30	B	618	BCR	C28-C27-C26	-4.12	106.69	113.78
30	P	516	BCR	C7-C8-C9	-4.11	120.04	126.21
30	P	516	BCR	C28-C27-C26	-4.05	106.82	113.78
30	K	101	BCR	C38-C26-C25	-4.04	119.99	124.51
30	C	515	BCR	C28-C27-C26	-4.02	106.86	113.78
30	Z	101	BCR	C15-C14-C13	-4.00	121.60	127.31
22	A	404	PHO	C3D-C2D-C1D	-3.99	99.91	105.82
22	G	405	PHO	C3D-C2D-C1D	-3.97	99.93	105.82
30	W	101	BCR	C33-C5-C6	-3.97	120.07	124.51
22	Q	403	PHO	C3D-C2D-C1D	-3.92	100.00	105.82
30	c	101	BCR	C38-C26-C25	-3.88	120.16	124.51
22	D	402	PHO	C3D-C2D-C1D	-3.87	100.08	105.82
30	B	620	BCR	C24-C23-C22	-3.86	120.41	126.21
30	H	101	BCR	C33-C5-C6	-3.85	120.19	124.51
21	N	610	CLA	O1D-CGD-CBD	-3.80	117.77	124.60
30	P	514	BCR	C7-C6-C5	-3.78	112.52	121.54
21	N	611	CLA	O1D-CGD-CBD	-3.78	117.82	124.60
30	P	516	BCR	C38-C26-C25	-3.78	120.28	124.51
34	E	101	HEM	CBA-CAA-C2A	-3.75	105.31	112.48
30	P	515	BCR	C15-C14-C13	-3.75	121.96	127.31
30	C	515	BCR	C38-C26-C25	-3.75	120.31	124.51
30	B	617	BCR	C7-C8-C9	-3.74	120.60	126.21
30	C	514	BCR	C7-C6-C5	-3.73	112.64	121.54
30	C	515	BCR	C7-C8-C9	-3.73	120.60	126.21
30	T	101	BCR	C33-C5-C6	-3.72	120.35	124.51
21	B	607	CLA	O1D-CGD-CBD	-3.70	117.96	124.60
30	P	514	BCR	C15-C14-C13	-3.69	122.05	127.31
30	b	102	BCR	C7-C8-C9	-3.67	120.69	126.21
26	N	601	SQD	C1-C2-C3	-3.66	103.18	109.98
30	B	620	BCR	C3-C4-C5	-3.65	107.50	113.78
30	B	618	BCR	C3-C4-C5	-3.63	107.54	113.78
30	S	101	BCR	C28-C27-C26	-3.63	107.54	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	101	BCR	C3-C4-C5	-3.60	107.60	113.78
30	B	617	BCR	C33-C5-C6	-3.59	120.49	124.51
30	D	405	BCR	C28-C27-C26	-3.57	107.64	113.78
30	T	101	BCR	C7-C8-C9	-3.57	120.85	126.21
24	C	517	DGD	C3G-O3G-C1D	-3.55	106.47	113.76
21	B	604	CLA	O1D-CGD-CBD	-3.54	118.24	124.60
30	C	514	BCR	C15-C14-C13	-3.54	122.26	127.31
24	P	518	DGD	C3G-O3G-C1D	-3.54	106.50	113.76
30	T	103	BCR	C3-C4-C5	-3.53	107.71	113.78
21	B	611	CLA	O1D-CGD-CBD	-3.52	118.28	124.60
30	T	102	BCR	C3-C4-C5	-3.50	107.75	113.78
27	N	622	LMG	C7-O1-C1	-3.50	106.58	113.76
30	K	101	BCR	C3-C4-C5	-3.48	107.80	113.78
21	N	608	CLA	O1D-CGD-CBD	-3.46	118.39	124.60
30	B	618	BCR	C38-C26-C25	-3.42	120.68	124.51
27	a	102	LMG	O6-C1-O1	-3.41	101.91	110.02
21	B	606	CLA	O1D-CGD-CBD	-3.41	118.48	124.60
21	N	618	CLA	O1D-CGD-CBD	-3.41	118.48	124.60
30	J	102	BCR	C7-C8-C9	-3.40	121.11	126.21
34	R	101	HEM	CBA-CAA-C2A	-3.39	106.00	112.48
21	N	615	CLA	O1D-CGD-CBD	-3.37	118.54	124.60
30	P	514	BCR	C16-C17-C18	-3.36	122.51	127.31
30	T	102	BCR	C38-C26-C25	-3.36	120.75	124.51
27	I	102	LMG	O6-C1-O1	-3.35	102.07	110.02
30	a	101	BCR	C38-C26-C25	-3.35	120.76	124.51
22	Q	403	PHO	C4C-C3C-C2C	-3.33	103.07	106.81
30	a	101	BCR	C33-C5-C6	-3.32	120.80	124.51
30	Z	101	BCR	C33-C5-C6	-3.30	120.82	124.51
30	C	514	BCR	C3-C4-C5	-3.29	108.12	113.78
30	P	514	BCR	C3-C4-C5	-3.28	108.14	113.78
21	B	616	CLA	O1D-CGD-CBD	-3.27	118.73	124.60
21	Q	404	CLA	O1D-CGD-CBD	-3.27	118.74	124.60
26	B	627	SQD	C1-C2-C3	-3.26	103.91	109.98
30	T	103	BCR	C38-C26-C25	-3.25	120.87	124.51
21	C	508	CLA	O1D-CGD-CBD	-3.25	118.77	124.60
30	B	620	BCR	C38-C26-C25	-3.25	120.87	124.51
30	Z	101	BCR	C24-C23-C22	-3.24	121.34	126.21
21	B	601	CLA	O1D-CGD-CBD	-3.24	118.79	124.60
30	C	515	BCR	C33-C5-C6	-3.23	120.89	124.51
21	N	610	CLA	O2D-CGD-O1D	-3.23	117.33	123.82
21	B	603	CLA	O1D-CGD-CBD	-3.23	118.81	124.60
34	R	101	HEM	C1D-C2D-C3D	-3.22	104.75	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	404	PHO	C4C-C3C-C2C	-3.22	103.19	106.81
30	P	515	BCR	C24-C23-C22	-3.21	121.39	126.21
26	G	410	SQD	C44-O6-C1	-3.20	107.19	113.76
30	N	621	BCR	C24-C23-C22	-3.20	121.41	126.21
21	C	512	CLA	O1D-CGD-CBD	-3.20	118.86	124.60
30	I	101	BCR	C33-C5-C6	-3.19	120.93	124.51
26	B	624	SQD	C45-O47-C7	-3.19	110.34	117.88
22	D	402	PHO	C4C-C3C-C2C	-3.19	103.23	106.81
30	S	101	BCR	C33-C5-C6	-3.18	120.94	124.51
30	I	101	BCR	C38-C26-C25	-3.18	120.95	124.51
22	G	405	PHO	C4C-C3C-C2C	-3.17	103.25	106.81
26	Q	408	SQD	C45-O47-C7	-3.15	110.42	117.88
21	A	401	CLA	O1D-CGD-CBD	-3.15	118.95	124.60
21	N	607	CLA	O1D-CGD-CBD	-3.13	118.98	124.60
26	A	409	SQD	C1-C2-C3	-3.13	104.16	109.98
30	P	515	BCR	C33-C5-C6	-3.13	121.01	124.51
30	I	101	BCR	C3-C4-C5	-3.12	108.41	113.78
21	A	405	CLA	O1D-CGD-CBD	-3.12	119.00	124.60
21	B	614	CLA	O1D-CGD-CBD	-3.10	119.04	124.60
21	D	403	CLA	O1D-CGD-CBD	-3.09	119.06	124.60
30	J	102	BCR	C35-C13-C14	-3.08	118.61	122.92
30	P	516	BCR	C33-C5-C6	-3.06	121.08	124.51
21	P	508	CLA	C2C-C1C-NC	-3.06	108.12	110.22
26	G	410	SQD	C1-C2-C3	-3.06	104.30	109.98
30	N	621	BCR	C15-C14-C13	-3.06	122.95	127.31
21	A	402	CLA	O1D-CGD-CBD	-3.06	119.11	124.60
30	b	102	BCR	C11-C10-C9	-3.05	122.95	127.31
30	C	514	BCR	C16-C17-C18	-3.05	122.96	127.31
21	G	403	CLA	O1D-CGD-CBD	-3.04	119.14	124.60
30	T	101	BCR	C15-C14-C13	-3.04	122.98	127.31
30	B	617	BCR	C15-C14-C13	-3.03	122.98	127.31
27	N	623	LMG	C8-O7-C10	-3.03	110.73	117.88
27	C	519	LMG	O6-C1-O1	-3.03	102.84	110.02
27	D	407	LMG	C8-O7-C10	-3.02	110.73	117.88
30	B	618	BCR	C11-C10-C9	-3.02	123.01	127.31
27	M	101	LMG	C7-O1-C1	-3.01	107.59	113.76
30	I	101	BCR	C15-C14-C13	-3.01	123.02	127.31
27	B	623	LMG	C8-O7-C10	-3.00	110.79	117.88
30	D	405	BCR	C33-C5-C6	-2.98	121.17	124.51
30	B	619	BCR	C33-C5-C6	-2.98	121.17	124.51
21	B	607	CLA	O2D-CGD-O1D	-2.98	117.83	123.82
27	B	622	LMG	C7-O1-C1	-2.97	107.66	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	SQD	C44-O6-C1	-2.97	107.66	113.76
21	B	610	CLA	O1D-CGD-CBD	-2.96	119.28	124.60
27	Q	407	LMG	C8-O7-C10	-2.95	110.91	117.88
21	C	503	CLA	O1D-CGD-CBD	-2.94	119.32	124.60
27	P	520	LMG	O6-C1-O1	-2.94	103.04	110.02
27	e	102	LMG	C7-O1-C1	-2.94	107.73	113.76
30	b	102	BCR	C35-C13-C14	-2.94	118.81	122.92
30	B	617	BCR	C38-C26-C25	-2.94	121.22	124.51
21	P	503	CLA	O1D-CGD-CBD	-2.94	119.33	124.60
34	E	101	HEM	C1D-C2D-C3D	-2.93	104.96	107.00
21	N	605	CLA	O1D-CGD-CBD	-2.93	119.34	124.60
22	A	404	PHO	CMD-C2D-C3D	-2.93	120.78	127.86
21	N	608	CLA	O2D-CGD-O1D	-2.92	117.94	123.82
26	Q	408	SQD	C1-C2-C3	-2.92	104.55	109.98
30	P	515	BCR	C3-C4-C5	-2.92	108.76	113.78
27	N	622	LMG	C9-C8-C7	-2.92	105.28	111.86
27	A	410	LMG	C8-O7-C10	-2.92	110.99	117.88
23	G	407	PL9	C22-C23-C24	-2.92	120.36	127.68
23	D	404	PL9	C22-C23-C24	-2.91	120.36	127.68
30	b	102	BCR	C28-C27-C26	-2.91	108.78	113.78
30	c	101	BCR	C10-C11-C12	-2.91	114.31	123.23
30	a	101	BCR	C24-C23-C22	-2.91	121.84	126.21
30	T	103	BCR	C7-C8-C9	-2.91	121.84	126.21
30	S	101	BCR	C3-C4-C5	-2.91	108.78	113.78
22	G	405	PHO	CMD-C2D-C3D	-2.90	120.83	127.86
30	a	101	BCR	C15-C14-C13	-2.90	123.17	127.31
30	N	621	BCR	C33-C5-C6	-2.90	121.26	124.51
27	B	623	LMG	C7-O1-C1	-2.90	107.81	113.76
30	B	619	BCR	C24-C23-C22	-2.90	121.86	126.21
21	N	620	CLA	O1D-CGD-CBD	-2.90	119.40	124.60
23	Q	405	PL9	C22-C23-C24	-2.89	120.41	127.68
22	G	405	PHO	C4D-ND-C1D	-2.89	101.77	106.98
23	A	406	PL9	C22-C23-C24	-2.89	120.43	127.68
26	A	414	SQD	C5-C6-S	-2.88	110.32	114.34
27	N	623	LMG	C7-O1-C1	-2.88	107.85	113.76
22	A	404	PHO	C4D-ND-C1D	-2.88	101.78	106.98
21	G	406	CLA	O1D-CGD-CBD	-2.88	119.43	124.60
30	B	619	BCR	C7-C8-C9	-2.88	121.89	126.21
30	H	101	BCR	C10-C11-C12	-2.88	114.41	123.23
22	D	402	PHO	C4D-ND-C1D	-2.87	101.80	106.98
21	B	612	CLA	C1-C2-C3	-2.86	120.68	125.96
30	K	101	BCR	C10-C11-C12	-2.86	114.45	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	613	CLA	C1-C2-C3	-2.86	120.69	125.96
30	B	619	BCR	C15-C14-C13	-2.84	123.25	127.31
21	C	505	CLA	O1D-CGD-CBD	-2.83	119.51	124.60
27	G	411	LMG	C8-O7-C10	-2.83	111.19	117.88
30	J	102	BCR	C28-C27-C26	-2.83	108.92	113.78
24	P	517	DGD	C3G-O3G-C1D	-2.82	107.96	113.76
30	C	514	BCR	C24-C23-C22	-2.82	121.97	126.21
27	N	622	LMG	C8-O7-C10	-2.82	111.21	117.88
30	N	621	BCR	C3-C4-C5	-2.82	108.94	113.78
21	B	604	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
30	B	620	BCR	C15-C14-C13	-2.81	123.30	127.31
30	W	101	BCR	C10-C11-C12	-2.81	114.62	123.23
30	Z	101	BCR	C3-C4-C5	-2.81	108.95	113.78
21	N	615	CLA	C1-C2-C3	-2.80	120.80	125.96
30	T	103	BCR	C16-C17-C18	-2.80	123.32	127.31
22	G	405	PHO	C1C-C2C-C3C	-2.79	103.27	106.51
21	B	611	CLA	C1-C2-C3	-2.79	120.81	125.96
21	G	404	CLA	O1D-CGD-CBD	-2.79	119.58	124.60
26	B	624	SQD	C1-C2-C3	-2.79	104.79	109.98
30	P	514	BCR	C28-C27-C26	-2.78	108.99	113.78
30	a	101	BCR	C3-C4-C5	-2.78	109.00	113.78
30	J	102	BCR	C11-C10-C9	-2.78	123.34	127.31
30	P	514	BCR	C24-C23-C22	-2.78	122.04	126.21
22	Q	403	PHO	C4D-ND-C1D	-2.77	101.97	106.98
21	B	602	CLA	O1D-CGD-CBD	-2.77	119.62	124.60
27	B	622	LMG	C9-C8-C7	-2.77	105.60	111.86
21	N	611	CLA	O2D-CGD-O1D	-2.77	118.25	123.82
30	C	515	BCR	C15-C14-C13	-2.77	123.36	127.31
30	B	620	BCR	C7-C8-C9	-2.77	122.06	126.21
30	P	516	BCR	C15-C14-C13	-2.76	123.36	127.31
30	D	405	BCR	C3-C4-C5	-2.76	109.03	113.78
30	T	103	BCR	C15-C14-C13	-2.76	123.37	127.31
30	D	405	BCR	C24-C23-C22	-2.76	122.07	126.21
30	T	101	BCR	C38-C26-C25	-2.75	121.43	124.51
21	A	403	CLA	O1D-CGD-CBD	-2.75	119.66	124.60
21	C	508	CLA	C2C-C1C-NC	-2.75	108.34	110.22
30	B	617	BCR	C16-C17-C18	-2.75	123.39	127.31
22	D	402	PHO	CMD-C2D-C3D	-2.75	121.21	127.86
30	T	102	BCR	C11-C10-C9	-2.74	123.40	127.31
21	P	512	CLA	O1D-CGD-CBD	-2.74	119.68	124.60
21	D	401	CLA	O1D-CGD-CBD	-2.74	119.68	124.60
21	N	609	CLA	O1D-CGD-CBD	-2.74	119.69	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	PL9	C37-C38-C39	-2.73	120.81	127.68
22	A	404	PHO	C1C-C2C-C3C	-2.72	103.35	106.51
21	N	613	CLA	C1-C2-C3	-2.72	120.94	125.96
27	B	623	LMG	O6-C1-O1	-2.72	103.56	110.02
22	D	402	PHO	C1C-C2C-C3C	-2.72	103.36	106.51
21	N	619	CLA	O1D-CGD-CBD	-2.71	119.72	124.60
30	P	516	BCR	C3-C4-C5	-2.71	109.12	113.78
30	T	101	BCR	C28-C27-C26	-2.71	109.12	113.78
21	N	617	CLA	C1-C2-C3	-2.70	120.98	125.96
30	K	101	BCR	C15-C14-C13	-2.70	123.45	127.31
21	D	401	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
21	N	616	CLA	C1-C2-C3	-2.70	120.98	125.96
30	C	514	BCR	C28-C27-C26	-2.70	109.15	113.78
30	b	102	BCR	C37-C22-C21	-2.69	119.15	122.92
27	P	520	LMG	C8-O7-C10	-2.68	111.54	117.88
22	Q	403	PHO	C1C-C2C-C3C	-2.68	103.40	106.51
21	P	508	CLA	C1-C2-C3	-2.68	121.02	125.96
23	G	407	PL9	C12-C13-C14	-2.68	120.95	127.68
23	Q	405	PL9	C37-C38-C39	-2.68	120.95	127.68
21	B	615	CLA	O1D-CGD-CBD	-2.68	119.79	124.60
21	C	511	CLA	O1D-CGD-CBD	-2.68	119.79	124.60
30	N	621	BCR	C7-C8-C9	-2.68	122.19	126.21
30	B	619	BCR	C3-C4-C5	-2.67	109.18	113.78
21	G	402	CLA	C2C-C1C-NC	-2.67	108.39	110.22
30	J	102	BCR	C37-C22-C21	-2.67	119.18	122.92
21	G	402	CLA	O1D-CGD-CBD	-2.67	119.81	124.60
27	C	519	LMG	C8-O7-C10	-2.67	111.58	117.88
21	C	510	CLA	O1D-CGD-CBD	-2.66	119.82	124.60
30	B	618	BCR	C21-C20-C19	-2.66	115.06	123.23
21	N	618	CLA	O2D-CGD-O1D	-2.66	118.47	123.82
21	N	614	CLA	O1D-CGD-CBD	-2.66	119.82	124.60
23	A	406	PL9	C12-C13-C14	-2.66	121.01	127.68
21	C	513	CLA	O1D-CGD-CBD	-2.65	119.83	124.60
22	G	405	PHO	O1D-CGD-CBD	-2.65	119.84	124.60
21	B	605	CLA	O1D-CGD-CBD	-2.65	119.84	124.60
21	Q	402	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
21	P	511	CLA	O1D-CGD-CBD	-2.65	119.84	124.60
30	S	101	BCR	C38-C26-C25	-2.65	121.55	124.51
21	B	606	CLA	O2D-CGD-O1D	-2.65	118.50	123.82
21	P	510	CLA	C1-C2-C3	-2.64	121.08	125.96
27	B	622	LMG	C8-O7-C10	-2.64	111.63	117.88
30	T	102	BCR	C21-C20-C19	-2.63	115.15	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	606	CLA	O1D-CGD-CBD	-2.63	119.88	124.60
30	D	405	BCR	C38-C26-C25	-2.62	121.57	124.51
21	N	616	CLA	C2C-C1C-NC	-2.62	108.42	110.22
30	C	514	BCR	C38-C26-C25	-2.62	121.58	124.51
21	P	513	CLA	O1D-CGD-CBD	-2.61	119.91	124.60
34	i	201	HEM	CAA-CBA-CGA	-2.61	108.21	112.66
30	T	101	BCR	C16-C17-C18	-2.60	123.60	127.31
26	N	601	SQD	C1-O5-C5	-2.60	108.82	113.72
21	N	606	CLA	C2C-C1C-NC	-2.60	108.44	110.22
21	Q	402	CLA	O1D-CGD-CBD	-2.60	119.94	124.60
30	Z	101	BCR	C20-C21-C22	-2.59	123.61	127.31
31	Q	410	LMT	C1B-O1B-C4'	-2.59	111.68	118.00
22	Q	403	PHO	CMD-C2D-C3D	-2.59	121.59	127.86
27	D	406	LMG	C8-O7-C10	-2.59	111.77	117.88
30	c	101	BCR	C15-C14-C13	-2.58	123.62	127.31
21	C	510	CLA	C1-C2-C3	-2.58	121.21	125.96
21	B	612	CLA	O1D-CGD-CBD	-2.57	119.98	124.60
24	C	516	DGD	C3G-O3G-C1D	-2.57	108.48	113.76
21	C	508	CLA	C1-C2-C3	-2.57	121.22	125.96
21	B	609	CLA	C1-C2-C3	-2.57	121.22	125.96
23	D	404	PL9	C7-C8-C9	-2.57	122.42	126.71
23	D	404	PL9	C36-C34-C33	-2.56	115.86	121.10
27	D	412	LMG	C8-O7-C10	-2.56	111.83	117.88
21	P	505	CLA	O1D-CGD-CBD	-2.56	120.01	124.60
21	B	614	CLA	O2D-CGD-O1D	-2.55	118.68	123.82
23	Q	405	PL9	C36-C34-C33	-2.54	115.90	121.10
23	Q	405	PL9	C7-C3-C2	-2.54	119.61	123.23
21	P	509	CLA	O1D-CGD-CBD	-2.54	120.04	124.60
