



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2016 – 09:42 PM EST

PDB ID : 5KAF
Title : RT XFEL structure of Photosystem II in the dark state at 3.0 Å resolution
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-06-01
Resolution : 3.00 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

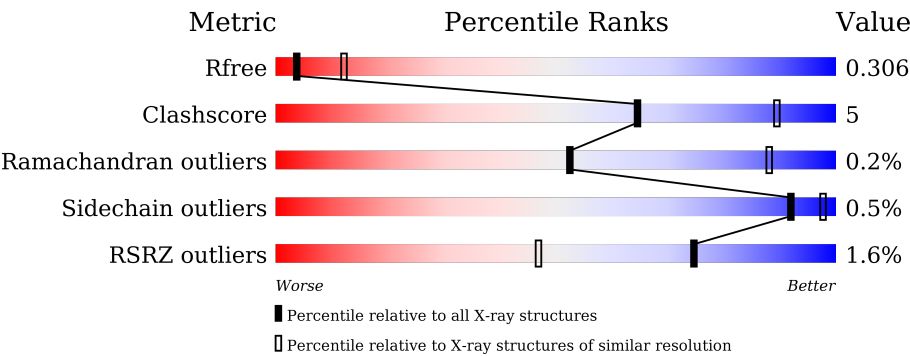
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



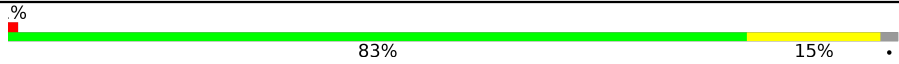
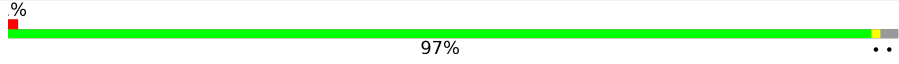
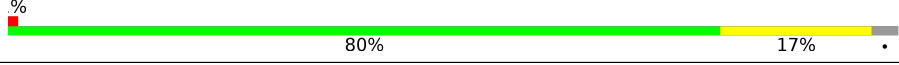
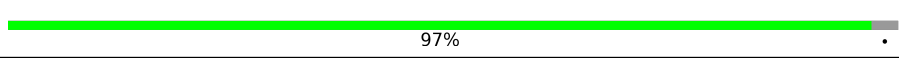
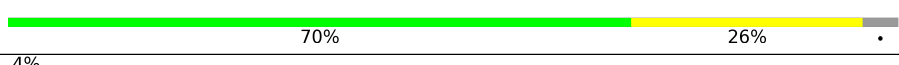
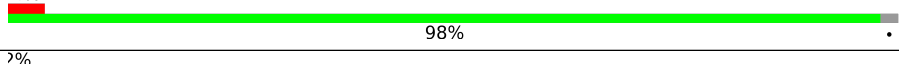
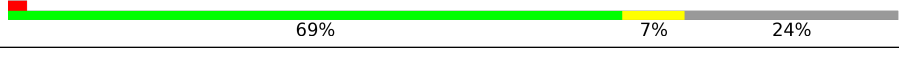

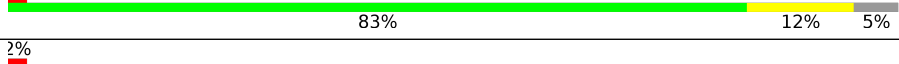
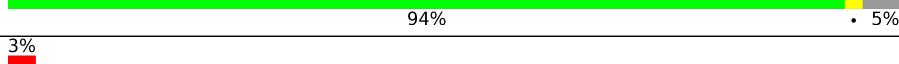

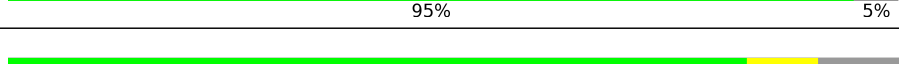
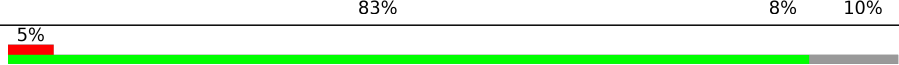
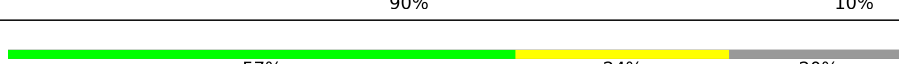

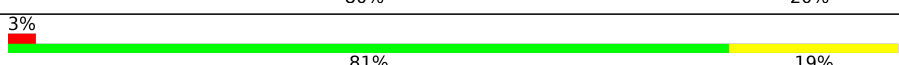
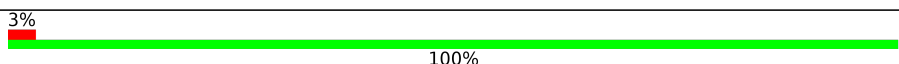
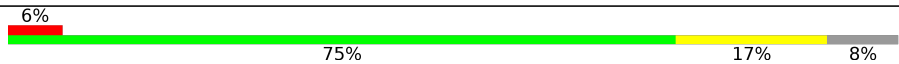
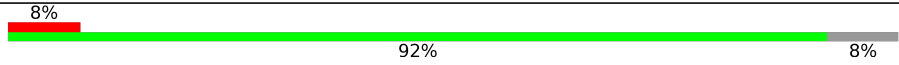