26	B	627	SQD	C1-O5-C5	-2.54	108.93	113.72
30	I	101	BCR	C24-C23-C22	-2.54	122.40	126.21
22	G	405	PHO	CHD-C1D-ND	-2.54	119.66	124.64
23	J	101	PL9	C7-C3-C2	-2.53	119.63	123.23
21	D	403	CLA	C1-C2-C3	-2.53	121.30	125.96
21	N	619	CLA	C1-C2-C3	-2.53	121.30	125.96
30	C	515	BCR	C3-C4-C5	-2.52	109.44	113.78
30	P	514	BCR	C35-C13-C14	-2.52	119.39	122.92
21	N	612	CLA	O1D-CGD-CBD	-2.52	120.08	124.60
23	b	101	PL9	C7-C3-C2	-2.52	119.65	123.23
30	N	621	BCR	C28-C27-C26	-2.52	109.46	113.78
30	P	515	BCR	C28-C27-C26	-2.52	109.46	113.78
22	A	404	PHO	CHD-C1D-ND	-2.51	119.71	124.64
23	Q	405	PL9	C12-C13-C14	-2.51	121.37	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	PHO	CHD-C1D-ND	-2.51	119.72	124.64
30	N	621	BCR	C38-C26-C25	-2.51	121.70	124.51
27	e	102	LMG	C8-O7-C10	-2.50	111.96	117.88
30	B	620	BCR	C16-C17-C18	-2.50	123.74	127.31
30	T	101	BCR	C3-C4-C5	-2.50	109.48	113.78
22	A	404	PHO	CAA-C2A-C3A	-2.50	105.95	112.81
21	B	601	CLA	C1-C2-C3	-2.50	121.35	125.96
30	B	619	BCR	C38-C26-C25	-2.50	121.71	124.51
21	Q	404	CLA	C1-C2-C3	-2.49	121.36	125.96
21	B	601	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
21	Q	404	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
21	D	403	CLA	O2D-CGD-O1D	-2.49	118.81	123.82
22	A	404	PHO	O1D-CGD-CBD	-2.49	120.13	124.60
24	B	621	DGD	C1E-C2E-C3E	-2.49	105.36	109.98
23	Q	405	PL9	C7-C8-C9	-2.49	122.55	126.71
21	P	507	CLA	O1D-CGD-CBD	-2.48	120.14	124.60
21	G	402	CLA	C1-C2-C3	-2.48	121.39	125.96
34	V	201	HEM	C1D-C2D-C3D	-2.48	105.27	107.00
31	D	409	LMT	C1B-O1B-C4'	-2.47	111.97	118.00
30	B	617	BCR	C28-C27-C26	-2.47	109.53	113.78
30	I	101	BCR	C16-C17-C18	-2.47	123.79	127.31
21	N	609	CLA	C2C-C1C-NC	-2.47	108.53	110.22
27	M	101	LMG	C8-O7-C10	-2.47	112.05	117.88
21	A	401	CLA	C1-C2-C3	-2.46	121.42	125.96
30	B	620	BCR	C28-C27-C26	-2.46	109.55	113.78
21	P	508	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
30	a	101	BCR	C20-C21-C22	-2.46	123.80	127.31
21	B	613	CLA	O1D-CGD-CBD	-2.46	120.19	124.60
21	P	502	CLA	O1D-CGD-CBD	-2.46	120.19	124.60
21	N	616	CLA	O1D-CGD-CBD	-2.45	120.19	124.60
27	Q	406	LMG	C8-O7-C10	-2.45	112.08	117.88
21	N	605	CLA	C1-C2-C3	-2.45	121.44	125.96
24	P	518	DGD	C3G-C2G-C1G	-2.45	106.33	111.86
30	Z	101	BCR	C28-C27-C26	-2.45	109.57	113.78
21	B	611	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
21	P	510	CLA	O1D-CGD-CBD	-2.45	120.21	124.60
30	C	514	BCR	C35-C13-C14	-2.44	119.50	122.92
21	C	509	CLA	O1D-CGD-CBD	-2.44	120.21	124.60
21	G	403	CLA	C1-C2-C3	-2.44	121.46	125.96
21	B	603	CLA	O2D-CGD-O1D	-2.44	118.91	123.82
24	P	518	DGD	C6E-C5E-C4E	-2.44	107.30	113.00
22	G	405	PHO	CAA-C2A-C3A	-2.43	106.14	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	617	BCR	C3-C4-C5	-2.43	109.60	113.78
21	B	608	CLA	C2C-C1C-NC	-2.43	108.56	110.22
21	G	404	CLA	C1-C2-C3	-2.43	121.48	125.96
22	Q	403	PHO	CHD-C1D-ND	-2.42	119.89	124.64
30	B	617	BCR	C11-C10-C9	-2.42	123.85	127.31
23	D	404	PL9	C12-C13-C14	-2.42	121.59	127.68
21	N	620	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
21	B	615	CLA	C1-C2-C3	-2.42	121.50	125.96
30	b	102	BCR	C33-C5-C6	-2.42	121.80	124.51
31	M	102	LMT	C1B-O1B-C4'	-2.41	112.11	118.00
27	N	623	LMG	O6-C1-O1	-2.40	104.32	110.02
21	N	607	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
30	T	101	BCR	C24-C23-C22	-2.39	122.62	126.21
30	P	514	BCR	C38-C26-C25	-2.39	121.83	124.51
24	C	517	DGD	C3G-C2G-C1G	-2.38	106.48	111.86
21	C	504	CLA	C2C-C1C-NC	-2.38	108.59	110.22
21	N	605	CLA	O2D-CGD-O1D	-2.38	119.02	123.82
26	N	601	SQD	C44-O6-C1	-2.38	108.87	113.76
23	J	101	PL9	C12-C13-C14	-2.38	121.69	127.68
21	B	603	CLA	C2C-C1C-NC	-2.38	108.59	110.22
21	A	402	CLA	C1-C2-C3	-2.37	121.58	125.96
24	Q	409	DGD	C6E-C5E-C4E	-2.37	107.45	113.00
21	N	608	CLA	C1-C2-C3	-2.37	121.59	125.96
21	C	513	CLA	C2C-C1C-NC	-2.37	108.60	110.22
30	W	101	BCR	C16-C17-C18	-2.37	123.93	127.31
21	P	513	CLA	C2C-C1C-NC	-2.37	108.60	110.22
27	Q	401	LMG	C8-O7-C10	-2.36	112.29	117.88
30	H	101	BCR	C3-C4-C5	-2.36	109.72	113.78
30	B	619	BCR	C28-C27-C26	-2.36	109.73	113.78
27	D	406	LMG	O2-C2-C1	-2.36	105.10	110.03
30	P	515	BCR	C20-C21-C22	-2.35	123.95	127.31
27	a	102	LMG	C7-O1-C1	-2.35	108.94	113.76
23	D	404	PL9	C42-C43-C44	-2.34	121.79	127.68
23	b	101	PL9	C12-C13-C14	-2.34	121.79	127.68
21	C	505	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
21	C	504	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
30	T	101	BCR	C11-C10-C9	-2.34	123.97	127.31
30	Z	101	BCR	C10-C11-C12	-2.34	116.06	123.23
21	C	502	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
30	J	102	BCR	C33-C5-C6	-2.33	121.90	124.51
30	S	101	BCR	C11-C10-C9	-2.33	123.98	127.31
23	D	404	PL9	C32-C33-C34	-2.33	121.83	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	619	CLA	O2D-CGD-O1D	-2.32	119.14	123.82
30	B	619	BCR	C16-C17-C18	-2.32	124.00	127.31
23	b	101	PL9	C22-C23-C24	-2.31	121.87	127.68
21	N	607	CLA	C2C-C1C-NC	-2.31	108.64	110.22
21	G	406	CLA	C1-C2-C3	-2.31	121.70	125.96
26	G	410	SQD	C45-O47-C7	-2.31	112.42	117.88
23	Q	405	PL9	C42-C43-C44	-2.31	121.88	127.68
21	B	605	CLA	C2C-C1C-NC	-2.30	108.64	110.22
21	B	604	CLA	C1-C2-C3	-2.30	121.72	125.96
21	B	606	CLA	C2C-C1C-NC	-2.30	108.64	110.22
30	D	405	BCR	C21-C20-C19	-2.30	116.19	123.23
30	C	515	BCR	C21-C20-C19	-2.29	116.19	123.23
21	C	506	CLA	C1-C2-C3	-2.29	121.73	125.96
30	D	405	BCR	C11-C10-C9	-2.29	124.04	127.31
23	G	407	PL9	C7-C3-C2	-2.29	119.97	123.23
21	C	509	CLA	C1-C2-C3	-2.29	121.74	125.96
21	B	602	CLA	C1-C2-C3	-2.29	121.74	125.96
21	A	401	CLA	C2C-C1C-NC	-2.29	108.65	110.22
30	P	514	BCR	C34-C9-C10	-2.29	119.72	122.92
21	B	616	CLA	O2D-CGD-O1D	-2.29	119.21	123.82
23	D	404	PL9	C45-C44-C43	-2.29	117.58	123.69
21	C	507	CLA	O1D-CGD-CBD	-2.29	120.50	124.60
23	Q	405	PL9	C32-C33-C34	-2.28	121.94	127.68
23	J	101	PL9	C22-C23-C24	-2.28	121.94	127.68
23	J	101	PL9	C7-C8-C9	-2.28	122.90	126.71
21	C	508	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
27	C	520	LMG	O8-C28-O10	-2.28	117.89	123.55
31	e	101	LMT	C1B-O1B-C4'	-2.28	112.44	118.00
30	C	514	BCR	C34-C9-C10	-2.28	119.73	122.92
24	P	517	DGD	O3D-C3D-C4D	-2.28	105.40	110.36
21	N	610	CLA	C2C-C1C-NC	-2.27	108.66	110.22
24	C	517	DGD	C6E-C5E-C4E	-2.27	107.69	113.00
30	B	618	BCR	C4-C5-C6	-2.27	119.41	122.74
30	P	515	BCR	C10-C11-C12	-2.27	116.28	123.23
30	S	101	BCR	C21-C20-C19	-2.26	116.28	123.23
27	R	102	LMG	C9-C8-C7	-2.26	106.75	111.86
30	I	101	BCR	C28-C27-C26	-2.26	109.89	113.78
21	G	406	CLA	C2C-C1C-NC	-2.26	108.67	110.22
30	T	103	BCR	C28-C27-C26	-2.26	109.89	113.78
21	P	506	CLA	C2C-C1C-NC	-2.26	108.67	110.22
23	A	406	PL9	C11-C9-C8	-2.26	116.48	121.10
30	T	102	BCR	C4-C5-C6	-2.26	119.43	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	101	BCR	C7-C8-C9	-2.26	122.82	126.21
30	B	617	BCR	C24-C23-C22	-2.26	122.82	126.21
30	B	618	BCR	C15-C16-C17	-2.25	118.66	123.46
21	P	501	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
23	A	406	PL9	C7-C8-C9	-2.25	122.95	126.71
30	b	102	BCR	C36-C18-C17	-2.25	119.78	122.92
21	A	402	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
21	P	503	CLA	C1-C2-C3	-2.25	121.82	125.96
21	Q	402	CLA	C2C-C1C-NC	-2.24	108.68	110.22
23	b	101	PL9	C7-C8-C9	-2.24	122.96	126.71
21	P	504	CLA	O1D-CGD-CBD	-2.24	120.57	124.60
30	Z	101	BCR	C11-C10-C9	-2.24	124.11	127.31
24	W	102	DGD	C1E-C2E-C3E	-2.24	105.81	109.98
21	N	615	CLA	O2D-CGD-O1D	-2.23	119.32	123.82
21	B	615	CLA	C2C-C1C-NC	-2.23	108.69	110.22
24	C	516	DGD	O3D-C3D-C4D	-2.23	105.50	110.36
21	D	403	CLA	C2C-C1C-NC	-2.23	108.69	110.22
23	Q	405	PL9	C45-C44-C43	-2.23	117.75	123.69
24	D	408	DGD	O5D-C1E-C2E	-2.23	104.60	108.23
22	A	404	PHO	C3B-C2B-C1B	-2.23	101.81	106.30
30	H	101	BCR	C16-C17-C18	-2.23	124.13	127.31
21	P	506	CLA	C1-C2-C3	-2.22	121.86	125.96
27	N	623	LMG	O2-C2-C3	-2.22	105.52	110.36
30	P	515	BCR	C8-C7-C6	-2.22	121.04	127.25
30	H	101	BCR	C28-C27-C26	-2.22	109.96	113.78
30	c	101	BCR	C1-C6-C5	-2.22	119.47	122.59
27	B	623	LMG	O2-C2-C3	-2.22	105.53	110.36
30	K	101	BCR	C1-C6-C5	-2.22	119.47	122.59
21	P	504	CLA	C2C-C1C-NC	-2.22	108.70	110.22
21	A	405	CLA	O2D-CGD-O1D	-2.22	119.36	123.82
21	C	512	CLA	O2D-CGD-O1D	-2.22	119.36	123.82
21	A	401	CLA	O2D-CGD-O1D	-2.21	119.37	123.82
22	Q	403	PHO	CAA-C2A-C3A	-2.21	106.75	112.81
21	C	501	CLA	C1-C2-C3	-2.21	121.88	125.96
27	N	622	LMG	O3-C3-C4	-2.21	105.55	110.36
22	G	405	PHO	C3B-C2B-C1B	-2.21	101.84	106.30
21	B	605	CLA	C1-C2-C3	-2.21	121.89	125.96
24	D	408	DGD	C6E-C5E-C4E	-2.21	107.84	113.00
30	B	617	BCR	C20-C21-C22	-2.21	124.16	127.31
21	P	510	CLA	C2C-C1C-NC	-2.20	108.71	110.22
23	G	407	PL9	C17-C18-C19	-2.20	122.14	127.68
21	B	602	CLA	C2C-C1C-NC	-2.20	108.71	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	606	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
30	a	101	BCR	C28-C27-C26	-2.20	110.00	113.78
26	A	409	SQD	C45-O47-C7	-2.20	112.68	117.88
21	C	503	CLA	C2C-C1C-NC	-2.20	108.71	110.22
21	B	612	CLA	C2C-C1C-NC	-2.20	108.71	110.22
21	C	502	CLA	C2C-C1C-NC	-2.20	108.72	110.22
30	P	514	BCR	C21-C20-C19	-2.20	116.50	123.23
21	B	605	CLA	O2D-CGD-O1D	-2.19	119.41	123.82
30	N	621	BCR	C20-C21-C22	-2.19	124.18	127.31
21	B	607	CLA	C2C-C1C-NC	-2.19	108.72	110.22
21	P	509	CLA	C1-C2-C3	-2.19	121.92	125.96
30	N	621	BCR	C16-C17-C18	-2.19	124.18	127.31
30	N	621	BCR	C35-C13-C14	-2.19	119.85	122.92
21	N	609	CLA	O2D-CGD-O1D	-2.19	119.41	123.82
21	N	617	CLA	C2C-C1C-NC	-2.19	108.72	110.22
27	N	622	LMG	O6-C1-O1	-2.19	104.82	110.02
30	P	515	BCR	C38-C26-C25	-2.19	122.06	124.51
26	F	101	SQD	O8-S-O7	-2.19	106.36	111.37
22	Q	403	PHO	C3B-C2B-C1B	-2.19	101.89	106.30
22	G	405	PHO	C1-C2-C3	-2.18	121.93	125.96
23	D	404	PL9	C7-C3-C2	-2.18	120.12	123.23
21	C	503	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
23	A	406	PL9	C17-C18-C19	-2.18	122.20	127.68
23	A	406	PL9	C27-C28-C29	-2.18	122.20	127.68
23	G	407	PL9	C7-C8-C9	-2.18	123.06	126.71
21	B	610	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
30	P	516	BCR	C16-C17-C18	-2.18	124.20	127.31
30	Z	101	BCR	C38-C26-C25	-2.18	122.07	124.51
23	A	406	PL9	C7-C3-C2	-2.18	120.13	123.23
30	T	103	BCR	C20-C21-C22	-2.18	124.20	127.31
30	a	101	BCR	C16-C17-C18	-2.18	124.20	127.31
26	N	601	SQD	C45-O47-C7	-2.18	112.73	117.88
30	H	101	BCR	C21-C20-C19	-2.18	116.55	123.23
23	Q	405	PL9	C17-C18-C19	-2.18	122.21	127.68
22	D	402	PHO	C3B-C2B-C1B	-2.17	101.92	106.30
21	P	501	CLA	C1-C2-C3	-2.17	121.96	125.96
21	N	617	CLA	O1D-CGD-CBD	-2.17	120.70	124.60
27	D	406	LMG	O3-C3-C4	-2.17	105.64	110.36
21	C	501	CLA	O1D-CGD-CBD	-2.17	120.71	124.60
21	N	609	CLA	C1-C2-C3	-2.17	121.97	125.96
24	B	628	DGD	C2G-O2G-C1B	-2.17	112.76	117.88
21	C	506	CLA	C2C-C1C-NC	-2.16	108.74	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	610	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
21	G	402	CLA	O2D-CGD-O1D	-2.16	119.47	123.82
30	Z	101	BCR	C16-C17-C18	-2.16	124.22	127.31
30	P	516	BCR	C35-C13-C14	-2.16	119.90	122.92
21	G	403	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
34	i	201	HEM	C1D-C2D-C3D	-2.16	105.50	107.00
21	N	611	CLA	C2C-C1C-NC	-2.15	108.74	110.22
21	B	608	CLA	CMB-C2B-C1B	-2.15	125.15	128.46
21	N	613	CLA	C2C-C1C-NC	-2.15	108.75	110.22
21	N	606	CLA	C1-C2-C3	-2.15	121.99	125.96
21	B	608	CLA	O1D-CGD-CBD	-2.15	120.74	124.60
21	P	502	CLA	C2C-C1C-NC	-2.15	108.75	110.22
30	b	102	BCR	C39-C30-C25	-2.15	106.83	110.31
30	S	101	BCR	C24-C23-C22	-2.15	122.98	126.21
21	P	505	CLA	C1-C2-C3	-2.15	122.00	125.96
23	G	407	PL9	C27-C28-C29	-2.15	122.29	127.68
21	P	503	CLA	O2D-CGD-O1D	-2.15	119.50	123.82
21	G	406	CLA	O2D-CGD-O1D	-2.15	119.50	123.82
21	D	401	CLA	C2C-C1C-NC	-2.14	108.75	110.22
27	B	622	LMG	O6-C1-O1	-2.14	104.93	110.02
21	P	505	CLA	C2C-C1C-NC	-2.14	108.75	110.22
21	N	615	CLA	CBA-CAA-C2A	-2.14	107.39	113.80
21	P	509	CLA	C2C-C1C-NC	-2.14	108.75	110.22
23	G	407	PL9	C36-C34-C33	-2.14	116.73	121.10
21	C	506	CLA	CBA-CAA-C2A	-2.14	107.40	113.80
30	K	101	BCR	C15-C16-C17	-2.14	118.90	123.46
22	D	402	PHO	CAA-C2A-C3A	-2.14	106.95	112.81
30	Z	101	BCR	C8-C7-C6	-2.13	121.28	127.25
21	Q	404	CLA	C2C-C1C-NC	-2.13	108.76	110.22
21	C	509	CLA	C2C-C1C-NC	-2.13	108.76	110.22
30	I	101	BCR	C7-C8-C9	-2.13	123.01	126.21
21	B	613	CLA	C2C-C1C-NC	-2.13	108.76	110.22
21	C	510	CLA	C2C-C1C-NC	-2.13	108.76	110.22
27	E	102	LMG	C9-C8-C7	-2.13	107.05	111.86
22	G	405	PHO	C9-C8-C10	-2.13	103.59	111.36
21	A	403	CLA	C1-C2-C3	-2.13	122.04	125.96
30	T	103	BCR	C33-C5-C6	-2.13	122.13	124.51
21	N	612	CLA	C2C-C1C-NC	-2.13	108.76	110.22
21	P	508	CLA	CMB-C2B-C1B	-2.13	125.20	128.46
34	V	201	HEM	CAA-CBA-CGA	-2.12	109.03	112.66
22	D	402	PHO	O1D-CGD-CBD	-2.12	120.79	124.60
21	A	405	CLA	C2C-C1C-NC	-2.12	108.77	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	605	CLA	CMC-C2C-C1C	-2.12	121.80	125.02
30	N	621	BCR	C11-C10-C9	-2.12	124.28	127.31
21	C	505	CLA	C2C-C1C-NC	-2.12	108.77	110.22
27	Q	406	LMG	O2-C2-C1	-2.12	105.60	110.03
21	P	507	CLA	C5-C3-C2	-2.12	116.77	121.10
21	N	615	CLA	C2C-C1C-NC	-2.12	108.77	110.22
21	C	507	CLA	C5-C3-C2	-2.12	116.77	121.10
30	P	515	BCR	C15-C16-C17	-2.11	118.95	123.46
25	G	409	LHG	C5-O7-C7	-2.11	112.88	117.88
21	P	513	CLA	C1-C2-C3	-2.11	122.06	125.96
21	B	615	CLA	O2D-CGD-O1D	-2.11	119.57	123.82
30	C	514	BCR	C21-C20-C19	-2.11	116.76	123.23
26	S	102	SQD	O8-S-O7	-2.11	106.54	111.37
30	K	101	BCR	C24-C23-C22	-2.11	123.05	126.21
23	G	407	PL9	C11-C9-C8	-2.10	116.80	121.10
21	N	615	CLA	C5-C3-C2	-2.10	116.80	121.10
30	W	101	BCR	C28-C27-C26	-2.10	110.17	113.78
30	B	620	BCR	C20-C21-C22	-2.10	124.31	127.31
30	I	101	BCR	C21-C20-C19	-2.09	116.81	123.23
27	B	622	LMG	O3-C3-C4	-2.09	105.80	110.36
24	G	408	DGD	C2G-O2G-C1B	-2.09	112.93	117.88
23	A	406	PL9	C36-C34-C33	-2.09	116.82	121.10
21	N	619	CLA	C2C-C1C-NC	-2.09	108.79	110.22
30	J	102	BCR	C39-C30-C25	-2.09	106.92	110.31
23	Q	405	PL9	C27-C28-C29	-2.09	122.44	127.68
21	C	503	CLA	C1-C2-C3	-2.08	122.12	125.96
21	N	616	CLA	O2D-CGD-O1D	-2.08	119.63	123.82
30	I	101	BCR	C20-C21-C22	-2.08	124.34	127.31
30	W	101	BCR	C21-C20-C19	-2.08	116.85	123.23
21	P	508	CLA	O2D-CGD-O1D	-2.08	119.63	123.82
30	P	515	BCR	C11-C10-C9	-2.08	124.34	127.31
30	B	618	BCR	C34-C9-C10	-2.08	120.01	122.92
30	H	101	BCR	C24-C23-C22	-2.08	123.09	126.21
21	C	506	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
21	C	512	CLA	C2C-C1C-NC	-2.08	108.80	110.22
30	W	101	BCR	C3-C4-C5	-2.08	110.21	113.78
24	B	628	DGD	O6D-C1D-O3G	-2.07	105.09	110.02
21	P	506	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
24	A	407	DGD	C2G-O2G-C1B	-2.07	112.98	117.88
27	R	102	LMG	O1-C7-C8	-2.07	106.06	110.99
30	P	516	BCR	C23-C24-C25	-2.07	121.45	127.25
21	N	614	CLA	O2D-CGD-O1D	-2.07	119.65	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	611	CLA	CBA-CAA-C2A	-2.07	107.60	113.80
27	P	521	LMG	O8-C28-O10	-2.07	118.42	123.55
24	N	602	DGD	C2G-O2G-C1B	-2.07	113.00	117.88
21	B	616	CLA	C2C-C1C-NC	-2.06	108.81	110.22
21	N	612	CLA	C1-C2-C3	-2.06	122.16	125.96
21	B	611	CLA	C5-C3-C2	-2.06	116.89	121.10
27	D	412	LMG	O7-C10-O9	-2.05	118.56	123.68
21	P	503	CLA	C2C-C1C-NC	-2.05	108.81	110.22
30	a	101	BCR	C21-C20-C19	-2.05	116.95	123.23
23	D	404	PL9	C27-C28-C29	-2.04	122.54	127.68
27	M	101	LMG	O7-C10-O9	-2.04	118.58	123.68
26	F	101	SQD	C45-O47-C7	-2.04	113.05	117.88
30	T	102	BCR	C34-C9-C10	-2.04	120.06	122.92
21	B	609	CLA	C2C-C1C-NC	-2.04	108.82	110.22
30	P	516	BCR	C21-C20-C19	-2.04	116.97	123.23
21	A	405	CLA	C1-C2-C3	-2.04	122.20	125.96
22	Q	403	PHO	O1D-CGD-CBD	-2.04	120.94	124.60
27	Q	401	LMG	O7-C10-O9	-2.04	118.60	123.68
21	A	402	CLA	O2D-CGD-O1D	-2.03	119.72	123.82
21	B	601	CLA	CMC-C2C-C1C	-2.03	121.94	125.02
27	P	520	LMG	C9-C8-C7	-2.03	107.27	111.86
30	Z	101	BCR	C15-C16-C17	-2.03	119.12	123.46
27	e	102	LMG	O7-C10-O9	-2.03	118.61	123.68
21	C	508	CLA	CBA-CAA-C2A	-2.03	107.72	113.80
30	T	101	BCR	C20-C21-C22	-2.03	124.41	127.31
21	B	611	CLA	C2C-C1C-NC	-2.03	108.83	110.22
21	B	602	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
26	B	627	SQD	C44-O6-C1	-2.03	109.60	113.76
30	J	102	BCR	C36-C18-C17	-2.03	120.08	122.92
21	C	505	CLA	C5-C3-C2	-2.03	116.96	121.10
21	N	606	CLA	CAA-CBA-CGA	-2.02	107.25	113.35
30	c	101	BCR	C28-C27-C26	-2.02	110.30	113.78
30	J	102	BCR	C1-C6-C5	-2.02	119.75	122.59
30	I	101	BCR	C10-C11-C12	-2.02	117.03	123.23
21	N	607	CLA	CAA-C2A-C3A	-2.02	107.27	112.81
26	G	410	SQD	O5-C1-C2	-2.02	106.40	110.30
30	S	101	BCR	C15-C14-C13	-2.02	124.43	127.31
30	P	516	BCR	C11-C10-C9	-2.02	124.43	127.31
21	P	511	CLA	C2C-C1C-NC	-2.02	108.84	110.22
34	E	101	HEM	C3B-C4B-NB	-2.02	106.60	109.21
27	C	520	LMG	C7-O1-C1	-2.01	109.63	113.76
21	B	602	CLA	O2D-CGD-O1D	-2.01	119.77	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	102	LMG	C8-O7-C10	-2.01	113.13	117.88
34	i	201	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
30	a	101	BCR	C10-C11-C12	-2.01	117.07	123.23
25	A	408	LHG	C5-O7-C7	-2.01	113.13	117.88
30	C	515	BCR	C23-C24-C25	-2.01	121.63	127.25
21	C	513	CLA	C1-C2-C3	-2.01	122.26	125.96
21	B	616	CLA	C1-C2-C3	-2.01	122.26	125.96
23	A	406	PL9	C26-C24-C23	-2.01	117.00	121.10
30	C	514	BCR	C20-C21-C22	-2.01	124.45	127.31
21	C	508	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
30	C	515	BCR	C35-C13-C14	-2.00	120.11	122.92
21	P	506	CLA	CBA-CAA-C2A	-2.00	107.80	113.80
21	B	606	CLA	C1-C2-C3	-2.00	122.26	125.96
21	N	614	CLA	C2C-C1C-NC	-2.00	108.85	110.22
24	Q	409	DGD	O5D-C1E-C2E	-2.00	104.97	108.23
21	P	509	CLA	O2D-CGD-O1D	-2.00	119.79	123.82
21	A	401	CLA	C1D-CHD-C4C	2.00	125.22	122.48
21	N	607	CLA	C4-C3-C5	2.00	118.76	115.29
21	B	615	CLA	C1D-CHD-C4C	2.00	125.22	122.48
21	B	603	CLA	C3A-C2A-C1A	2.00	104.34	101.34
24	W	102	DGD	O6E-C5E-C6E	2.01	111.22	106.41
21	P	506	CLA	C4-C3-C5	2.01	118.77	115.29
21	N	620	CLA	CED-O2D-CGD	2.01	120.68	115.97
21	N	619	CLA	C1D-CHD-C4C	2.01	125.23	122.48
21	Q	402	CLA	CAA-C2A-C1A	2.01	118.56	111.97
23	b	101	PL9	C10-C9-C11	2.01	118.78	115.29
30	P	515	BCR	C36-C18-C19	2.02	121.31	118.10
23	b	101	PL9	C53-C6-C1	2.02	119.12	114.84
21	B	614	CLA	C1D-CHD-C4C	2.02	125.25	122.48
23	Q	405	PL9	C53-C6-C1	2.02	119.13	114.84
24	B	628	DGD	O6E-C5E-C6E	2.02	111.25	106.41
26	G	410	SQD	O5-C5-C4	2.02	113.39	109.66
30	B	618	BCR	C33-C5-C4	2.02	117.29	113.45
23	G	407	PL9	C10-C9-C11	2.03	118.80	115.29
23	D	404	PL9	C51-C49-C50	2.03	119.34	114.60
21	B	602	CLA	C1D-CHD-C4C	2.03	125.26	122.48
21	C	506	CLA	CED-O2D-CGD	2.03	120.74	115.97
30	C	514	BCR	C33-C5-C4	2.03	117.31	113.45
30	T	101	BCR	C29-C30-C25	2.03	113.66	110.48
21	B	605	CLA	CED-O2D-CGD	2.04	120.74	115.97
21	P	512	CLA	C1D-CHD-C4C	2.04	125.27	122.48
30	c	101	BCR	C36-C18-C19	2.04	121.34	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	609	CLA	CED-O2D-CGD	2.04	120.74	115.97
22	G	405	PHO	CMC-C2C-C1C	2.04	128.21	125.04
21	P	507	CLA	O2A-CGA-CBA	2.04	117.83	111.90
21	N	610	CLA	C1D-CHD-C4C	2.04	125.27	122.48
21	N	608	CLA	C4-C3-C5	2.04	118.83	115.29
23	A	406	PL9	C41-C39-C40	2.04	119.36	114.60
24	Q	409	DGD	O3G-C1D-C2D	2.04	111.57	108.23
21	N	607	CLA	C1D-CHD-C4C	2.04	125.28	122.48
21	N	618	CLA	C1D-CHD-C4C	2.05	125.28	122.48
27	N	622	LMG	O8-C28-C29	2.05	117.86	111.90
21	B	611	CLA	C1D-CHD-C4C	2.05	125.28	122.48
21	P	501	CLA	C1D-CHD-C4C	2.05	125.28	122.48
21	B	603	CLA	C1-O2A-CGA	2.05	121.69	116.77
21	A	402	CLA	C1D-CHD-C4C	2.05	125.29	122.48
21	B	606	CLA	C1D-CHD-C4C	2.05	125.29	122.48
21	P	502	CLA	CED-O2D-CGD	2.05	120.78	115.97
30	W	101	BCR	C35-C13-C12	2.05	121.37	118.10
21	N	606	CLA	O2A-CGA-CBA	2.06	117.88	111.90
21	P	507	CLA	C4-C3-C5	2.06	118.86	115.29
21	A	403	CLA	O2A-CGA-CBA	2.06	117.88	111.90
26	F	101	SQD	O6-C1-C2	2.06	111.59	108.23
21	G	403	CLA	C1D-CHD-C4C	2.06	125.30	122.48
21	P	508	CLA	C4-C3-C5	2.06	118.86	115.29
27	Q	406	LMG	O4-C4-C3	2.06	114.84	110.36
30	T	102	BCR	C33-C5-C4	2.07	117.37	113.45
24	Q	409	DGD	O6E-C5E-C6E	2.07	111.36	106.41
23	Q	405	PL9	C51-C49-C50	2.07	119.42	114.60
26	S	102	SQD	O6-C1-C2	2.07	111.61	108.23
21	C	513	CLA	C1D-CHD-C4C	2.07	125.31	122.48
21	C	504	CLA	C1-O2A-CGA	2.07	121.74	116.77
21	C	501	CLA	C4-C3-C5	2.07	118.88	115.29
21	P	501	CLA	C4-C3-C5	2.08	118.89	115.29
27	D	406	LMG	O4-C4-C3	2.08	114.88	110.36
23	G	407	PL9	C41-C39-C40	2.08	119.45	114.60
21	B	610	CLA	C4-C3-C5	2.08	118.90	115.29
24	B	621	DGD	O6E-C5E-C6E	2.09	111.41	106.41
23	D	404	PL9	C20-C19-C21	2.09	118.92	115.29
30	B	618	BCR	C36-C18-C19	2.10	121.44	118.10
30	P	516	BCR	C30-C25-C24	2.10	121.62	115.73
24	P	519	DGD	O5D-C6D-C5D	2.10	112.46	108.94
30	C	514	BCR	C35-C13-C12	2.10	121.45	118.10
21	N	606	CLA	CED-O2D-CGD	2.10	120.90	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	505	CLA	C1D-CHD-C4C	2.10	125.36	122.48
30	I	101	BCR	C2-C1-C6	2.11	113.77	110.48
30	W	101	BCR	C33-C5-C4	2.11	117.45	113.45
24	P	518	DGD	C1D-O6D-C5D	2.11	117.69	113.72
27	B	622	LMG	O8-C28-C29	2.11	118.03	111.90
24	P	519	DGD	O6E-C1E-O5D	2.11	115.03	110.02
21	P	509	CLA	C4-C3-C5	2.11	118.95	115.29
24	P	518	DGD	C6D-C5D-C4D	2.11	116.50	112.00
30	J	102	BCR	C23-C22-C21	2.11	122.19	118.94
24	W	102	DGD	O6D-C5D-C4D	2.12	113.56	109.66
30	P	514	BCR	C29-C30-C25	2.12	113.79	110.48
23	Q	405	PL9	C15-C14-C16	2.12	118.97	115.29
30	H	101	BCR	C35-C13-C12	2.12	121.48	118.10
21	B	615	CLA	C4-C3-C5	2.12	118.97	115.29
21	B	604	CLA	C1D-CHD-C4C	2.13	125.39	122.48
21	C	509	CLA	C4-C3-C5	2.13	118.98	115.29
21	C	507	CLA	O2A-CGA-CBA	2.13	118.11	111.90
21	B	602	CLA	C4-C3-C5	2.14	119.00	115.29
21	P	512	CLA	C4-C3-C5	2.14	119.01	115.29
24	W	102	DGD	C1D-O6D-C5D	2.14	117.75	113.72
21	C	504	CLA	O2A-CGA-CBA	2.15	118.15	111.90
30	K	101	BCR	C36-C18-C19	2.15	121.53	118.10
30	P	516	BCR	C38-C26-C27	2.16	117.54	113.45
24	C	517	DGD	O6E-C1E-O5D	2.16	115.14	110.02
30	B	620	BCR	C33-C5-C4	2.16	117.55	113.45
24	B	621	DGD	O4D-C4D-C3D	2.16	115.06	110.36
31	N	604	LMT	O1B-C4'-C3'	2.16	112.40	107.19
27	P	521	LMG	O1-C1-C2	2.16	111.76	108.23
30	T	103	BCR	C33-C5-C4	2.17	117.56	113.45
26	F	101	SQD	O48-C23-C24	2.17	118.21	111.90
30	P	514	BCR	C33-C5-C4	2.17	117.57	113.45
30	C	515	BCR	C38-C26-C27	2.17	117.57	113.45
21	C	504	CLA	C4-C3-C5	2.17	119.05	115.29
30	K	101	BCR	C38-C26-C27	2.17	117.57	113.45
23	Q	405	PL9	C40-C39-C41	2.17	119.06	115.29
27	C	520	LMG	C9-O8-C28	2.17	123.67	117.13
30	P	516	BCR	C2-C1-C6	2.17	113.88	110.48
27	E	102	LMG	C1-O6-C5	2.18	117.81	113.72
26	S	102	SQD	O48-C23-C24	2.18	118.23	111.90
21	N	614	CLA	C4-C3-C5	2.18	119.06	115.29
21	P	506	CLA	CED-O2D-CGD	2.18	121.07	115.97
30	H	101	BCR	C33-C5-C4	2.18	117.58	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	404	CLA	O2A-CGA-CBA	2.18	118.23	111.90
21	P	513	CLA	C1D-CHD-C4C	2.18	125.46	122.48
21	A	401	CLA	C2A-C1A-CHA	2.18	127.78	123.92
30	c	101	BCR	C38-C26-C27	2.18	117.59	113.45
23	A	406	PL9	C53-C6-C1	2.18	119.47	114.84
24	C	517	DGD	C6D-C5D-C4D	2.18	116.65	112.00
22	Q	403	PHO	CMC-C2C-C1C	2.18	128.44	125.04
21	P	504	CLA	O2A-CGA-CBA	2.19	118.27	111.90
21	B	605	CLA	O2A-CGA-CBA	2.19	118.28	111.90
27	R	102	LMG	C1-O6-C5	2.19	117.85	113.72
30	C	514	BCR	C29-C30-C25	2.19	113.91	110.48
27	P	521	LMG	C9-O8-C28	2.20	123.74	117.13
24	P	518	DGD	O6E-C1E-O5D	2.20	115.25	110.02
27	E	102	LMG	O7-C10-C11	2.20	116.13	111.55
21	P	504	CLA	C1-O2A-CGA	2.21	122.08	116.77
21	B	602	CLA	O2A-CGA-CBA	2.21	118.34	111.90
30	D	405	BCR	C37-C22-C23	2.21	121.63	118.10
26	N	601	SQD	O48-C23-C24	2.22	118.35	111.90
30	T	102	BCR	C30-C25-C24	2.22	121.96	115.73
30	T	102	BCR	C36-C18-C19	2.22	121.64	118.10
21	N	609	CLA	O2A-CGA-CBA	2.23	118.38	111.90
21	C	512	CLA	C4-C3-C5	2.23	119.15	115.29
23	D	404	PL9	C15-C14-C16	2.23	119.15	115.29
30	b	102	BCR	C23-C22-C21	2.23	122.36	118.94
22	A	404	PHO	CMC-C2C-C1C	2.23	128.51	125.04
21	B	614	CLA	C4-C3-C5	2.23	119.16	115.29
21	C	507	CLA	C4-C3-C5	2.24	119.17	115.29
21	C	506	CLA	C4-C3-C5	2.24	119.18	115.29
26	A	409	SQD	O5-C5-C4	2.24	113.79	109.66
21	N	619	CLA	C4-C3-C5	2.24	119.18	115.29
21	B	611	CLA	O2A-CGA-CBA	2.25	118.44	111.90
21	B	605	CLA	C4-C3-C5	2.25	119.19	115.29
24	C	517	DGD	C1D-O6D-C5D	2.25	117.95	113.72
30	C	515	BCR	C2-C1-C6	2.25	114.00	110.48
26	F	101	SQD	C3-C4-C5	2.26	114.20	110.22
21	N	607	CLA	C1-O2A-CGA	2.26	122.20	116.77
30	C	515	BCR	C30-C25-C24	2.26	122.09	115.73
26	S	102	SQD	C3-C4-C5	2.27	114.21	110.22
21	P	513	CLA	C2A-C1A-CHA	2.27	127.94	123.92
21	P	503	CLA	C4-C3-C5	2.27	119.22	115.29
27	M	101	LMG	O8-C28-C29	2.27	118.50	111.90
21	N	613	CLA	CED-O2D-CGD	2.27	121.29	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	603	CLA	C4-C3-C5	2.27	119.22	115.29
25	A	408	LHG	O8-C23-C24	2.27	118.52	111.90
26	N	601	SQD	O5-C1-O6	2.28	115.43	110.02
21	N	615	CLA	O2A-CGA-CBA	2.28	118.53	111.90
30	S	101	BCR	C37-C22-C23	2.28	121.73	118.10
26	B	627	SQD	O48-C23-C24	2.28	118.53	111.90
23	G	407	PL9	C53-C6-C1	2.28	119.69	114.84
30	N	621	BCR	C2-C1-C6	2.29	114.06	110.48
21	G	402	CLA	C2A-C1A-CHA	2.29	127.98	123.92
30	b	102	BCR	C12-C13-C14	2.29	122.46	118.94
30	K	101	BCR	C29-C30-C25	2.30	114.07	110.48
30	B	618	BCR	C30-C25-C24	2.30	122.19	115.73
31	B	626	LMT	O1B-C1B-C2B	2.30	113.29	108.11
21	C	503	CLA	C4-C3-C5	2.30	119.28	115.29
24	C	518	DGD	O6E-C1E-O5D	2.30	115.49	110.02
25	G	409	LHG	O8-C23-C24	2.30	118.60	111.90
31	a	103	LMT	O1B-C4'-C3'	2.31	112.74	107.19