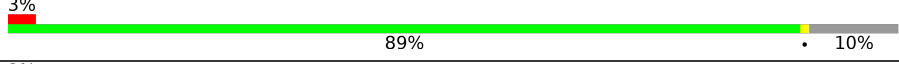
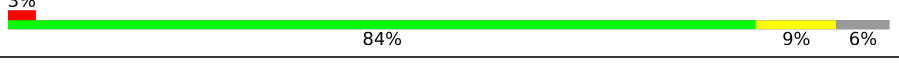
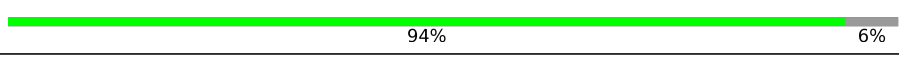


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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></div><div>77%20%.</div></div>
1	a	344	<div><div></div><div>97%. .</div></div>
2	B	510	<div><div>2%</div><div>85%14%. .</div></div>
2	b	510	<div><div>%</div><div>99%. .</div></div>

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
23	SQD	A	619	-	-	-	X
23	SQD	I	101	-	-	-	X
23	SQD	b	601	-	-	-	X
23	SQD	c	501	-	-	-	X
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	615	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	X
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	604	X	-	-	X
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
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25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	b	618	X	-	-	-
25	CLA	b	619	X	-	-	-
25	CLA	c	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	X
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	c	514	X	-	-	-
25	CLA	c	515	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
27	BCR	B	627	-	-	-	X
27	BCR	T	101	-	-	-	X
27	BCR	b	622	-	-	-	X
28	PL9	A	611	-	-	-	X
28	PL9	a	611	-	-	-	X
29	LMG	A	612	-	-	-	X
29	LMG	A	613	-	-	-	X
29	LMG	B	621	-	-	-	X
29	LMG	B	625	-	-	-	X
29	LMG	C	520	-	-	-	X
29	LMG	D	405	-	-	-	X
29	LMG	b	623	-	-	-	X
29	LMG	b	624	-	-	-	X
29	LMG	c	502	-	-	-	X
29	LMG	c	521	-	-	-	X
29	LMG	c	522	-	-	-	X
29	LMG	d	409	-	-	-	X
30	UNL	C	521	-	-	-	X
30	UNL	b	602	-	-	-	X
30	UNL	b	603	-	-	-	X
30	UNL	d	402	-	-	-	X
30	UNL	t	101	-	-	-	X
31	LHG	A	617	-	-	-	X
31	LHG	A	618	-	-	-	X
31	LHG	a	615	-	-	-	X
33	DGD	c	520	-	-	-	X
33	DGD	h	102	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50162 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2618	1715	431	457	15			
1	a	334	Total	C	N	O	S	0	0	0
			2613	1713	428	457	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3953	2596	658	686	13			
2	b	504	Total	C	N	O	S	3	1	0
			3960	2600	658	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			
4	d	341	Total	C	N	O	S	0	0	0
			2709	1798	441	458	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			657	429	106	122			
5	e	82	Total	C	N	O	0	0	0
			665	434	108	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			
6	f	34	Total	C	N	O	S	0	0	0
			274	187	45	41	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	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			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	0	0
			1845	1154	309	378	4			
13	o	244	Total	C	N	O	S	0	0	0
			1853	1160	312	377	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			279	187	45	47				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

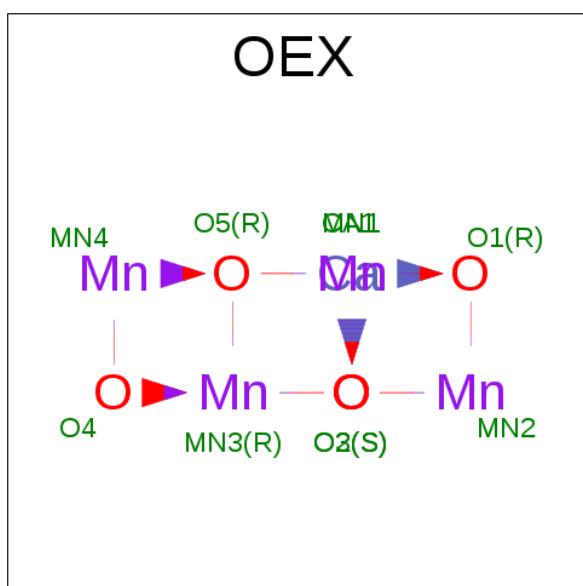
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			273	186	47	40				
20	r	34	Total	C	N	O		0	0	0
			273	186	47	40				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