23	J	101	PL9	C15-C14-C16	2.31	119.29	115.29
23	Q	405	PL9	C20-C19-C21	2.31	119.30	115.29
23	G	407	PL9	C15-C14-C16	2.31	119.30	115.29
23	G	407	PL9	C30-C29-C31	2.32	119.31	115.29
30	P	514	BCR	C35-C13-C12	2.32	121.80	118.10
27	M	101	LMG	O6-C5-C6	2.33	111.99	106.41
21	D	401	CLA	C4-C3-C5	2.33	119.33	115.29
30	c	101	BCR	C29-C30-C25	2.33	114.12	110.48
30	J	102	BCR	C12-C13-C14	2.34	122.53	118.94
22	D	402	PHO	CMC-C2C-C1C	2.34	128.69	125.04
26	B	627	SQD	O5-C1-O6	2.35	115.59	110.02
26	B	627	SQD	C3-C4-C5	2.35	114.36	110.22
21	N	614	CLA	O2A-CGA-CBA	2.36	118.75	111.90
21	G	403	CLA	O2A-CGA-CBA	2.36	118.75	111.90
31	N	625	LMT	O1B-C1B-C2B	2.36	113.42	108.11
21	P	504	CLA	C2A-C1A-CHA	2.36	128.10	123.92
21	N	618	CLA	C4-C3-C5	2.36	119.38	115.29
26	Q	408	SQD	O8-S-C6	2.37	108.90	106.01
23	D	404	PL9	C40-C39-C41	2.37	119.39	115.29
21	C	513	CLA	C2A-C1A-CHA	2.37	128.11	123.92
27	D	412	LMG	O8-C28-C29	2.37	118.79	111.90
27	C	520	LMG	O1-C1-C2	2.37	112.10	108.23
21	B	610	CLA	O2A-CGA-CBA	2.38	118.82	111.90
24	C	516	DGD	O5D-C1E-C2E	2.38	112.12	108.23
26	G	410	SQD	O48-C23-C24	2.39	118.84	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	101	PL9	C15-C14-C16	2.39	119.43	115.29
30	B	618	BCR	C38-C26-C27	2.39	117.98	113.45
21	A	402	CLA	O2A-CGA-CBA	2.39	118.85	111.90
30	T	102	BCR	C35-C13-C12	2.39	121.91	118.10
26	B	624	SQD	O7-S-C6	2.40	108.87	106.83
21	N	609	CLA	C4-C3-C5	2.40	119.45	115.29
21	B	605	CLA	C2A-C1A-CHA	2.40	128.17	123.92
23	b	101	PL9	C20-C19-C21	2.40	119.46	115.29
21	C	510	CLA	C2A-C1A-CHA	2.41	128.19	123.92
31	I	103	LMT	O1B-C4'-C3'	2.41	113.00	107.19
27	Q	401	LMG	O8-C28-C29	2.41	118.92	111.90
21	B	609	CLA	CED-O2D-CGD	2.42	121.64	115.97
21	B	607	CLA	O2A-CGA-CBA	2.42	118.95	111.90
23	A	406	PL9	C15-C14-C16	2.43	119.50	115.29
21	Q	402	CLA	C4-C3-C5	2.43	119.51	115.29
21	C	510	CLA	O2A-CGA-CBA	2.43	118.98	111.90
21	P	502	CLA	O2A-CGA-CBA	2.43	118.98	111.90
30	B	619	BCR	C2-C1-C6	2.44	114.28	110.48
27	B	623	LMG	O6-C5-C6	2.44	112.24	106.41
21	P	503	CLA	O2A-CGA-CBA	2.44	118.99	111.90
27	a	102	LMG	O8-C28-C29	2.45	119.02	111.90
21	N	618	CLA	C2A-C1A-CHA	2.45	128.26	123.92
30	T	102	BCR	C38-C26-C27	2.45	118.10	113.45
21	P	511	CLA	C4-C3-C5	2.46	119.55	115.29
21	C	502	CLA	C2A-C1A-CHA	2.46	128.27	123.92
21	A	401	CLA	O2A-CGA-CBA	2.46	119.06	111.90
21	C	502	CLA	O2A-CGA-CBA	2.46	119.06	111.90
27	R	102	LMG	O8-C28-C29	2.46	119.07	111.90
24	B	628	DGD	O5D-C1E-C2E	2.46	112.25	108.23
26	Q	408	SQD	O48-C23-C24	2.46	119.07	111.90
21	P	503	CLA	C2A-C1A-CHA	2.47	128.29	123.92
24	N	602	DGD	O5D-C1E-C2E	2.47	112.26	108.23
27	e	102	LMG	O6-C5-C6	2.47	112.32	106.41
21	N	616	CLA	C2A-C1A-CHA	2.47	128.29	123.92
21	C	503	CLA	O2A-CGA-CBA	2.47	119.08	111.90
21	A	401	CLA	C4-C3-C5	2.47	119.57	115.29
27	N	623	LMG	O8-C28-C29	2.47	119.09	111.90
21	C	504	CLA	C2A-C1A-CHA	2.48	128.31	123.92
21	N	613	CLA	O2A-CGA-CBA	2.48	119.11	111.90
21	C	505	CLA	O2A-CGA-CBA	2.48	119.11	111.90
21	N	608	CLA	C2A-C1A-CHA	2.48	128.31	123.92
21	A	403	CLA	C4-C3-C5	2.48	119.59	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	503	CLA	C2A-C1A-CHA	2.48	128.31	123.92
21	N	615	CLA	C2A-C1A-CHA	2.48	128.31	123.92
22	A	404	PHO	C4-C3-C5	2.48	119.59	115.29
21	P	509	CLA	O2A-CGA-CBA	2.48	119.12	111.90
21	P	510	CLA	C2A-C1A-CHA	2.48	128.32	123.92
21	N	614	CLA	C2A-C1A-CHA	2.49	128.32	123.92
21	C	511	CLA	C4-C3-C5	2.49	119.60	115.29
21	P	505	CLA	O2A-CGA-CBA	2.49	119.15	111.90
23	A	406	PL9	C30-C29-C31	2.50	119.62	115.29
26	B	624	SQD	O48-C23-C24	2.50	119.17	111.90
26	Q	408	SQD	O7-S-C6	2.50	108.96	106.83
21	B	614	CLA	C2A-C1A-CHA	2.50	128.35	123.92
21	N	609	CLA	C2A-C1A-CHA	2.50	128.35	123.92
27	B	623	LMG	O8-C28-C29	2.50	119.18	111.90
23	G	407	PL9	C20-C19-C21	2.50	119.63	115.29
26	A	409	SQD	O48-C23-C24	2.50	119.18	111.90
27	E	102	LMG	O8-C28-C29	2.50	119.19	111.90
27	C	520	LMG	O6-C5-C6	2.50	112.41	106.41
21	P	508	CLA	O2A-CGA-CBA	2.51	119.19	111.90
21	A	405	CLA	C4-C3-C5	2.51	119.64	115.29
22	A	404	PHO	C3C-C4C-NC	2.51	114.29	110.19
27	C	519	LMG	O1-C1-C2	2.51	112.32	108.23
21	C	508	CLA	O2A-CGA-CBA	2.51	119.20	111.90
21	B	604	CLA	C2A-C1A-CHA	2.52	128.38	123.92
27	P	521	LMG	O6-C5-C6	2.52	112.45	106.41
21	P	502	CLA	C2A-C1A-CHA	2.52	128.39	123.92
27	e	102	LMG	O8-C28-C29	2.53	119.27	111.90
21	B	606	CLA	C2A-C1A-CHA	2.53	128.41	123.92
21	B	613	CLA	O2A-CGA-CBA	2.54	119.30	111.90
21	B	611	CLA	C2A-C1A-CHA	2.54	128.43	123.92
21	C	510	CLA	C4-C3-C5	2.55	119.71	115.29
22	D	402	PHO	C3C-C4C-NC	2.55	114.36	110.19
23	J	101	PL9	C20-C19-C21	2.55	119.72	115.29
22	G	405	PHO	C3C-C4C-NC	2.55	114.36	110.19
21	G	404	CLA	C4-C3-C5	2.55	119.72	115.29
21	C	509	CLA	O2A-CGA-CBA	2.55	119.33	111.90
21	G	402	CLA	O2A-CGA-CBA	2.55	119.33	111.90
21	G	406	CLA	O2A-CGA-CBA	2.55	119.33	111.90
21	P	508	CLA	C2A-C1A-CHA	2.56	128.45	123.92
21	C	511	CLA	O2A-CGA-CBA	2.56	119.34	111.90
21	N	612	CLA	C2A-C1A-CHA	2.56	128.46	123.92
21	B	610	CLA	C2A-C1A-CHA	2.56	128.46	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	405	CLA	O2A-CGA-CBA	2.56	119.36	111.90
24	N	602	DGD	C3D-C4D-C5D	2.56	114.73	110.22
21	N	610	CLA	O2A-CGA-CBA	2.56	119.36	111.90
21	B	614	CLA	O2A-CGA-CBA	2.57	119.36	111.90
27	I	102	LMG	O8-C28-C29	2.57	119.37	111.90
21	P	510	CLA	C4-C3-C5	2.57	119.74	115.29
21	Q	402	CLA	C2A-C1A-CHA	2.57	128.47	123.92
21	N	618	CLA	O2A-CGA-CBA	2.57	119.38	111.90
21	B	612	CLA	C2A-C1A-CHA	2.57	128.48	123.92
30	B	618	BCR	C2-C1-C6	2.57	114.50	110.48
30	c	101	BCR	C2-C1-C6	2.58	114.52	110.48
30	H	101	BCR	C29-C30-C25	2.58	114.52	110.48
24	B	628	DGD	C3D-C4D-C5D	2.58	114.77	110.22
21	G	402	CLA	C4-C3-C5	2.58	119.77	115.29
30	P	516	BCR	C29-C30-C25	2.58	114.52	110.48
24	G	408	DGD	C3E-C4E-C5E	2.58	114.77	110.22
21	C	508	CLA	C2A-C1A-CHA	2.59	128.50	123.92
27	N	623	LMG	O1-C1-C2	2.59	112.46	108.23
21	N	620	CLA	O2A-CGA-CBA	2.59	119.44	111.90
21	D	401	CLA	C2A-C1A-CHA	2.59	128.51	123.92
24	Q	409	DGD	O1G-C1A-C2A	2.60	119.46	111.90
21	B	616	CLA	O2A-CGA-CBA	2.60	119.46	111.90
24	A	407	DGD	C3E-C4E-C5E	2.60	114.80	110.22
30	T	102	BCR	C2-C1-C6	2.60	114.55	110.48
26	B	624	SQD	O8-S-C6	2.60	109.19	106.01
21	A	403	CLA	C2A-C1A-CHA	2.61	128.54	123.92
21	D	403	CLA	O2A-CGA-CBA	2.61	119.49	111.90
30	B	618	BCR	C35-C13-C12	2.61	122.26	118.10
27	B	623	LMG	O1-C1-C2	2.61	112.50	108.23
21	N	610	CLA	C4-C3-C5	2.61	119.82	115.29
21	N	617	CLA	O2A-CGA-CBA	2.62	119.51	111.90
27	N	623	LMG	O6-C5-C6	2.62	112.68	106.41
22	G	405	PHO	CAC-C3C-C4C	2.62	128.29	125.21
25	G	412	LHG	O8-C23-C24	2.62	119.54	111.90
21	B	609	CLA	O2A-CGA-CBA	2.63	119.54	111.90
30	D	405	BCR	C29-C30-C25	2.63	114.59	110.48
21	B	606	CLA	C4-C3-C5	2.63	119.85	115.29
21	C	505	CLA	C2A-C1A-CHA	2.64	128.59	123.92
22	Q	403	PHO	CMB-C2B-C1B	2.64	129.15	125.04
21	B	608	CLA	C2A-C1A-CHA	2.64	128.60	123.92
27	D	407	LMG	O8-C28-C29	2.64	119.58	111.90
21	B	603	CLA	O2A-CGA-CBA	2.64	119.59	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	PL9	C20-C19-C21	2.64	119.88	115.29
21	P	509	CLA	C2A-C1A-CHA	2.65	128.61	123.92
21	Q	404	CLA	O2A-CGA-CBA	2.65	119.60	111.90
21	B	615	CLA	O2A-CGA-CBA	2.65	119.60	111.90
21	C	509	CLA	C2A-C1A-CHA	2.65	128.61	123.92
24	P	517	DGD	O5D-C1E-C2E	2.65	112.56	108.23
21	P	501	CLA	O2A-CGA-CBA	2.65	119.61	111.90
24	D	408	DGD	O1G-C1A-C2A	2.65	119.61	111.90
26	N	601	SQD	C3-C4-C5	2.65	114.89	110.22
25	A	411	LHG	O8-C23-C24	2.66	119.62	111.90
24	C	517	DGD	C3E-C4E-C5E	2.66	114.90	110.22
21	G	406	CLA	C2A-C1A-CHA	2.66	128.63	123.92
21	P	505	CLA	C2A-C1A-CHA	2.67	128.64	123.92
30	C	515	BCR	C29-C30-C25	2.67	114.64	110.48
22	Q	403	PHO	C3C-C4C-NC	2.67	114.56	110.19
21	B	613	CLA	C2A-C1A-CHA	2.68	128.66	123.92
21	C	501	CLA	O2A-CGA-CBA	2.68	119.69	111.90
21	P	513	CLA	O2A-CGA-CBA	2.68	119.69	111.90
21	A	405	CLA	C2A-C3A-C4A	2.68	106.19	101.87
21	B	607	CLA	C2A-C1A-CHA	2.68	128.67	123.92
21	B	606	CLA	O2A-CGA-CBA	2.68	119.70	111.90
27	Q	407	LMG	O8-C28-C29	2.68	119.70	111.90
21	N	605	CLA	C2A-C1A-CHA	2.68	128.67	123.92
21	B	602	CLA	C2A-C1A-CHA	2.68	128.67	123.92
22	D	402	PHO	CAC-C3C-C4C	2.69	128.37	125.21
21	N	611	CLA	O2A-CGA-CBA	2.70	119.75	111.90
24	P	518	DGD	C3E-C4E-C5E	2.70	114.97	110.22
21	P	506	CLA	C2A-C1A-CHA	2.70	128.70	123.92
21	N	617	CLA	C2A-C1A-CHA	2.70	128.71	123.92
22	D	402	PHO	CMB-C2B-C1B	2.70	129.25	125.04
21	C	513	CLA	O2A-CGA-CBA	2.71	119.77	111.90
30	S	101	BCR	C29-C30-C25	2.71	114.71	110.48
27	P	520	LMG	O1-C1-C2	2.71	112.65	108.23
21	N	607	CLA	O2A-CGA-CBA	2.71	119.78	111.90
21	A	405	CLA	C2A-C1A-CHA	2.71	128.73	123.92
21	P	510	CLA	O2A-CGA-CBA	2.71	119.79	111.90
22	Q	403	PHO	O2A-CGA-CBA	2.71	119.80	111.90
21	N	610	CLA	C2A-C1A-CHA	2.72	128.74	123.92
27	Q	401	LMG	O6-C5-C6	2.72	112.93	106.41
21	N	606	CLA	C2A-C3A-C4A	2.73	106.27	101.87
21	G	406	CLA	C2A-C3A-C4A	2.73	106.28	101.87
21	N	619	CLA	O2A-CGA-CBA	2.73	119.85	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	619	BCR	C29-C30-C25	2.74	114.75	110.48
21	B	608	CLA	O2A-CGA-CBA	2.74	119.86	111.90
30	W	101	BCR	C29-C30-C25	2.74	114.76	110.48
21	C	506	CLA	C2A-C1A-CHA	2.74	128.77	123.92
21	B	602	CLA	C2A-C3A-C4A	2.74	106.30	101.87
22	G	405	PHO	CMB-C2B-C1B	2.75	129.32	125.04
21	C	501	CLA	C2A-C1A-CHA	2.75	128.79	123.92
21	G	406	CLA	C4-C3-C5	2.75	120.05	115.29
21	B	609	CLA	C2A-C1A-CHA	2.75	128.79	123.92
21	C	506	CLA	O2A-CGA-CBA	2.75	119.90	111.90
21	N	611	CLA	C2A-C1A-CHA	2.76	128.81	123.92
21	B	601	CLA	C2A-C1A-CHA	2.76	128.81	123.92
21	G	404	CLA	C2A-C1A-CHA	2.76	128.82	123.92
30	T	102	BCR	C29-C30-C25	2.76	114.80	110.48
21	N	606	CLA	C2A-C1A-CHA	2.77	128.82	123.92
22	Q	403	PHO	CAC-C3C-C4C	2.77	128.46	125.21
21	B	610	CLA	C2A-C3A-C4A	2.77	106.34	101.87
21	P	511	CLA	C2A-C3A-C4A	2.77	106.34	101.87
21	B	607	CLA	C2A-C3A-C4A	2.77	106.35	101.87
21	A	402	CLA	C2A-C3A-C4A	2.77	106.35	101.87
21	C	511	CLA	C2A-C1A-CHA	2.77	128.84	123.92
21	N	613	CLA	C2A-C1A-CHA	2.78	128.84	123.92
27	G	411	LMG	O8-C28-C29	2.78	119.99	111.90
21	B	615	CLA	C2A-C1A-CHA	2.78	128.84	123.92
26	G	401	SQD	O48-C23-C24	2.78	119.99	111.90
21	B	612	CLA	O2A-CGA-CBA	2.79	120.01	111.90
21	N	607	CLA	C2A-C3A-C4A	2.79	106.37	101.87
21	P	511	CLA	C2A-C1A-CHA	2.79	128.87	123.92
24	C	518	DGD	O5D-C6D-C5D	2.79	113.62	108.94
21	C	511	CLA	C2A-C3A-C4A	2.80	106.40	101.87
21	B	603	CLA	C2A-C3A-C4A	2.80	106.40	101.87
21	Q	404	CLA	C2A-C1A-CHA	2.81	128.90	123.92
26	A	414	SQD	O8-S-C6	2.81	109.44	106.01
22	D	402	PHO	O2A-CGA-CBA	2.81	120.08	111.90
22	A	404	PHO	C2B-C1B-NB	2.81	113.99	109.82
21	N	611	CLA	C2A-C3A-C4A	2.81	106.42	101.87
30	N	621	BCR	C29-C30-C25	2.81	114.88	110.48
22	G	405	PHO	C4-C3-C5	2.82	120.17	115.29
21	G	403	CLA	C2A-C3A-C4A	2.82	106.42	101.87
21	P	512	CLA	C2A-C1A-CHA	2.82	128.92	123.92
21	B	604	CLA	O2A-CGA-CBA	2.82	120.12	111.90
21	N	619	CLA	C2A-C1A-CHA	2.83	128.93	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	511	CLA	O2A-CGA-CBA	2.83	120.14	111.90
21	D	403	CLA	C2A-C1A-CHA	2.83	128.94	123.92
22	D	402	PHO	C4-C3-C5	2.84	120.21	115.29
24	B	621	DGD	C1E-O6E-C5E	2.84	119.06	113.72
21	P	506	CLA	O2A-CGA-CBA	2.84	120.16	111.90
21	P	501	CLA	C2A-C1A-CHA	2.84	128.95	123.92
24	A	407	DGD	O1G-C1A-C2A	2.85	120.19	111.90
21	N	608	CLA	O2A-CGA-CBA	2.85	120.19	111.90
21	N	618	CLA	C2A-C3A-C4A	2.85	106.47	101.87
21	G	403	CLA	C2A-C1A-CHA	2.85	128.97	123.92
21	A	402	CLA	C2A-C1A-CHA	2.85	128.98	123.92
21	C	512	CLA	C2A-C1A-CHA	2.86	128.98	123.92
21	G	404	CLA	C2A-C3A-C4A	2.86	106.48	101.87
30	B	618	BCR	C29-C30-C25	2.86	114.95	110.48
24	D	408	DGD	C1E-O6E-C5E	2.86	119.10	113.72
22	Q	403	PHO	C4D-C3D-CAD	2.86	110.71	105.41
27	D	412	LMG	O6-C5-C6	2.86	113.26	106.41
27	D	406	LMG	O8-C28-C29	2.86	120.22	111.90
24	P	518	DGD	O6D-C5D-C6D	2.86	112.35	106.64
21	N	614	CLA	C2A-C3A-C4A	2.86	106.50	101.87
21	C	506	CLA	C2A-C3A-C4A	2.87	106.50	101.87
21	N	612	CLA	O2A-CGA-CBA	2.87	120.25	111.90
21	C	507	CLA	C2A-C1A-CHA	2.87	129.01	123.92
24	G	408	DGD	O1G-C1A-C2A	2.87	120.26	111.90
24	A	407	DGD	O5D-C6D-C5D	2.87	113.75	108.94
21	C	508	CLA	C2A-C3A-C4A	2.88	106.52	101.87
26	A	414	SQD	O48-C23-C24	2.88	120.28	111.90
21	P	502	CLA	C2A-C3A-C4A	2.88	106.53	101.87
21	B	614	CLA	C2A-C3A-C4A	2.88	106.53	101.87
22	A	404	PHO	CAC-C3C-C4C	2.89	128.60	125.21
21	P	507	CLA	C2A-C3A-C4A	2.89	106.53	101.87
21	C	505	CLA	C2A-C3A-C4A	2.89	106.54	101.87
21	P	506	CLA	C2A-C3A-C4A	2.89	106.54	101.87
24	G	408	DGD	O5D-C6D-C5D	2.89	113.78	108.94
21	N	617	CLA	C2A-C3A-C4A	2.89	106.54	101.87
22	G	405	PHO	C2B-C1B-NB	2.90	114.11	109.82
22	Q	403	PHO	C4-C3-C5	2.90	120.32	115.29
24	B	628	DGD	O1G-C1A-C2A	2.90	120.34	111.90
21	P	508	CLA	C2A-C3A-C4A	2.90	106.56	101.87
22	A	404	PHO	CMB-C2B-C1B	2.91	129.57	125.04
22	D	402	PHO	C2B-C1B-NB	2.91	114.12	109.82
24	B	621	DGD	O1G-C1A-C2A	2.91	120.37	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	502	CLA	C2A-C3A-C4A	2.91	106.57	101.87
22	D	402	PHO	C4D-C3D-CAD	2.91	110.81	105.41
21	P	501	CLA	C2A-C3A-C4A	2.91	106.58	101.87
24	A	407	DGD	C1D-O6D-C5D	2.92	119.21	113.72
22	D	402	PHO	C2D-C1D-ND	2.92	114.14	109.82
21	C	501	CLA	C2A-C3A-C4A	2.92	106.58	101.87
21	N	619	CLA	C2A-C3A-C4A	2.92	106.58	101.87
21	B	611	CLA	C2A-C3A-C4A	2.92	106.59	101.87
24	C	517	DGD	O6D-C5D-C6D	2.92	112.47	106.64
21	B	601	CLA	C2A-C3A-C4A	2.93	106.60	101.87
22	Q	403	PHO	C2D-C1D-ND	2.93	114.16	109.82
21	A	403	CLA	C2A-C3A-C4A	2.93	106.60	101.87
24	P	517	DGD	O1G-C1A-C2A	2.93	120.44	111.90
21	D	401	CLA	O2A-CGA-CBA	2.94	120.44	111.90
27	Q	406	LMG	O8-C28-C29	2.94	120.46	111.90
21	N	620	CLA	C2A-C1A-CHA	2.94	129.14	123.92
21	P	503	CLA	C2A-C3A-C4A	2.95	106.63	101.87
24	W	102	DGD	O1G-C1A-C2A	2.95	120.48	111.90
21	N	605	CLA	C2A-C3A-C4A	2.95	106.64	101.87
21	N	612	CLA	C2A-C3A-C4A	2.95	106.64	101.87
30	T	103	BCR	C2-C1-C6	2.95	115.09	110.48
24	C	516	DGD	O1G-C1A-C2A	2.96	120.50	111.90
21	C	507	CLA	C2A-C3A-C4A	2.96	106.64	101.87
27	a	102	LMG	O6-C5-C6	2.96	113.50	106.41
21	P	507	CLA	C2A-C1A-CHA	2.96	129.17	123.92
21	C	503	CLA	C2A-C3A-C4A	2.96	106.65	101.87
21	Q	404	CLA	C2A-C3A-C4A	2.96	106.66	101.87
22	Q	403	PHO	C2B-C1B-NB	2.97	114.21	109.82
21	N	610	CLA	C2A-C3A-C4A	2.97	106.66	101.87
27	G	411	LMG	O6-C5-C6	2.97	113.52	106.41
21	C	512	CLA	C2A-C3A-C4A	2.97	106.67	101.87
21	P	509	CLA	C2A-C3A-C4A	2.97	106.67	101.87
21	B	616	CLA	C2A-C3A-C4A	2.98	106.69	101.87
21	N	613	CLA	C2A-C3A-C4A	2.98	106.69	101.87
21	Q	402	CLA	O2A-CGA-CBA	2.98	120.58	111.90
21	D	403	CLA	C2A-C3A-C4A	2.99	106.70	101.87
21	C	509	CLA	C2A-C3A-C4A	2.99	106.70	101.87
22	A	404	PHO	C2D-C1D-ND	2.99	114.25	109.82
21	B	615	CLA	C2A-C3A-C4A	2.99	106.70	101.87
27	A	410	LMG	O8-C28-C29	2.99	120.61	111.90
21	B	616	CLA	C2A-C1A-CHA	2.99	129.23	123.92
30	K	101	BCR	C2-C1-C6	3.00	115.16	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	512	CLA	C2A-C3A-C4A	3.00	106.71	101.87
21	P	505	CLA	C2A-C3A-C4A	3.00	106.71	101.87
22	D	402	PHO	C2C-C1C-NC	3.00	114.26	109.82
21	N	615	CLA	C2A-C3A-C4A	3.00	106.72	101.87
21	B	608	CLA	C2A-C3A-C4A	3.01	106.73	101.87
26	S	102	SQD	O7-S-C6	3.01	109.40	106.83
22	Q	403	PHO	C2C-C1C-NC	3.01	114.28	109.82
21	N	616	CLA	O2A-CGA-CBA	3.01	120.67	111.90
22	D	402	PHO	C4A-NA-C1A	3.02	110.60	108.16
24	C	518	DGD	C3E-C4E-C5E	3.02	115.53	110.22
27	I	102	LMG	O6-C5-C6	3.02	113.64	106.41
22	G	405	PHO	C2D-C1D-ND	3.02	114.29	109.82
21	C	513	CLA	C2A-C3A-C4A	3.02	106.75	101.87
21	B	604	CLA	C2A-C3A-C4A	3.02	106.75	101.87
30	J	102	BCR	C31-C1-C2	3.03	120.74	108.80
21	B	609	CLA	C2A-C3A-C4A	3.03	106.76	101.87
31	B	629	LMT	O1B-C4'-C3'	3.03	114.48	107.19
22	Q	403	PHO	C4A-NA-C1A	3.03	110.61	108.16
23	Q	405	PL9	C35-C34-C36	3.03	120.55	115.29
21	B	603	CLA	C2A-C1A-CHA	3.03	129.30	123.92
21	P	504	CLA	C2A-C3A-C4A	3.04	106.77	101.87
21	C	504	CLA	C2A-C3A-C4A	3.04	106.78	101.87
22	G	405	PHO	C4A-NA-C1A	3.04	110.62	108.16
22	A	404	PHO	C2C-C1C-NC	3.04	114.32	109.82
21	N	607	CLA	C2A-C1A-CHA	3.04	129.31	123.92
21	P	513	CLA	C2A-C3A-C4A	3.05	106.79	101.87
21	N	608	CLA	C2A-C3A-C4A	3.05	106.79	101.87
21	P	510	CLA	C2A-C3A-C4A	3.05	106.79	101.87
24	N	602	DGD	O1G-C1A-C2A	3.05	120.78	111.90
30	b	102	BCR	C31-C1-C2	3.05	120.85	108.80
21	C	510	CLA	C2A-C3A-C4A	3.07	106.82	101.87
21	B	613	CLA	C2A-C3A-C4A	3.07	106.82	101.87
24	G	408	DGD	C1D-O6D-C5D	3.07	119.50	113.72
21	B	606	CLA	C2A-C3A-C4A	3.07	106.83	101.87
24	P	519	DGD	O1G-C1A-C2A	3.08	120.85	111.90
24	W	102	DGD	C1E-O6E-C5E	3.08	119.51	113.72
24	C	516	DGD	O5D-C6D-C5D	3.08	114.09	108.94
30	B	620	BCR	C2-C1-C6	3.08	115.29	110.48
24	B	628	DGD	C3E-C4E-C5E	3.08	115.65	110.22
21	N	609	CLA	C2A-C3A-C4A	3.08	106.85	101.87
21	A	401	CLA	C2A-C3A-C4A	3.09	106.85	101.87
27	P	520	LMG	O8-C28-C29	3.09	120.88	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	627	SQD	O6-C1-C2	3.09	113.27	108.23
22	A	404	PHO	C4D-C3D-CAD	3.09	111.14	105.41
21	N	620	CLA	C2A-C3A-C4A	3.09	106.86	101.87
22	G	405	PHO	C2C-C1C-NC	3.09	114.40	109.82
21	N	605	CLA	O2A-CGA-CBA	3.09	120.89	111.90
22	G	405	PHO	C4D-C3D-CAD	3.10	111.15	105.41
21	Q	402	CLA	C2A-C3A-C4A	3.10	106.87	101.87
21	B	601	CLA	O2A-CGA-CBA	3.10	120.92	111.90
22	A	404	PHO	C4A-NA-C1A	3.10	110.67	108.16
21	G	402	CLA	C2A-C3A-C4A	3.10	106.88	101.87
24	P	519	DGD	C3E-C4E-C5E	3.11	115.70	110.22
27	I	102	LMG	O1-C1-C2	3.12	113.32	108.23
23	D	404	PL9	C35-C34-C36	3.12	120.71	115.29
27	P	520	LMG	O6-C5-C6	3.13	113.90	106.41
31	N	603	LMT	O1B-C4'-C3'	3.13	114.73	107.19
24	P	517	DGD	C3E-C4E-C5E	3.13	115.74	110.22
24	C	517	DGD	O1G-C1A-C2A	3.14	121.04	111.90
24	C	518	DGD	O1G-C1A-C2A	3.15	121.06	111.90
27	C	519	LMG	O8-C28-C29	3.16	121.11	111.90
24	C	517	DGD	O5D-C6D-C5D	3.17	114.24	108.94
24	P	518	DGD	O5D-C6D-C5D	3.17	114.25	108.94
24	Q	409	DGD	O6D-C5D-C6D	3.17	112.97	106.64
23	Q	405	PL9	C25-C24-C26	3.18	120.80	115.29
26	F	101	SQD	O7-S-C6	3.18	109.55	106.83
22	G	405	PHO	O2A-CGA-CBA	3.18	121.16	111.90
21	B	605	CLA	C2A-C3A-C4A	3.18	107.01	101.87
27	E	102	LMG	O6-C5-C6	3.19	114.04	106.41
21	B	612	CLA	C2A-C3A-C4A	3.19	107.02	101.87
24	C	516	DGD	C1E-O6E-C5E	3.20	119.73	113.72
30	C	514	BCR	C34-C9-C8	3.20	123.19	118.10
21	D	401	CLA	C2A-C3A-C4A	3.20	107.04	101.87
24	P	518	DGD	O1G-C1A-C2A	3.20	121.22	111.90
23	D	404	PL9	C25-C24-C26	3.20	120.85	115.29
27	A	410	LMG	O6-C5-C6	3.21	114.09	106.41
27	a	102	LMG	O1-C1-C2	3.21	113.47	108.23
30	J	102	BCR	C29-C30-C25	3.21	115.50	110.48
30	b	102	BCR	C29-C30-C25	3.21	115.50	110.48
27	C	519	LMG	O6-C5-C6	3.21	114.10	106.41
26	F	101	SQD	O9-S-C6	3.22	109.58	106.83
24	C	516	DGD	C3E-C4E-C5E	3.22	115.90	110.22
22	A	404	PHO	O2A-CGA-CBA	3.24	121.33	111.90
24	N	602	DGD	C3E-C4E-C5E	3.24	115.93	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	409	DGD	C1E-O6E-C5E	3.25	119.83	113.72
27	Q	406	LMG	O6-C5-C6	3.25	114.20	106.41
24	P	517	DGD	O5D-C6D-C5D	3.26	114.39	108.94
23	J	101	PL9	C25-C24-C26	3.27	120.96	115.29
26	A	409	SQD	O6-C1-C2	3.27	113.57	108.23
27	R	102	LMG	O6-C5-C6	3.28	114.27	106.41
24	B	628	DGD	O6E-C5E-C4E	3.30	115.75	109.66
21	N	616	CLA	C2A-C3A-C4A	3.32	107.23	101.87
23	b	101	PL9	C25-C24-C26	3.32	121.05	115.29
30	P	514	BCR	C34-C9-C8	3.34	123.41	118.10
26	S	102	SQD	O9-S-C6	3.35	109.69	106.83
24	D	408	DGD	O6D-C5D-C6D	3.35	113.33	106.64
27	a	102	LMG	O7-C10-C11	3.35	118.52	111.55
27	B	622	LMG	O6-C5-C6	3.37	114.48	106.41
24	B	621	DGD	C3E-C4E-C5E	3.37	116.16	110.22
27	P	521	LMG	O8-C28-C29	3.37	121.71	111.90
27	I	102	LMG	O7-C10-C11	3.38	118.58	111.55
27	C	519	LMG	O7-C10-C11	3.39	118.60	111.55
27	D	406	LMG	O6-C5-C6	3.41	114.59	106.41
26	G	401	SQD	O8-S-C6	3.41	110.18	106.01
27	P	520	LMG	O7-C10-C11	3.42	118.65	111.55
24	Q	409	DGD	C3E-C4E-C5E	3.43	116.26	110.22
24	P	519	DGD	C1E-O6E-C5E	3.46	120.22	113.72
24	N	602	DGD	O6E-C5E-C4E	3.46	116.03	109.66
24	W	102	DGD	C3E-C4E-C5E	3.46	116.31	110.22
21	B	604	CLA	O2D-CGD-CBD	3.47	117.49	111.30
25	G	409	LHG	O7-C7-C8	3.48	118.78	111.55
21	B	611	CLA	O2D-CGD-CBD	3.48	117.52	111.30
24	D	408	DGD	C3E-C4E-C5E	3.49	116.37	110.22
24	D	408	DGD	O2G-C1B-C2B	3.50	118.82	111.55
26	B	627	SQD	O47-C7-C8	3.51	118.83	111.55
26	N	601	SQD	O6-C1-C2	3.51	113.96	108.23
21	D	401	CLA	O2D-CGD-CBD	3.52	117.58	111.30
26	F	101	SQD	O47-C7-C8	3.52	118.86	111.55
22	Q	403	PHO	O2D-CGD-CBD	3.53	117.61	111.30
21	P	512	CLA	O2A-CGA-CBA	3.53	122.18	111.90
21	C	512	CLA	O2A-CGA-CBA	3.57	122.30	111.90
21	Q	402	CLA	O2D-CGD-CBD	3.58	117.69	111.30
27	N	622	LMG	O6-C5-C6	3.58	114.98	106.41
25	A	408	LHG	O7-C7-C8	3.58	119.00	111.55
23	G	407	PL9	C25-C24-C26	3.59	121.51	115.29
21	N	613	CLA	O2D-CGD-CBD	3.61	117.75	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	PL9	C35-C34-C36	3.61	121.55	115.29
21	N	608	CLA	O2D-CGD-CBD	3.62	117.76	111.30
27	N	623	LMG	O7-C10-C11	3.62	119.07	111.55
26	N	601	SQD	O47-C7-C8	3.62	119.07	111.55
24	Q	409	DGD	O2G-C1B-C2B	3.63	119.08	111.55
24	G	408	DGD	C1E-O6E-C5E	3.63	120.55	113.72
27	C	520	LMG	O8-C28-C29	3.63	122.46	111.90
24	C	518	DGD	O2G-C1B-C2B	3.63	119.09	111.55
21	N	610	CLA	O2D-CGD-CBD	3.64	117.80	111.30
21	B	613	CLA	O2D-CGD-CBD	3.64	117.80	111.30
24	P	519	DGD	O2G-C1B-C2B	3.65	119.13	111.55
23	A	406	PL9	C25-C24-C26	3.66	121.63	115.29
22	D	402	PHO	O2D-CGD-CBD	3.67	117.85	111.30
27	B	622	LMG	O7-C10-C11	3.67	119.17	111.55
26	A	414	SQD	O47-C7-C8	3.67	119.17	111.55
24	P	517	DGD	C1E-O6E-C5E	3.67	120.63	113.72
26	S	102	SQD	O47-C7-C8	3.67	119.17	111.55
23	G	407	PL9	C35-C34-C36	3.67	121.66	115.29
24	N	602	DGD	O5D-C6D-C5D	3.68	115.10	108.94
24	B	628	DGD	O6D-C5D-C6D	3.68	113.99	106.64
30	C	514	BCR	C1-C6-C7	3.69	126.11	115.73
24	N	602	DGD	O6D-C5D-C6D	3.69	114.02	106.64
21	P	506	CLA	O2D-CGD-CBD	3.70	117.91	111.30
26	G	401	SQD	O47-C7-C8	3.70	119.24	111.55
27	B	623	LMG	O7-C10-C11	3.72	119.29	111.55
24	A	407	DGD	C1E-O6E-C5E	3.73	120.75	113.72
21	B	609	CLA	O2D-CGD-CBD	3.74	117.99	111.30
26	G	410	SQD	O6-C1-C2	3.76	114.36	108.23
30	P	514	BCR	C1-C6-C7	3.79	126.39	115.73
26	A	409	SQD	O47-C7-C8	3.82	119.48	111.55
26	B	624	SQD	O47-C7-C8	3.82	119.49	111.55
26	G	410	SQD	O47-C7-C8	3.83	119.50	111.55
23	D	404	PL9	C7-C3-C4	3.83	119.99	116.88
24	B	621	DGD	O2G-C1B-C2B	3.84	119.53	111.55
27	N	622	LMG	O7-C10-C11	3.87	119.59	111.55
26	Q	408	SQD	O47-C7-C8	3.87	119.59	111.55
24	B	628	DGD	O5D-C6D-C5D	3.88	115.43	108.94
24	C	516	DGD	O2G-C1B-C2B	3.88	119.61	111.55
21	B	605	CLA	O2D-CGD-CBD	3.89	118.24	111.30
21	N	607	CLA	O2D-CGD-CBD	3.90	118.27	111.30
21	N	615	CLA	O2D-CGD-CBD	3.90	118.27	111.30
21	B	603	CLA	O2D-CGD-CBD	3.91	118.29	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	102	DGD	O2G-C1B-C2B	3.93	119.71	111.55
24	C	518	DGD	C1E-O6E-C5E	3.93	121.13	113.72
25	G	412	LHG	O7-C7-C8	3.94	119.73	111.55
21	C	505	CLA	O2D-CGD-CBD	3.96	118.37	111.30
21	N	609	CLA	O2D-CGD-CBD	3.97	118.39	111.30
25	A	411	LHG	O7-C7-C8	3.97	119.79	111.55
21	N	617	CLA	O2D-CGD-CBD	3.97	118.39	111.30
21	P	505	CLA	O2D-CGD-CBD	3.98	118.40	111.30
23	A	406	PL9	C7-C3-C4	3.99	120.12	116.88
24	P	518	DGD	O2G-C1B-C2B	3.99	119.84	111.55
24	P	517	DGD	O2G-C1B-C2B	4.00	119.85	111.55
21	B	614	CLA	O2D-CGD-CBD	4.01	118.46	111.30
21	C	506	CLA	O2D-CGD-CBD	4.05	118.54	111.30
30	b	102	BCR	C2-C1-C6	4.06	116.82	110.48
21	B	601	CLA	O2D-CGD-CBD	4.06	118.56	111.30
21	B	606	CLA	O2D-CGD-CBD	4.08	118.58	111.30
21	N	618	CLA	O2D-CGD-CBD	4.09	118.61	111.30
24	C	517	DGD	O2G-C1B-C2B	4.10	120.07	111.55
27	D	407	LMG	O6-C5-C6	4.12	116.27	106.41
27	Q	407	LMG	O6-C5-C6	4.12	116.28	106.41
24	C	517	DGD	O6E-C5E-C4E	4.13	117.27	109.66
26	G	410	SQD	O8-S-C6	4.14	111.06	106.01
30	J	102	BCR	C2-C1-C6	4.17	116.99	110.48
24	G	408	DGD	O6D-C5D-C6D	4.17	114.96	106.64
24	A	407	DGD	O6D-C5D-C6D	4.18	114.98	106.64
24	P	518	DGD	O6E-C5E-C4E	4.21	117.41	109.66
26	B	624	SQD	O6-C1-C2	4.23	115.13	108.23
23	G	407	PL9	C7-C3-C4	4.23	120.31	116.88
21	N	612	CLA	O2D-CGD-CBD	4.23	118.86	111.30
27	D	407	LMG	O7-C10-C11	4.24	120.36	111.55
24	B	621	DGD	O6E-C5E-C4E	4.25	117.48	109.66
21	A	401	CLA	O2D-CGD-CBD	4.25	118.90	111.30
24	B	628	DGD	C1E-O6E-C5E	4.26	121.75	113.72
24	N	602	DGD	C1E-O6E-C5E	4.28	121.78	113.72
21	B	608	CLA	O2D-CGD-CBD	4.28	118.95	111.30
24	W	102	DGD	O6D-C5D-C6D	4.29	115.19	106.64
21	N	611	CLA	O2D-CGD-CBD	4.29	118.96	111.30
21	P	504	CLA	O2D-CGD-CBD	4.29	118.97	111.30
21	C	504	CLA	O2D-CGD-CBD	4.30	118.98	111.30
21	C	509	CLA	O2D-CGD-CBD	4.31	118.99	111.30
26	Q	408	SQD	O6-C1-C2	4.31	115.27	108.23
24	B	621	DGD	O6D-C5D-C6D	4.32	115.25	106.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	401	CLA	C4A-NA-C1A	4.32	111.82	106.45
24	W	102	DGD	O6E-C5E-C4E	4.33	117.63	109.66
21	P	509	CLA	O2D-CGD-CBD	4.33	119.03	111.30
21	N	605	CLA	O2D-CGD-CBD	4.34	119.06	111.30
21	B	602	CLA	O2D-CGD-CBD	4.34	119.06	111.30
21	C	508	CLA	O2D-CGD-CBD	4.34	119.06	111.30
24	P	517	DGD	O6D-C5D-C6D	4.35	115.33	106.64
21	B	616	CLA	O2D-CGD-CBD	4.35	119.08	111.30
26	B	624	SQD	O9-S-C6	4.36	110.55	106.83
21	P	501	CLA	O2D-CGD-CBD	4.36	119.09	111.30
24	C	516	DGD	O6E-C5E-C4E	4.37	117.70	109.66
22	A	404	PHO	O2D-CGD-CBD	4.38	119.12	111.30
27	Q	407	LMG	O7-C10-C11	4.39	120.67	111.55
24	P	519	DGD	O6D-C5D-C6D	4.39	115.40	106.64
21	C	503	CLA	O2D-CGD-CBD	4.42	119.19	111.30
21	P	507	CLA	O2D-CGD-CBD	4.42	119.20	111.30
21	A	403	CLA	C4A-NA-C1A	4.42	111.94	106.45
23	J	101	PL9	C7-C3-C4	4.43	120.48	116.88
21	B	606	CLA	C4A-NA-C1A	4.43	111.95	106.45
21	N	618	CLA	C4A-NA-C1A	4.44	111.97	106.45
27	P	521	LMG	O7-C10-C11	4.45	120.79	111.55
21	C	513	CLA	O2D-CGD-CBD	4.46	119.27	111.30
21	C	509	CLA	C4A-NA-C1A	4.46	111.99	106.45
21	C	507	CLA	O2D-CGD-CBD	4.47	119.28	111.30
21	G	403	CLA	C4A-NA-C1A	4.48	112.01	106.45
21	B	612	CLA	C4A-NA-C1A	4.48	112.01	106.45
21	G	402	CLA	O2D-CGD-CBD	4.48	119.31	111.30
21	C	506	CLA	C4A-NA-C1A	4.49	112.02	106.45
21	P	512	CLA	C4A-NA-C1A	4.49	112.03	106.45
24	P	518	DGD	C1E-O6E-C5E	4.49	122.18	113.72
24	B	628	DGD	O2G-C1B-C2B	4.50	120.90	111.55
21	N	607	CLA	C4A-NA-C1A	4.50	112.04	106.45
21	C	510	CLA	C4A-NA-C1A	4.50	112.04	106.45
21	P	513	CLA	O2D-CGD-CBD	4.50	119.35	111.30
24	P	517	DGD	O6E-C5E-C4E	4.51	117.96	109.66
21	G	402	CLA	C4A-NA-C1A	4.51	112.05	106.45
21	G	404	CLA	C4A-NA-C1A	4.51	112.05	106.45
21	P	506	CLA	C4A-NA-C1A	4.51	112.05	106.45
21	P	503	CLA	C4A-NA-C1A	4.52	112.06	106.45
21	P	503	CLA	O2D-CGD-CBD	4.52	119.38	111.30
26	Q	408	SQD	O9-S-C6	4.52	110.69	106.83
21	G	406	CLA	O2D-CGD-CBD	4.53	119.39	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	602	DGD	O2G-C1B-C2B	4.53	120.95	111.55
24	C	517	DGD	C1E-O6E-C5E	4.53	122.25	113.72
24	C	518	DGD	O6D-C5D-C6D	4.53	115.68	106.64
24	G	408	DGD	O2G-C1B-C2B	4.53	120.96	111.55
21	C	512	CLA	C4A-NA-C1A	4.53	112.08	106.45
24	C	516	DGD	O6D-C5D-C6D	4.53	115.69	106.64
21	C	510	CLA	O2D-CGD-CBD	4.53	119.40	111.30
21	N	610	CLA	C4A-NA-C1A	4.54	112.08	106.45
21	N	611	CLA	C4A-NA-C1A	4.54	112.08	106.45
27	Q	406	LMG	O7-C10-C11	4.54	120.98	111.55
21	P	510	CLA	C4A-NA-C1A	4.54	112.09	106.45
21	P	509	CLA	C4A-NA-C1A	4.54	112.09	106.45
21	C	502	CLA	O2D-CGD-CBD	4.55	119.42	111.30
21	C	501	CLA	O2D-CGD-CBD	4.55	119.43	111.30
21	N	614	CLA	C4A-NA-C1A	4.55	112.10	106.45
24	P	519	DGD	O6E-C5E-C4E	4.55	118.05	109.66
26	F	101	SQD	O8-S-C6	4.55	111.57	106.01
21	B	602	CLA	C4A-NA-C1A	4.56	112.11	106.45
21	A	405	CLA	O2D-CGD-CBD	4.56	119.45	111.30
21	Q	404	CLA	C4A-NA-C1A	4.56	112.11	106.45
21	N	605	CLA	C4A-NA-C1A	4.56	112.12	106.45
21	D	403	CLA	C4A-NA-C1A	4.56	112.12	106.45
21	B	607	CLA	O2D-CGD-CBD	4.57	119.47	111.30
21	Q	402	CLA	C4A-NA-C1A	4.57	112.13	106.45
23	Q	405	PL9	C7-C3-C4	4.58	120.60	116.88
21	B	614	CLA	C4A-NA-C1A	4.58	112.14	106.45
21	A	402	CLA	C4A-NA-C1A	4.58	112.14	106.45
27	C	520	LMG	O7-C10-C11	4.59	121.09	111.55
21	N	606	CLA	O2D-CGD-CBD	4.59	119.51	111.30
21	P	507	CLA	C4A-NA-C1A	4.59	112.15	106.45
27	D	412	LMG	O7-C10-C11	4.60	121.09	111.55
27	Q	401	LMG	O7-C10-C11	4.60	121.11	111.55
21	P	513	CLA	C4A-NA-C1A	4.61	112.17	106.45
21	N	612	CLA	C4A-NA-C1A	4.61	112.17	106.45
21	B	607	CLA	C4A-NA-C1A	4.61	112.18	106.45
21	N	615	CLA	C4A-NA-C1A	4.62	112.18	106.45
21	C	507	CLA	C4A-NA-C1A	4.62	112.19	106.45
21	B	613	CLA	C4A-NA-C1A	4.63	112.20	106.45
21	G	406	CLA	C4A-NA-C1A	4.64	112.21	106.45
21	A	405	CLA	C4A-NA-C1A	4.64	112.21	106.45
21	P	504	CLA	C4A-NA-C1A	4.64	112.21	106.45
21	N	620	CLA	C4A-NA-C1A	4.65	112.22	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	609	CLA	C4A-NA-C1A	4.65	112.22	106.45
21	C	502	CLA	C4A-NA-C1A	4.65	112.23	106.45
21	D	401	CLA	C4A-NA-C1A	4.65	112.23	106.45
21	P	511	CLA	C4A-NA-C1A	4.65	112.23	106.45
21	N	617	CLA	C4A-NA-C1A	4.66	112.23	106.45
21	P	508	CLA	C4A-NA-C1A	4.66	112.23	106.45
21	B	603	CLA	C4A-NA-C1A	4.66	112.24	106.45
21	P	502	CLA	O2D-CGD-CBD	4.66	119.63	111.30
21	N	606	CLA	C4A-NA-C1A	4.66	112.24	106.45
21	B	615	CLA	C4A-NA-C1A	4.66	112.24	106.45
21	B	616	CLA	C4A-NA-C1A	4.67	112.24	106.45
21	C	508	CLA	C4A-NA-C1A	4.67	112.25	106.45
21	P	502	CLA	C4A-NA-C1A	4.68	112.26	106.45
21	C	513	CLA	C4A-NA-C1A	4.68	112.26	106.45
27	D	406	LMG	O7-C10-C11	4.68	121.27	111.55
21	B	601	CLA	C4A-NA-C1A	4.68	112.26	106.45
21	C	504	CLA	C4A-NA-C1A	4.69	112.27	106.45
21	C	503	CLA	C4A-NA-C1A	4.69	112.27	106.45
21	N	608	CLA	C4A-NA-C1A	4.69	112.28	106.45
27	A	410	LMG	O7-C10-C11	4.70	121.30	111.55
27	G	411	LMG	O7-C10-C11	4.70	121.30	111.55
21	B	604	CLA	C4A-NA-C1A	4.70	112.28	106.45
21	N	616	CLA	O2D-CGD-CBD	4.70	119.70	111.30
24	C	518	DGD	O6E-C5E-C4E	4.70	118.32	109.66
26	S	102	SQD	O8-S-C6	4.70	111.75	106.01
21	B	610	CLA	C4A-NA-C1A	4.70	112.29	106.45
23	b	101	PL9	C7-C3-C4	4.71	120.71	116.88
21	N	613	CLA	C4A-NA-C1A	4.71	112.30	106.45
21	B	605	CLA	C4A-NA-C1A	4.72	112.31	106.45
21	N	620	CLA	O2D-CGD-CBD	4.73	119.76	111.30
21	N	619	CLA	C4A-NA-C1A	4.73	112.33	106.45
26	G	401	SQD	O9-S-C6	4.74	110.88	106.83
21	B	608	CLA	C4A-NA-C1A	4.74	112.34	106.45
21	B	612	CLA	O2D-CGD-CBD	4.75	119.78	111.30
22	G	405	PHO	O2D-CGD-CBD	4.75	119.78	111.30
21	C	501	CLA	C4A-NA-C1A	4.76	112.36	106.45
24	Q	409	DGD	O6E-C5E-C4E	4.76	118.43	109.66
26	A	409	SQD	O8-S-C6	4.77	111.83	106.01
21	P	510	CLA	O2D-CGD-CBD	4.77	119.83	111.30
21	C	511	CLA	C4A-NA-C1A	4.77	112.38	106.45
21	N	616	CLA	C4A-NA-C1A	4.77	112.38	106.45
24	A	407	DGD	O2G-C1B-C2B	4.78	121.47	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	403	CLA	O2D-CGD-CBD	4.80	119.87	111.30
21	B	610	CLA	O2D-CGD-CBD	4.83	119.92	111.30
21	P	501	CLA	C4A-NA-C1A	4.84	112.46	106.45
21	N	609	CLA	C4A-NA-C1A	4.85	112.47	106.45
21	B	611	CLA	C4A-NA-C1A	4.85	112.47	106.45
24	D	408	DGD	O6E-C5E-C4E	4.86	118.60	109.66
26	A	414	SQD	O9-S-C6	4.90	111.01	106.83
27	M	101	LMG	O7-C10-C11	4.90	121.73	111.55
21	C	512	CLA	O2D-CGD-CBD	4.95	120.14	111.30
21	P	505	CLA	C4A-NA-C1A	4.95	112.60	106.45
21	P	511	CLA	O2D-CGD-CBD	4.95	120.15	111.30
27	e	102	LMG	O7-C10-C11	4.95	121.84	111.55
21	N	614	CLA	O2D-CGD-CBD	4.96	120.16	111.30
21	G	404	CLA	O2D-CGD-CBD	4.96	120.16	111.30
21	P	508	CLA	O2D-CGD-CBD	4.97	120.17	111.30
24	A	407	DGD	O6E-C5E-C4E	5.00	118.88	109.66
21	C	505	CLA	C4A-NA-C1A	5.01	112.67	106.45
21	C	511	CLA	O2D-CGD-CBD	5.01	120.25	111.30
30	P	514	BCR	C8-C7-C6	5.08	141.49	127.25
21	P	512	CLA	O2D-CGD-CBD	5.09	120.39	111.30
24	G	408	DGD	O6E-C5E-C4E	5.11	119.08	109.66
30	C	514	BCR	C8-C7-C6	5.11	141.57	127.25
21	Q	404	CLA	O2D-CGD-CBD	5.13	120.47	111.30
21	B	615	CLA	O2D-CGD-CBD	5.17	120.54	111.30
21	D	403	CLA	O2D-CGD-CBD	5.19	120.58	111.30
26	A	409	SQD	O9-S-C6	5.19	111.27	106.83
21	N	619	CLA	O2D-CGD-CBD	5.21	120.61	111.30
21	G	403	CLA	O2D-CGD-CBD	5.37	120.90	111.30
21	A	402	CLA	O2D-CGD-CBD	5.45	121.03	111.30
26	G	410	SQD	O9-S-C6	5.74	111.74	106.83
30	J	102	BCR	C31-C1-C6	6.60	121.02	110.31
30	b	102	BCR	C31-C1-C6	6.62	121.04	110.31
26	B	627	SQD	O9-S-C6	8.25	113.88	106.83
26	N	601	SQD	O9-S-C6	8.38	113.99	106.83
22	Q	403	PHO	CMD-C2D-C1D	8.58	138.40	125.04
22	D	402	PHO	CMD-C2D-C1D	8.78	138.71	125.04
22	G	405	PHO	CMD-C2D-C1D	9.11	139.23	125.04
22	A	404	PHO	CMD-C2D-C1D	9.16	139.31	125.04
30	P	514	BCR	C7-C8-C9	9.28	140.16	126.21
30	C	514	BCR	C7-C8-C9	9.47	140.43	126.21

All (296) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	B	628	DGD	C2D
24	B	628	DGD	C5D
24	B	628	DGD	C5E
21	B	615	CLA	NC
21	B	615	CLA	ND
21	B	615	CLA	NA
21	Q	404	CLA	NC
21	Q	404	CLA	ND
21	Q	404	CLA	NA
27	I	102	LMG	C2
27	I	102	LMG	C5
21	P	512	CLA	NC
21	P	512	CLA	ND
21	P	512	CLA	NA
24	A	407	DGD	C2D
24	A	407	DGD	C5D
24	A	407	DGD	C5E
24	B	621	DGD	C2D
24	B	621	DGD	C5D
24	B	621	DGD	C5E
27	D	412	LMG	C2
27	D	412	LMG	C5
21	B	603	CLA	NC
21	B	603	CLA	ND
21	B	603	CLA	NA
21	B	609	CLA	NC
21	B	609	CLA	ND
21	B	609	CLA	NA
21	P	502	CLA	NC
21	P	502	CLA	ND
21	P	502	CLA	NA
27	G	411	LMG	C2
27	G	411	LMG	C5
21	C	506	CLA	NC
21	C	506	CLA	ND
21	C	506	CLA	NA
21	C	503	CLA	NC
21	C	503	CLA	ND
21	C	503	CLA	NA
27	N	622	LMG	C2
27	N	622	LMG	C5
21	N	605	CLA	NC
21	N	605	CLA	ND

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Mol	Chain	Res	Type	Atom
21	N	605	CLA	NA
21	D	401	CLA	NC
21	D	401	CLA	ND
21	D	401	CLA	NA
21	G	404	CLA	NC
21	G	404	CLA	ND
21	G	404	CLA	NA
21	B	611	CLA	NC
21	B	611	CLA	ND
21	B	611	CLA	NA
21	N	614	CLA	NC
21	N	614	CLA	ND
21	N	614	CLA	NA
27	R	102	LMG	C2
27	R	102	LMG	C5
21	N	608	CLA	NC
21	N	608	CLA	ND
21	N	608	CLA	NA
21	P	511	CLA	NC
21	P	511	CLA	ND
21	P	511	CLA	NA
21	N	609	CLA	NC
21	N	609	CLA	ND
21	N	609	CLA	NA
21	C	505	CLA	NC
21	C	505	CLA	ND
21	C	505	CLA	NA
27	P	520	LMG	C2
27	P	520	LMG	C5
27	A	410	LMG	C2
27	A	410	LMG	C5
21	C	511	CLA	NC
21	C	511	CLA	ND
21	C	511	CLA	NA
27	e	102	LMG	C2
27	e	102	LMG	C5
27	Q	401	LMG	C2
27	Q	401	LMG	C5
21	P	510	CLA	NC
21	P	510	CLA	ND
21	P	510	CLA	NA
21	A	405	CLA	NC

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Mol	Chain	Res	Type	Atom
21	A	405	CLA	ND
21	A	405	CLA	NA
21	B	607	CLA	NC
21	B	607	CLA	ND
21	B	607	CLA	NA
21	N	610	CLA	NC
21	N	610	CLA	ND
21	N	610	CLA	NA
24	P	517	DGD	C2D
24	P	517	DGD	C5D
24	P	517	DGD	C5E
27	D	406	LMG	C2
27	D	406	LMG	C5
21	P	501	CLA	NC
21	P	501	CLA	ND
21	P	501	CLA	NA
21	C	501	CLA	NC
21	C	501	CLA	ND
21	C	501	CLA	NA
21	C	507	CLA	NC
21	C	507	CLA	ND
21	C	507	CLA	NA
21	N	607	CLA	NC
21	N	607	CLA	ND
21	N	607	CLA	NA
27	Q	407	LMG	C2
27	Q	407	LMG	C5
21	B	608	CLA	NC
21	B	608	CLA	ND
21	B	608	CLA	NA
21	Q	402	CLA	NC
21	Q	402	CLA	ND
21	Q	402	CLA	NA
21	C	512	CLA	NC
21	C	512	CLA	ND
21	C	512	CLA	NA
21	C	502	CLA	NC
21	C	502	CLA	ND
21	C	502	CLA	NA
21	B	614	CLA	NC
21	B	614	CLA	ND
21	B	614	CLA	NA

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Mol	Chain	Res	Type	Atom
21	B	604	CLA	NC
21	B	604	CLA	ND
21	B	604	CLA	NA
21	P	505	CLA	NC
21	P	505	CLA	ND
21	P	505	CLA	NA
21	N	606	CLA	NC
21	N	606	CLA	ND
21	N	606	CLA	NA
24	P	519	DGD	C2D
24	P	519	DGD	C5D
24	P	519	DGD	C5E
21	P	503	CLA	NC
21	P	503	CLA	ND
21	P	503	CLA	NA
27	D	407	LMG	C2
27	D	407	LMG	C5
24	G	408	DGD	C2D
24	G	408	DGD	C5D
24	G	408	DGD	C5E
21	G	403	CLA	NC
21	G	403	CLA	ND
21	G	403	CLA	NA
21	D	403	CLA	NC
21	D	403	CLA	ND
21	D	403	CLA	NA
21	B	612	CLA	NC
21	B	612	CLA	ND
21	B	612	CLA	NA
21	A	401	CLA	NC
21	A	401	CLA	ND
21	A	401	CLA	NA
27	Q	406	LMG	C2
27	Q	406	LMG	C5
21	A	403	CLA	NC
21	A	403	CLA	ND
21	A	403	CLA	NA
21	N	615	CLA	NC
21	N	615	CLA	ND
21	N	615	CLA	NA
27	M	101	LMG	C2
27	M	101	LMG	C5

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Mol	Chain	Res	Type	Atom
27	B	622	LMG	C2
27	B	622	LMG	C5
21	P	506	CLA	NC
21	P	506	CLA	ND
21	P	506	CLA	NA
24	Q	409	DGD	C2D
24	Q	409	DGD	C5D
24	Q	409	DGD	C5E
21	C	509	CLA	NC
21	C	509	CLA	ND
21	C	509	CLA	NA
24	W	102	DGD	C2D
24	W	102	DGD	C5D
24	W	102	DGD	C5E
21	G	406	CLA	NC
21	G	406	CLA	ND
21	G	406	CLA	NA
21	P	507	CLA	NC
21	P	507	CLA	ND
21	P	507	CLA	NA
21	P	508	CLA	NC
21	P	508	CLA	ND
21	P	508	CLA	NA
27	C	519	LMG	C2
27	C	519	LMG	C5
24	N	602	DGD	C2D
24	N	602	DGD	C5D
24	N	602	DGD	C5E
21	N	620	CLA	NC
21	N	620	CLA	ND
21	N	620	CLA	NA
24	C	518	DGD	C2D
24	C	518	DGD	C5D
24	C	518	DGD	C5E
24	P	518	DGD	C2D
24	P	518	DGD	C5D
24	P	518	DGD	C5E
21	N	611	CLA	NC
21	N	611	CLA	ND
21	N	611	CLA	NA
27	N	623	LMG	C2
27	N	623	LMG	C5

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Mol	Chain	Res	Type	Atom
21	N	613	CLA	NC
21	N	613	CLA	ND
21	N	613	CLA	NA
24	C	516	DGD	C2D
24	C	516	DGD	C5D
24	C	516	DGD	C5E
21	P	504	CLA	NC
21	P	504	CLA	ND
21	P	504	CLA	NA
21	B	610	CLA	NC
21	B	610	CLA	ND
21	B	610	CLA	NA
21	B	602	CLA	NC
21	B	602	CLA	ND
21	B	602	CLA	NA
21	C	510	CLA	NC
21	C	510	CLA	ND
21	C	510	CLA	NA
21	A	402	CLA	NC
21	A	402	CLA	ND
21	A	402	CLA	NA
27	B	623	LMG	C2
27	B	623	LMG	C5
21	B	601	CLA	NC
21	B	601	CLA	ND
21	B	601	CLA	NA
21	G	402	CLA	NC
21	G	402	CLA	ND
21	G	402	CLA	NA
27	P	521	LMG	C2
27	P	521	LMG	C5
27	E	102	LMG	C2
27	E	102	LMG	C5
24	C	517	DGD	C2D
24	C	517	DGD	C5D
24	C	517	DGD	C5E
21	C	504	CLA	NC
21	C	504	CLA	ND
21	C	504	CLA	NA
21	N	617	CLA	NC
21	N	617	CLA	ND
21	N	617	CLA	NA

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Mol	Chain	Res	Type	Atom
21	N	616	CLA	NC
21	N	616	CLA	ND
21	N	616	CLA	NA
27	C	520	LMG	C2
27	C	520	LMG	C5
21	P	513	CLA	NC
21	P	513	CLA	ND
21	P	513	CLA	NA
21	B	606	CLA	NC
21	B	606	CLA	ND
21	B	606	CLA	NA
21	P	509	CLA	NC
21	P	509	CLA	ND
21	P	509	CLA	NA
24	D	408	DGD	C2D
24	D	408	DGD	C5D
24	D	408	DGD	C5E
21	B	605	CLA	NC
21	B	605	CLA	ND
21	B	605	CLA	NA
27	a	102	LMG	C2
27	a	102	LMG	C5
21	N	619	CLA	NC
21	N	619	CLA	ND
21	N	619	CLA	NA
21	N	618	CLA	NC
21	N	618	CLA	ND
21	N	618	CLA	NA
21	B	613	CLA	NC
21	B	613	CLA	ND
21	B	613	CLA	NA
21	C	508	CLA	NC
21	C	508	CLA	ND
21	C	508	CLA	NA
21	C	513	CLA	NC
21	C	513	CLA	ND
21	C	513	CLA	NA
21	B	616	CLA	NC
21	B	616	CLA	ND
21	B	616	CLA	NA
21	N	612	CLA	NC
21	N	612	CLA	ND

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Mol	Chain	Res	Type	Atom
21	N	612	CLA	NA

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	C	505	CLA	C1-C2-C3-C4
21	P	513	CLA	C1-C2-C3-C4
21	C	513	CLA	C1-C2-C3-C4
21	N	610	CLA	C1-C2-C3-C4
21	C	509	CLA	C1-C2-C3-C4
21	P	510	CLA	C1-C2-C3-C4
21	C	510	CLA	C1-C2-C3-C4
27	Q	407	LMG	C7-O1-C1-O6
27	D	407	LMG	C7-O1-C1-O6
26	Q	408	SQD	C45-O47-C7-C8
26	B	624	SQD	C45-O47-C7-C8

There are no ring outliers.

154 monomers are involved in 576 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	401	CLA	13	0
21	A	402	CLA	11	0
21	A	403	CLA	8	0
22	A	404	PHO	7	0
21	A	405	CLA	3	0
23	A	406	PL9	5	0
24	A	407	DGD	1	0
25	A	408	LHG	2	0
26	A	409	SQD	4	0
27	A	410	LMG	2	0
25	A	411	LHG	2	0
26	A	414	SQD	7	0
21	B	601	CLA	1	0
21	B	602	CLA	4	0
21	B	603	CLA	8	0
21	B	604	CLA	5	0
21	B	605	CLA	7	0
21	B	606	CLA	9	0
21	B	607	CLA	6	0
21	B	608	CLA	10	0
21	B	609	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	610	CLA	4	0
21	B	611	CLA	2	0
21	B	612	CLA	7	0
21	B	613	CLA	5	0
21	B	614	CLA	6	0
21	B	615	CLA	3	0
21	B	616	CLA	7	0
30	B	617	BCR	8	0
30	B	618	BCR	4	0
30	B	619	BCR	2	0
30	B	620	BCR	2	0
24	B	621	DGD	2	0
27	B	622	LMG	1	0
27	B	623	LMG	1	0
26	B	624	SQD	5	0
31	B	625	LMT	1	0
31	B	626	LMT	1	0
26	B	627	SQD	5	0
24	B	628	DGD	3	0
31	B	629	LMT	2	0
31	B	630	LMT	3	0
21	C	501	CLA	8	0
21	C	503	CLA	6	0
21	C	504	CLA	6	0
21	C	505	CLA	6	0
21	C	506	CLA	3	0
21	C	507	CLA	5	0
21	C	508	CLA	6	0
21	C	509	CLA	8	0
21	C	510	CLA	7	0
21	C	511	CLA	9	0
21	C	512	CLA	3	0
21	C	513	CLA	3	0
30	C	514	BCR	12	0
30	C	515	BCR	6	0
24	C	516	DGD	2	0
24	C	517	DGD	7	0
24	C	518	DGD	7	0
27	C	520	LMG	4	0
21	D	401	CLA	8	0
22	D	402	PHO	4	0
21	D	403	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	404	PL9	7	0
30	D	405	BCR	3	0
27	D	406	LMG	4	0
27	D	407	LMG	9	0
31	D	409	LMT	1	0
27	D	412	LMG	2	0
34	E	101	HEM	7	0
27	E	102	LMG	3	0
26	F	101	SQD	2	0
26	G	401	SQD	6	0
21	G	402	CLA	13	0
21	G	403	CLA	9	0
21	G	404	CLA	6	0
22	G	405	PHO	7	0
21	G	406	CLA	3	0
23	G	407	PL9	6	0
24	G	408	DGD	2	0
25	G	409	LHG	1	0
26	G	410	SQD	6	0
25	G	412	LHG	3	0
30	H	101	BCR	3	0
30	I	101	BCR	5	0
27	I	102	LMG	4	0
31	I	103	LMT	2	0
30	J	102	BCR	4	0
30	K	101	BCR	11	0
27	M	101	LMG	3	0
31	M	102	LMT	1	0
26	N	601	SQD	7	0
24	N	602	DGD	4	0
31	N	603	LMT	3	0
31	N	604	LMT	4	0
21	N	605	CLA	2	0
21	N	606	CLA	5	0
21	N	607	CLA	9	0
21	N	608	CLA	6	0
21	N	609	CLA	8	0
21	N	610	CLA	6	0
21	N	611	CLA	5	0
21	N	612	CLA	8	0
21	N	613	CLA	4	0
21	N	614	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	615	CLA	2	0
21	N	616	CLA	9	0
21	N	617	CLA	4	0
21	N	618	CLA	9	0
21	N	619	CLA	4	0
21	N	620	CLA	5	0
30	N	621	BCR	4	0
27	N	622	LMG	2	0
31	N	624	LMT	1	0
31	N	625	LMT	1	0
21	P	501	CLA	5	0
21	P	502	CLA	2	0
21	P	503	CLA	7	0
21	P	504	CLA	5	0
21	P	505	CLA	5	0
21	P	506	CLA	2	0
21	P	507	CLA	5	0
21	P	508	CLA	5	0
21	P	509	CLA	7	0
21	P	510	CLA	7	0
21	P	511	CLA	7	0
21	P	512	CLA	4	0
21	P	513	CLA	3	0
30	P	514	BCR	8	0
30	P	515	BCR	4	0
30	P	516	BCR	5	0
24	P	517	DGD	2	0
24	P	518	DGD	4	0
24	P	519	DGD	6	0
27	P	521	LMG	4	0
27	Q	401	LMG	2	0
21	Q	402	CLA	11	0
22	Q	403	PHO	6	0
21	Q	404	CLA	3	0
23	Q	405	PL9	6	0
27	Q	406	LMG	2	0
27	Q	407	LMG	6	0
26	Q	408	SQD	3	0
24	Q	409	DGD	1	0
34	R	101	HEM	6	0
27	R	102	LMG	2	0
30	S	101	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	T	101	BCR	3	0
30	T	102	BCR	9	0
30	T	103	BCR	3	0
34	V	201	HEM	4	0
30	W	101	BCR	4	0
24	W	102	DGD	3	0
30	Z	101	BCR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.46	28 (8%)	12 18	131, 152, 182, 204	0
1	G	335/344 (97%)	0.29	20 (5%)	23 26	128, 156, 184, 213	0
2	B	490/510 (96%)	0.57	57 (11%)	5 13	128, 158, 178, 195	0
2	N	490/510 (96%)	0.62	64 (13%)	4 11	129, 160, 180, 207	0
3	C	447/461 (96%)	0.30	22 (4%)	30 33	129, 164, 183, 211	0
3	P	447/461 (96%)	0.66	69 (15%)	2 10	139, 165, 183, 197	0
4	D	340/352 (96%)	0.33	25 (7%)	15 21	125, 152, 176, 198	0
4	Q	340/352 (96%)	0.18	13 (3%)	41 40	130, 155, 175, 184	0
5	E	82/83 (98%)	0.16	2 (2%)	59 57	148, 171, 188, 198	0
5	R	82/83 (98%)	-0.15	0	100 100	148, 171, 188, 195	0
6	F	35/44 (79%)	-0.19	1 (2%)	52 50	140, 168, 185, 199	0
6	S	35/44 (79%)	0.37	0	100 100	148, 165, 187, 188	0
7	H	65/65 (100%)	0.78	7 (10%)	6 13	154, 172, 189, 195	0
7	W	65/65 (100%)	0.85	16 (24%)	1 7	154, 173, 188, 196	0
8	I	35/38 (92%)	0.19	2 (5%)	24 28	147, 163, 174, 178	0
8	a	35/38 (92%)	0.03	0	100 100	148, 164, 179, 190	0
9	J	34/39 (87%)	0.04	0	100 100	155, 165, 183, 189	0
9	b	34/39 (87%)	1.20	8 (23%)	1 7	156, 176, 190, 190	0
10	K	37/37 (100%)	0.20	3 (8%)	13 19	158, 170, 181, 185	0
10	c	37/37 (100%)	1.36	10 (27%)	1 6	152, 171, 187, 195	0
11	L	37/37 (100%)	0.27	4 (10%)	6 13	137, 155, 186, 190	0
11	d	37/37 (100%)	0.26	4 (10%)	6 13	143, 158, 194, 201	0
12	M	34/36 (94%)	0.37	5 (14%)	3 10	147, 163, 179, 195	0
12	e	34/36 (94%)	0.43	7 (20%)	1 7	147, 159, 176, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/246 (98%)	0.83	39 (16%) 2 9	132, 162, 190, 201	0
13	f	243/246 (98%)	0.54	15 (6%) 21 25	127, 164, 191, 211	0
14	T	32/32 (100%)	0.21	0 100 100	144, 157, 187, 198	0
14	g	32/32 (100%)	0.28	3 (9%) 9 16	145, 158, 179, 198	0
15	U	97/104 (93%)	0.87	10 (10%) 7 14	136, 154, 173, 177	0
15	h	97/104 (93%)	1.72	32 (32%) 0 6	140, 154, 165, 174	0
16	V	137/137 (100%)	0.45	11 (8%) 13 19	135, 156, 170, 180	0
16	i	137/137 (100%)	0.54	11 (8%) 13 19	131, 158, 176, 185	0
17	m	28/46 (60%)	2.13	17 (60%) 0 3	167, 183, 198, 205	0
17	y	28/46 (60%)	0.46	2 (7%) 17 21	164, 182, 197, 201	0
18	X	37/40 (92%)	1.19	6 (16%) 2 9	158, 173, 188, 190	0
18	j	37/40 (92%)	0.76	2 (5%) 26 30	161, 175, 191, 202	0
19	Y	0/28	-	-	-	-
19	k	0/28	-	-	-	-
20	Z	62/62 (100%)	1.55	17 (27%) 1 6	159, 178, 198, 208	0
20	l	62/62 (100%)	0.97	5 (8%) 13 19	164, 178, 199, 208	0
All	All	5214/5482 (95%)	0.53	537 (10%) 7 14	125, 161, 185, 213	0

All (537) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	295	SER	7.7
12	M	2	GLU	6.5
16	i	132	ASN	6.5
15	U	123	GLU	6.2
2	N	393	GLU	6.0
9	b	15	THR	6.0
2	B	412	THR	5.8
2	N	388	SER	5.8
4	Q	295	SER	5.7
2	B	438	ASN	5.6
2	N	306	PRO	5.4
13	O	269	ILE	5.4
12	M	4	ASN	5.4
2	N	483	ASP	5.3
13	f	175	PRO	5.2
2	B	322	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
2	N	305	ILE	5.1
3	P	328	VAL	5.1
18	X	47	GLN	5.0
2	N	382	PRO	5.0
15	h	44	ASP	4.9
3	P	329	GLY	4.9
15	U	38	GLU	4.9
15	U	39	LEU	4.8
13	O	176	SER	4.8
13	O	56	TYR	4.8
13	f	176	SER	4.7
17	m	29	GLY	4.7
2	N	484	PRO	4.7
3	P	340	TYR	4.7
15	U	40	VAL	4.7
13	O	161	SER	4.6
2	N	408	GLY	4.6
4	D	294	ARG	4.6
3	C	137	PRO	4.5
2	B	326	ARG	4.5
11	L	37	ASN	4.5
3	P	330	SER	4.5
3	P	373	ASN	4.4
2	B	305	ILE	4.3
12	e	5	GLN	4.3
3	P	228	ASN	4.2
2	N	407	ASN	4.2
1	A	69	GLY	4.2
9	b	18	GLY	4.2
4	D	194	ASN	4.1
2	B	417	VAL	4.1
2	B	411	PHE	4.1
2	B	421	ALA	4.1
13	O	175	PRO	4.0
4	D	296	TYR	4.0
3	P	44	ASN	4.0
13	O	57	PRO	4.0
2	B	306	PRO	4.0
7	W	14	LEU	4.0
2	B	397	VAL	4.0
2	B	420	TYR	4.0
17	m	32	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	323	GLY	3.9
12	M	5	GLN	3.9
11	L	33	SER	3.9
18	X	46	VAL	3.9
12	e	7	GLY	3.9
3	P	341	LEU	3.8
13	O	162	ILE	3.8
13	f	221	GLY	3.8
13	O	90	GLU	3.8
2	B	418	LYS	3.8
17	m	28	ILE	3.8
2	N	405	GLU	3.8
10	c	32	PHE	3.8
15	h	52	GLY	3.7
1	A	79	THR	3.7
2	B	127	ARG	3.7
17	m	31	ALA	3.7
3	C	167	VAL	3.7
9	b	20	GLY	3.7
2	B	327	THR	3.7
17	m	21	GLN	3.7
4	D	297	ASP	3.6
17	m	27	MET	3.6
13	O	235	GLY	3.6
13	O	58	ILE	3.6
2	B	347	ARG	3.6
1	G	69	GLY	3.6
15	U	124	GLY	3.6
13	O	84	ASN	3.6
2	B	128	THR	3.6
13	O	217	SER	3.6
1	A	81	ALA	3.6
15	U	121	LEU	3.6
1	G	75	ASN	3.6
7	H	2	ALA	3.6
16	i	49	GLU	3.6
3	C	27	ASP	3.6
3	P	369	LEU	3.6
4	Q	294	ARG	3.5
9	b	14	ALA	3.5
1	G	81	ALA	3.5
2	N	343	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
3	P	146	PHE	3.5
11	L	34	TYR	3.5
3	C	328	VAL	3.5
9	b	17	ALA	3.5
2	N	385	ARG	3.5
15	U	122	VAL	3.5
2	N	381	ILE	3.5
3	P	325	GLY	3.5
7	W	27	THR	3.5
15	h	113	THR	3.5
2	N	307	GLU	3.5
2	N	212	ALA	3.5
20	Z	1	MET	3.4
7	W	9	ASP	3.4
13	f	190	LEU	3.4
3	P	147	PHE	3.4
2	N	409	GLN	3.4
13	f	216	PHE	3.4
3	C	327	ASN	3.4
1	G	80	GLY	3.4
2	B	352	GLU	3.4
3	P	138	GLU	3.3
1	A	266	ASN	3.3
17	m	33	PRO	3.3
2	N	394	GLN	3.3
20	Z	4	LEU	3.3
10	K	14	ALA	3.3
4	Q	194	ASN	3.3
2	N	219	VAL	3.3
15	h	47	LEU	3.3
17	m	35	ILE	3.3
2	B	348	ASN	3.3
2	N	404	GLY	3.3
1	A	10	SER	3.3
2	B	346	PHE	3.3
5	E	3	GLY	3.3
3	P	367	GLU	3.3
2	N	487	SER	3.2
17	m	34	MET	3.2
1	G	76	ASN	3.2
3	C	149	TYR	3.2
3	P	385	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
13	O	88	GLU	3.2
3	P	331	ALA	3.2
13	O	268	SER	3.2
7	W	11	LEU	3.2
16	i	78	LEU	3.2
2	B	296	ALA	3.2
2	N	380	ASP	3.2
13	O	87	GLN	3.2
13	O	85	LYS	3.2
13	O	89	ALA	3.2
16	V	49	GLU	3.2
15	h	51	TYR	3.2
8	I	3	THR	3.2
1	A	229	GLU	3.2
2	N	489	GLU	3.2
18	X	45	LYS	3.2
2	N	414	PRO	3.2
3	P	139	THR	3.2
5	E	4	THR	3.2
2	B	345	VAL	3.1
3	P	370	ARG	3.1
20	Z	2	THR	3.1
17	m	26	ALA	3.1
20	Z	62	VAL	3.1
2	N	488	PRO	3.1
2	N	295	GLY	3.1
2	N	302	TRP	3.1
3	C	326	ALA	3.1
14	g	2	GLU	3.1
2	N	403	GLY	3.1
13	O	55	ALA	3.1
2	N	490	GLN	3.1
2	N	410	THR	3.1
2	B	398	THR	3.1
15	h	108	ASN	3.1
15	U	110	GLU	3.1
1	A	268	SER	3.1
3	P	326	ALA	3.0
4	Q	344	GLU	3.0
7	W	5	THR	3.0
7	W	6	TRP	3.0
13	O	216	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
15	h	115	THR	3.0
1	G	10	SER	3.0
15	h	74	THR	3.0
1	G	79	THR	3.0
17	m	24	MET	3.0
4	Q	282	SER	3.0
10	c	26	PRO	3.0
3	C	332	GLN	3.0
9	b	26	GLY	3.0
13	O	160	THR	3.0
2	B	295	GLY	3.0
13	O	82	PRO	3.0
7	H	56	ASP	3.0
4	D	227	GLU	3.0
2	N	304	ALA	3.0
2	N	402	TYR	3.0
16	i	131	ARG	3.0
10	c	29	PRO	3.0
1	A	75	ASN	3.0
10	c	23	ASP	2.9
2	N	136	PRO	2.9
7	H	57	GLY	2.9
3	P	116	VAL	2.9
7	W	10	ILE	2.9
3	P	315	MET	2.9
7	W	4	ARG	2.9
1	A	298	ASN	2.9
7	W	13	PRO	2.9
3	P	324	LEU	2.9
13	O	86	ARG	2.9
20	Z	57	LEU	2.9
3	C	449	ARG	2.9
2	B	382	PRO	2.9
20	Z	17	PHE	2.9
1	G	171	GLY	2.9
4	D	140	PRO	2.9
3	P	351	PHE	2.9
13	f	191	ALA	2.9
16	i	47	LEU	2.9
2	B	413	ASP	2.9
3	P	342	MET	2.9
2	N	294	SER	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	190	ASN	2.8
16	i	158	GLY	2.8
15	h	69	ARG	2.8
4	D	132	ILE	2.8
2	N	204	ALA	2.8
3	P	362	ARG	2.8
7	H	6	TRP	2.8
2	N	368	VAL	2.8
13	O	244	GLU	2.8
2	B	350	GLU	2.8
13	O	207	GLU	2.8
2	B	396	GLY	2.8
1	A	177	SER	2.8
2	B	353	GLU	2.8
13	O	243	SER	2.8
15	h	55	ILE	2.8
1	A	178	GLY	2.8
2	B	444	ARG	2.8
3	P	27	ASP	2.8
13	O	236	GLU	2.8
2	B	388	SER	2.8
12	M	3	VAL	2.8
20	l	23	VAL	2.8
3	P	365	TRP	2.7
1	A	80	GLY	2.7
1	A	254	TYR	2.7
3	P	363	GLY	2.7
3	P	142	GLU	2.7
2	B	126	PRO	2.7
2	B	410	THR	2.7
3	C	164	HIS	2.7
2	N	232	GLY	2.7
3	P	137	PRO	2.7
20	Z	6	GLN	2.7
1	A	175	GLY	2.7
12	e	1	MET	2.7
2	N	435	GLU	2.7
15	h	54	LYS	2.7
2	B	416	THR	2.7
3	P	388	GLN	2.7
6	F	44	GLN	2.7
7	W	30	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
16	V	78	LEU	2.7
2	B	354	LEU	2.7
1	G	43	ALA	2.7
2	B	304	ALA	2.7
3	P	145	SER	2.7
20	Z	3	ILE	2.7
1	G	173	PRO	2.7
2	N	386	ALA	2.7
15	U	120	ALA	2.7
1	G	179	THR	2.7
2	B	439	SER	2.7
2	N	391	SER	2.7
2	N	392	PHE	2.7
3	C	148	GLY	2.7
13	f	217	SER	2.7
1	A	267	ASN	2.6
2	B	351	GLY	2.6
12	e	4	ASN	2.6
2	B	307	GLU	2.6
2	N	398	THR	2.6
3	P	210	PHE	2.6
15	h	75	LEU	2.6
13	f	153	ALA	2.6
3	P	140	LEU	2.6
16	i	77	SER	2.6
1	A	247	ASN	2.6
1	A	16	ARG	2.6
2	B	414	PRO	2.6
10	c	24	VAL	2.6
4	D	59	TYR	2.6
2	B	491	VAL	2.6
11	d	33	SER	2.6
4	D	193	LEU	2.6
3	P	349	ILE	2.6
3	P	372	PRO	2.6
13	O	68	ARG	2.6
3	P	368	PRO	2.6
1	A	222	SER	2.6
15	h	56	ASP	2.6
3	P	180	MET	2.6
1	A	179	THR	2.6
3	P	45	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
15	h	101	GLN	2.6
4	D	313	THR	2.6
17	m	19	ILE	2.6
3	P	375	LEU	2.6
2	N	412	THR	2.6
3	P	295	THR	2.6
2	N	340	TRP	2.6
12	e	2	GLU	2.6
13	f	220	LYS	2.6
11	d	37	ASN	2.6
15	h	60	THR	2.6
20	l	20	VAL	2.5
4	D	197	HIS	2.5
20	l	17	PHE	2.5
3	P	213	LEU	2.5
4	Q	342	PRO	2.5
17	m	23	THR	2.5
7	H	3	ARG	2.5
7	H	4	ARG	2.5
20	Z	8	ALA	2.5
2	N	322	GLY	2.5
4	Q	197	HIS	2.5
11	L	2	GLU	2.5
4	D	292	ASN	2.5
3	P	211	GLY	2.5
16	i	111	GLU	2.5
2	B	392	PHE	2.5
17	m	30	ILE	2.5
2	N	387	GLU	2.5
11	d	36	PHE	2.5
1	G	68	SER	2.5
4	D	241	GLU	2.5
7	W	29	PRO	2.5
9	b	16	VAL	2.5
13	O	67	ALA	2.5
3	P	62	PHE	2.4
7	W	7	LEU	2.4
3	P	209	ILE	2.4
4	D	195	PRO	2.4
7	W	8	GLY	2.4
2	B	297	THR	2.4
3	P	321	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
7	W	35	MET	2.4
15	h	68	TYR	2.4
13	f	207	GLU	2.4
1	A	190	HIS	2.4
15	h	43	VAL	2.4
13	f	222	GLN	2.4
13	O	234	THR	2.4
16	i	159	GLY	2.4
15	h	70	GLY	2.4
20	Z	5	PHE	2.4
3	P	371	GLY	2.4
12	M	7	GLY	2.4
9	b	19	MET	2.4
13	O	46	PRO	2.4
14	g	1	MET	2.4
14	g	3	THR	2.4
2	N	406	LEU	2.4
3	C	268	GLY	2.4
7	H	55	LEU	2.4
3	P	126	GLY	2.4
4	D	198	MET	2.4
3	P	208	VAL	2.4
3	P	374	GLY	2.4
2	N	68	ARG	2.4
2	N	438	ASN	2.4
10	c	20	PRO	2.4
2	N	211	ILE	2.3
15	h	41	ASN	2.3
13	O	218	LEU	2.3
3	P	332	GLN	2.3
16	V	77	SER	2.3
1	G	61	ASP	2.3
3	P	78	GLU	2.3
3	P	117	VAL	2.3
10	c	28	ILE	2.3
3	P	296	VAL	2.3
20	Z	61	VAL	2.3
17	y	45	ASN	2.3
4	D	239	GLN	2.3
13	O	270	GLU	2.3
3	C	400	PRO	2.3
4	Q	191	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
20	Z	7	LEU	2.3
3	P	174	LEU	2.3
1	G	175	GLY	2.3
20	Z	43	GLY	2.3
2	B	472	ARG	2.3
3	P	350	ILE	2.3
16	i	51	GLN	2.3
2	N	70	GLY	2.3
1	A	11	ALA	2.3
15	h	46	LYS	2.3
13	O	64	TYR	2.3
10	c	19	ASP	2.3
2	N	485	GLU	2.3
16	V	48	THR	2.3
2	N	299	GLU	2.3
7	W	15	ASN	2.3
2	B	405	GLU	2.2
2	B	325	PHE	2.2
3	C	147	PHE	2.2
16	i	48	THR	2.2
3	C	470	PRO	2.2
20	l	21	ILE	2.2
13	O	91	PHE	2.2
2	N	418	LYS	2.2
4	D	142	ASN	2.2
15	h	97	LEU	2.2
4	D	192	THR	2.2
1	G	198	HIS	2.2
3	P	389	GLU	2.2
3	C	453	ALA	2.2
10	c	25	LEU	2.2
13	f	35	ASP	2.2
3	C	135	ARG	2.2
4	D	130	PHE	2.2
1	G	11	ALA	2.2
1	A	12	ASN	2.2
12	e	34	LYS	2.2
4	Q	313	THR	2.2
13	O	271	PRO	2.2
13	f	34	ASP	2.2
3	P	229	ASN	2.2
4	D	264	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
13	O	232	GLY	2.2
16	V	37	PRO	2.2
1	A	258	LEU	2.2
17	m	36	ILE	2.2
1	A	70	SER	2.2
2	B	187	PRO	2.2
3	P	361	PHE	2.2
4	Q	200	GLY	2.2
2	B	332	LYS	2.2
15	h	111	HIS	2.2
15	U	119	THR	2.2
2	B	309	LEU	2.2
16	V	47	LEU	2.2
3	P	114	VAL	2.2
20	Z	53	VAL	2.2
2	N	215	PHE	2.2
3	P	318	LEU	2.2
1	A	27	ARG	2.1
13	O	233	ARG	2.1
10	K	13	GLU	2.1
2	B	381	ILE	2.1
15	h	59	ASN	2.1
10	K	12	PRO	2.1
16	V	50	LYS	2.1
2	N	491	VAL	2.1
3	C	121	SER	2.1
15	h	116	GLU	2.1
2	B	44	THR	2.1
12	e	3	VAL	2.1
20	Z	38	GLN	2.1
1	A	74	GLY	2.1
1	G	189	GLU	2.1
18	X	44	ASP	2.1
2	N	482	ILE	2.1
2	N	303	SER	2.1
20	Z	27	TYR	2.1
2	N	326	ARG	2.1
1	A	230	THR	2.1
15	h	92	LEU	2.1
18	j	42	GLN	2.1
2	N	293	ALA	2.1
17	m	25	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	298	PHE	2.1
17	m	20	ALA	2.1
3	P	212	TYR	2.1
1	G	226	GLU	2.1
2	N	283	GLU	2.1
3	P	227	VAL	2.1
2	B	287	ARG	2.1
3	C	151	TRP	2.1
3	P	202	PRO	2.1
20	l	44	SER	2.1
1	G	56	PRO	2.1
4	D	300	SER	2.1
13	O	66	ILE	2.1
10	c	31	LEU	2.1
16	V	45	ILE	2.1
15	h	106	ARG	2.1
18	j	34	PHE	2.1
2	B	368	VAL	2.1
15	h	53	GLU	2.1
16	V	111	GLU	2.1
2	N	218	LEU	2.1
2	N	298	LEU	2.0
3	P	339	LYS	2.0
3	C	265	ILE	2.0
15	h	67	GLN	2.0
15	h	112	PHE	2.0
1	G	225	ARG	2.0
20	Z	56	VAL	2.0
2	B	409	GLN	2.0
3	P	179	ALA	2.0
7	W	2	ALA	2.0
11	d	32	SER	2.0
15	h	57	LEU	2.0
4	Q	192	THR	2.0
13	f	32	THR	2.0
18	X	32	LEU	2.0
2	B	435	GLU	2.0
2	N	421	ALA	2.0
13	f	173	ASN	2.0
17	y	31	ALA	2.0
16	V	40	SER	2.0
15	h	120	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	395	GLN	2.0
3	C	473	ASP	2.0
3	P	28	GLN	2.0
4	Q	300	SER	2.0
2	N	137	LYS	2.0
4	Q	296	TYR	2.0
15	h	82	ASN	2.0
16	V	36	VAL	2.0
18	X	20	PHE	2.0
1	A	76	ASN	2.0
3	C	325	GLY	2.0
13	O	177	TYR	2.0
3	P	112	PHE	2.0
8	I	7	THR	2.0
2	B	185	TRP	2.0
3	P	144	SER	2.0
4	D	129	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	CL	G	415	1/1	0.86	0.90	5.26	122,122,122,122	0
27	LMG	C	520	45/55	0.29	1.14	4.76	164,178,186,187	0
31	LMT	D	409	31/35	0.56	1.06	4.73	162,187,202,208	0
30	BCR	T	103	40/40	0.49	0.88	4.69	155,168,181,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	CL	D	411	1/1	0.71	0.87	4.62	121,121,121,121	0
30	BCR	B	620	40/40	0.61	0.76	4.44	161,168,186,196	0
31	LMT	Q	410	31/35	0.38	0.73	4.18	165,182,193,197	0
30	BCR	P	514	40/40	0.71	1.52	4.07	139,152,173,175	0
21	CLA	B	603	65/65	0.82	1.03	3.98	147,166,178,179	0
31	LMT	a	103	35/35	0.47	0.87	3.72	169,180,206,216	0
24	DGD	B	628	52/66	0.73	0.47	3.66	148,173,194,200	0
30	BCR	Z	101	40/40	0.85	1.17	3.64	163,178,192,197	0
24	DGD	D	408	63/66	0.58	0.78	3.46	167,181,198,212	0
21	CLA	P	503	65/65	0.78	1.06	3.36	144,174,187,195	0
21	CLA	P	501	65/65	0.81	0.97	3.26	149,170,185,188	0
30	BCR	D	405	40/40	0.65	0.69	3.23	145,161,176,179	0
27	LMG	P	521	45/55	0.43	1.10	3.09	149,175,191,198	0
30	BCR	P	515	40/40	0.84	1.38	3.08	165,176,185,189	0
30	BCR	C	514	40/40	0.74	0.84	3.04	153,160,171,173	0
21	CLA	B	610	65/65	0.82	0.57	2.94	146,163,174,176	0
21	CLA	B	605	65/65	0.75	0.75	2.88	156,167,176,179	0
31	LMT	N	604	35/35	0.59	0.51	2.85	145,180,209,212	0
31	LMT	B	630	35/35	0.64	0.54	2.81	157,169,199,220	0
21	CLA	D	403	65/65	0.82	0.89	2.69	153,160,181,189	0
32	BCT	Q	411	4/4	0.89	0.41	2.65	164,166,168,173	0
30	BCR	H	101	40/40	0.62	0.96	2.61	165,178,188,190	0
21	CLA	C	512	65/65	0.76	1.22	2.60	173,183,196,199	0
21	CLA	P	512	65/65	0.81	1.29	2.57	172,184,194,199	0
21	CLA	P	509	65/65	0.74	0.83	2.48	152,174,181,184	0
31	LMT	N	625	35/35	0.59	0.86	2.47	165,184,206,216	0
21	CLA	B	601	65/65	0.49	1.00	2.43	167,188,199,203	0
21	CLA	B	609	65/65	0.82	0.79	2.42	162,177,185,186	0
31	LMT	I	103	35/35	0.31	1.02	2.41	153,189,201,206	0
30	BCR	K	101	40/40	0.76	0.80	2.33	154,167,176,181	0
30	BCR	C	515	40/40	0.79	0.66	2.21	139,164,177,180	0
21	CLA	B	608	65/65	0.79	0.72	2.16	147,165,180,186	0
21	CLA	C	513	65/65	0.66	1.15	2.14	173,193,206,213	0
21	CLA	B	602	65/65	0.84	0.72	2.09	152,172,182,185	0
21	CLA	B	615	65/65	0.79	0.67	2.08	162,178,191,194	0
21	CLA	P	502	65/65	0.64	0.87	2.00	146,161,175,182	0
21	CLA	B	612	65/65	0.80	0.55	1.94	152,163,174,176	0
21	CLA	P	507	65/65	0.75	0.66	1.91	162,172,191,194	0
21	CLA	B	604	65/65	0.68	0.69	1.89	148,158,172,182	0
21	CLA	N	612	65/65	0.84	0.49	1.84	151,164,181,190	0
21	CLA	C	507	65/65	0.68	0.81	1.81	159,172,185,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	N	610	65/65	0.70	0.77	1.80	152,178,191,194	0
21	CLA	G	406	65/65	0.70	0.61	1.74	145,159,181,186	0
21	CLA	P	511	65/65	0.72	1.02	1.68	156,174,184,187	0
27	LMG	D	406	46/55	0.88	0.36	1.64	140,153,176,181	0
30	BCR	J	102	40/40	0.50	0.48	1.63	167,182,207,208	0
21	CLA	A	405	65/65	0.75	0.51	1.58	144,155,176,187	0
21	CLA	C	503	65/65	0.74	0.54	1.57	155,171,181,183	0
21	CLA	N	609	65/65	0.68	0.68	1.54	148,165,174,178	0
27	LMG	Q	401	42/55	0.60	0.65	1.54	131,168,174,183	0
21	CLA	Q	404	65/65	0.81	0.60	1.51	152,162,187,194	0
21	CLA	P	513	65/65	0.67	1.01	1.51	168,182,207,216	0
21	CLA	C	502	65/65	0.68	0.51	1.50	142,157,179,185	0
24	DGD	P	518	62/66	0.82	0.44	1.47	144,168,195,200	0
24	DGD	Q	409	63/66	0.67	0.54	1.46	157,183,208,238	0
21	CLA	N	616	65/65	0.78	0.56	1.44	156,167,181,184	0
31	LMT	N	603	35/35	0.54	0.61	1.44	153,179,189,190	0
21	CLA	N	607	65/65	0.69	0.71	1.43	133,163,170,175	0
30	BCR	a	101	40/40	0.40	0.56	1.41	139,159,176,181	0
24	DGD	B	621	58/66	0.74	0.49	1.36	142,158,168,171	0
21	CLA	C	501	65/65	0.75	0.55	1.35	160,174,184,185	0
21	CLA	C	509	65/65	0.70	0.80	1.27	145,170,180,183	0
26	SQD	N	601	47/54	0.70	0.44	1.25	141,176,198,202	0
24	DGD	N	602	52/66	0.74	0.46	1.23	154,176,204,206	0
30	BCR	P	516	40/40	0.68	0.85	1.23	164,173,180,187	0
30	BCR	I	101	40/40	0.47	0.54	1.23	143,155,171,183	0
27	LMG	R	102	44/55	0.67	0.42	1.18	161,177,189,192	0
31	LMT	B	629	35/35	0.57	0.74	1.17	153,166,181,185	0
23	PL9	J	101	35/55	0.46	0.50	1.14	177,190,200,204	0
21	CLA	N	605	65/65	0.46	0.79	1.13	170,189,202,205	0
26	SQD	F	101	45/54	0.77	0.60	1.09	157,176,196,198	0
30	BCR	W	101	40/40	0.78	0.79	1.09	164,176,182,186	0
27	LMG	C	519	48/55	0.69	0.39	1.05	132,169,183,188	0
30	BCR	S	101	40/40	0.83	0.63	1.03	145,159,176,178	0
26	SQD	A	414	54/54	0.63	0.57	0.99	139,173,190,200	0
26	SQD	S	102	45/54	0.81	0.58	0.97	160,188,201,203	0
23	PL9	G	407	45/55	0.72	0.44	0.97	148,160,183,188	0
21	CLA	N	619	65/65	0.75	0.86	0.95	158,180,190,193	0
26	SQD	Q	408	43/54	0.64	0.59	0.95	143,180,193,194	0
21	CLA	N	608	65/65	0.63	0.59	0.94	146,158,176,191	0
30	BCR	c	101	40/40	0.40	1.10	0.94	151,171,188,190	0
21	CLA	N	620	65/65	0.65	0.79	0.92	156,175,192,194	0
21	CLA	N	614	65/65	0.80	0.75	0.89	150,162,173,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	PHO	D	402	64/64	0.72	0.49	0.85	135,155,161,168	0
21	CLA	B	606	65/65	0.82	0.54	0.84	156,173,194,204	0
34	HEM	E	101	43/43	0.86	0.36	0.81	166,179,188,190	0
21	CLA	C	506	65/65	0.78	0.45	0.80	159,175,202,211	0
34	HEM	R	101	43/43	0.90	0.50	0.79	164,184,192,199	0
26	SQD	B	627	47/54	0.68	0.42	0.76	143,179,209,227	0
21	CLA	A	403	65/65	0.68	0.40	0.69	142,161,183,185	0
25	LHG	G	412	37/49	0.59	0.52	0.69	147,176,193,204	0
24	DGD	W	102	58/66	0.84	0.34	0.68	145,157,168,172	0
27	LMG	E	102	44/55	0.77	0.44	0.64	168,188,198,203	0
34	HEM	i	201	43/43	0.83	0.49	0.63	131,158,169,172	0
27	LMG	D	412	42/55	0.53	0.43	0.62	147,178,195,199	0
21	CLA	N	613	65/65	0.76	0.78	0.62	160,170,177,182	0
21	CLA	B	613	65/65	0.87	0.31	0.60	148,160,171,175	0
21	CLA	C	505	65/65	0.68	0.50	0.59	147,172,186,188	0
26	SQD	G	401	54/54	0.80	0.38	0.58	158,176,209,210	0
21	CLA	P	508	65/65	0.89	0.43	0.56	157,168,182,193	0
21	CLA	P	506	65/65	0.83	0.43	0.55	159,176,194,202	0
31	LMT	B	626	35/35	0.69	0.41	0.51	163,194,202,213	0
26	SQD	B	624	43/54	0.68	0.45	0.47	150,181,199,206	0
24	DGD	A	407	56/66	0.75	0.35	0.47	147,171,188,195	0
34	HEM	V	201	43/43	0.81	0.43	0.46	139,151,166,173	0
21	CLA	P	505	65/65	0.82	0.37	0.46	134,164,180,183	0
21	CLA	P	510	65/65	0.81	0.69	0.45	145,161,170,178	0
23	PL9	A	406	45/55	0.88	0.51	0.44	152,174,185,188	0
22	PHO	Q	403	64/64	0.80	0.37	0.43	144,155,164,168	0
25	LHG	A	408	39/49	0.83	0.35	0.43	146,167,179,179	0
21	CLA	B	616	65/65	0.79	0.46	0.42	155,166,199,214	0
21	CLA	N	618	65/65	0.85	0.31	0.39	153,171,180,185	0
25	LHG	G	409	39/49	0.88	0.39	0.38	156,168,188,191	0
27	LMG	M	101	42/55	0.84	0.32	0.37	166,174,184,188	0
21	CLA	N	617	65/65	0.89	0.28	0.35	149,168,182,188	0
21	CLA	D	401	65/65	0.68	0.42	0.34	137,149,176,181	0
21	CLA	P	504	65/65	0.83	0.46	0.33	155,169,181,186	0
21	CLA	N	606	65/65	0.86	0.37	0.27	152,172,178,182	0
21	CLA	C	511	65/65	0.79	0.46	0.25	155,172,181,184	0
27	LMG	Q	406	46/55	0.84	0.41	0.24	135,162,171,180	0
21	CLA	C	508	65/65	0.90	0.34	0.19	154,170,194,203	0
21	CLA	Q	402	65/65	0.77	0.50	0.12	136,144,158,169	0
24	DGD	G	408	56/66	0.74	0.43	0.11	163,179,188,193	0
27	LMG	e	102	42/55	0.85	0.30	0.09	155,166,183,191	0
24	DGD	C	516	53/66	0.83	0.34	0.06	141,158,168,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	G	402	65/65	0.84	0.43	0.05	136,148,155,166	0
28	OEC	A	412	5/9	0.96	0.47	-0.01	122,122,126,129	0
27	LMG	D	407	48/55	0.82	0.32	-0.05	145,159,169,175	0
28	OEC	G	413	5/9	0.91	0.47	-0.06	91,102,115,124	0
30	BCR	B	617	40/40	0.74	0.28	-0.07	151,158,176,180	0
30	BCR	B	618	40/40	0.71	0.29	-0.08	149,162,168,169	0
24	DGD	C	518	66/66	0.71	0.35	-0.08	139,157,179,185	0
27	LMG	B	622	49/55	0.78	0.36	-0.11	148,163,174,176	0
27	LMG	A	410	51/55	0.87	0.30	-0.12	138,157,168,171	0
21	CLA	C	504	65/65	0.85	0.29	-0.16	153,172,198,204	0
30	BCR	B	619	40/40	0.79	0.25	-0.18	140,156,169,178	0
31	LMT	e	101	35/35	0.65	0.52	-0.18	164,176,191,195	0
24	DGD	C	517	62/66	0.78	0.35	-0.21	145,169,193,200	0
26	SQD	G	410	51/54	0.77	0.39	-0.21	161,172,184,190	0
27	LMG	P	520	48/55	0.79	0.58	-0.21	147,168,177,184	0
21	CLA	C	510	65/65	0.89	0.27	-0.23	149,161,171,178	0
21	CLA	B	614	65/65	0.83	0.29	-0.24	157,172,181,184	0
26	SQD	A	409	51/54	0.80	0.35	-0.25	156,178,191,194	0
22	PHO	A	404	64/64	0.73	0.32	-0.25	129,151,167,177	0
21	CLA	B	611	65/65	0.89	0.32	-0.26	149,160,167,169	0
21	CLA	N	615	65/65	0.88	0.30	-0.26	152,158,168,173	0
30	BCR	b	102	40/40	0.63	0.55	-0.31	158,178,202,203	0
24	DGD	P	517	53/66	0.85	0.33	-0.31	141,160,173,176	0
27	LMG	B	623	49/55	0.74	0.36	-0.33	128,147,164,167	0
31	LMT	M	102	35/35	0.69	0.59	-0.37	134,165,196,205	0
30	BCR	T	102	40/40	0.80	0.29	-0.40	143,167,176,178	0
22	PHO	G	405	64/64	0.75	0.37	-0.40	131,149,159,162	0
32	BCT	D	410	4/4	0.87	0.36	-0.43	166,167,167,169	0
24	DGD	P	519	66/66	0.83	0.32	-0.43	142,157,177,186	0
21	CLA	G	404	65/65	0.74	0.36	-0.47	141,159,179,181	0
21	CLA	A	401	65/65	0.85	0.27	-0.51	138,146,156,160	0
30	BCR	T	101	40/40	0.75	0.29	-0.51	144,167,181,184	0
21	CLA	B	607	65/65	0.79	0.30	-0.62	135,152,161,165	0
27	LMG	N	622	49/55	0.88	0.28	-0.66	145,154,172,174	0
25	LHG	A	411	37/49	0.69	0.40	-0.68	156,178,214,232	0
21	CLA	N	611	65/65	0.88	0.29	-0.71	145,156,164,166	0
27	LMG	Q	407	48/55	0.81	0.25	-0.72	142,156,168,176	0
30	BCR	N	621	40/40	0.79	0.21	-0.73	132,154,165,172	0
27	LMG	N	623	49/55	0.83	0.27	-0.77	139,152,164,171	0
21	CLA	G	403	65/65	0.79	0.33	-0.81	123,139,149,162	0
23	PL9	D	404	55/55	0.86	0.23	-0.84	129,150,158,160	0
21	CLA	A	402	65/65	0.81	0.26	-0.89	139,147,158,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	LMG	G	411	51/55	0.85	0.24	-1.00	152,164,177,178	0
23	PL9	Q	405	55/55	0.79	0.22	-1.18	137,146,166,170	0
23	PL9	b	101	35/55	0.29	0.47	-1.59	168,188,199,208	0
29	FE2	A	413	1/1	0.88	0.17	-1.71	166,166,166,166	0
29	FE2	G	414	1/1	0.92	0.17	-1.78	149,149,149,149	0
31	LMT	N	624	35/35	0.43	0.92	-	166,201,210,213	0
27	LMG	a	102	43/55	0.72	0.64	-	160,179,196,200	0
27	LMG	I	102	43/55	0.60	0.79	-	152,184,203,207	0
35	CA	O	301	1/1	0.06	0.78	-	138,138,138,138	0
35	CA	f	301	1/1	0.30	0.81	-	210,210,210,210	0
31	LMT	B	625	35/35	0.49	0.88	-	163,196,218,227	0

6.5 Other polymers [i](#)

There are no such residues in this entry.