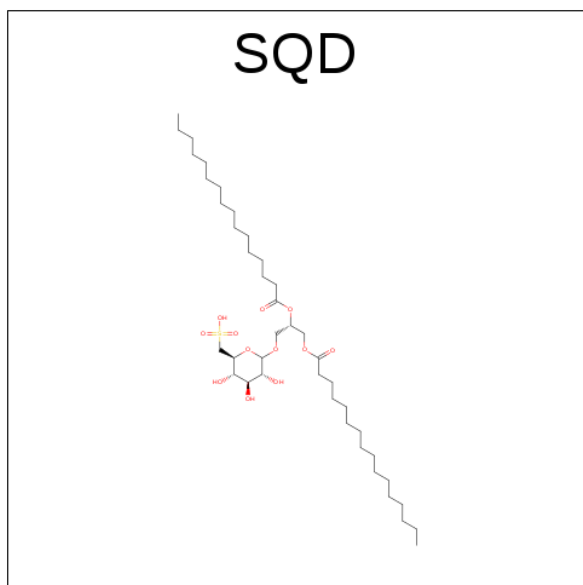
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	1	Total	Fe	0	0
			1	1		

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).

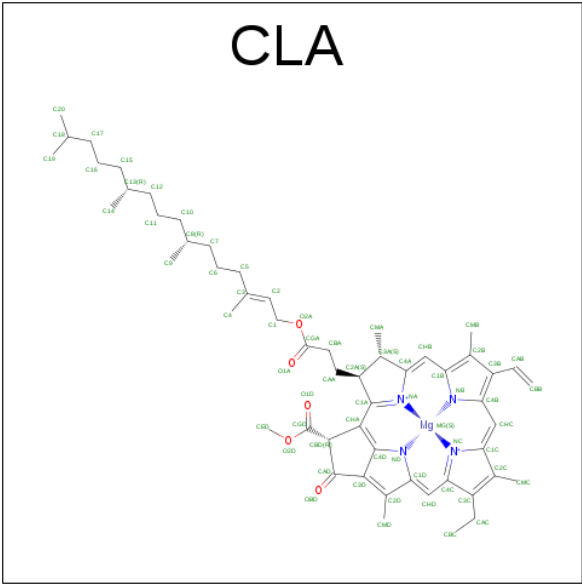


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	S	0	0
			52	39	12	1		
23	A	1	Total	C	O		0	0
			40	35	5			
23	B	1	Total	C	O	S	0	0
			54	41	12	1		
23	D	1	Total	C	O	S	0	0
			47	34	12	1		
23	D	1	Total	C	O	S	0	0
			43	30	12	1		
23	I	1	Total	C	O		0	0
			40	35	5			
23	b	1	Total	C	O	S	0	0
			54	41	12	1		
23	c	1	Total	C	O	S	0	0
			54	41	12	1		
23	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 57 47 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0

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

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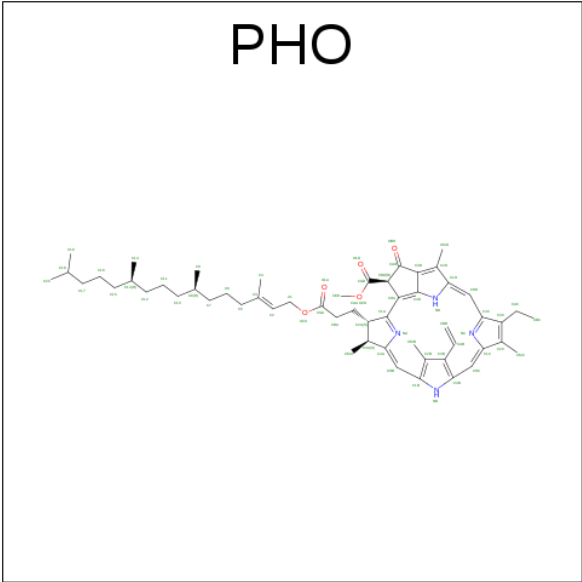
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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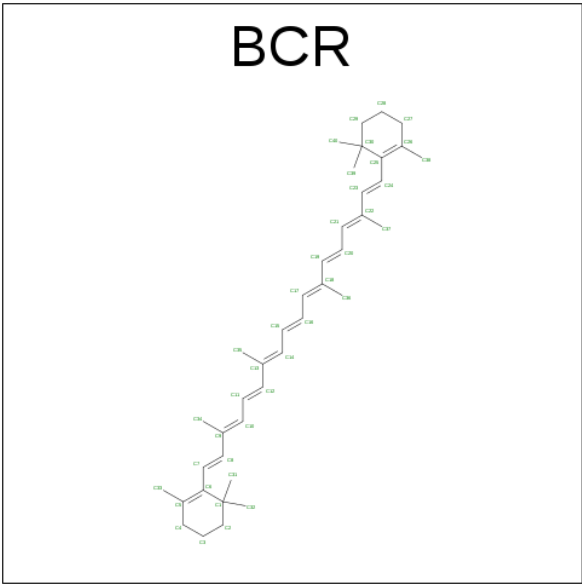
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



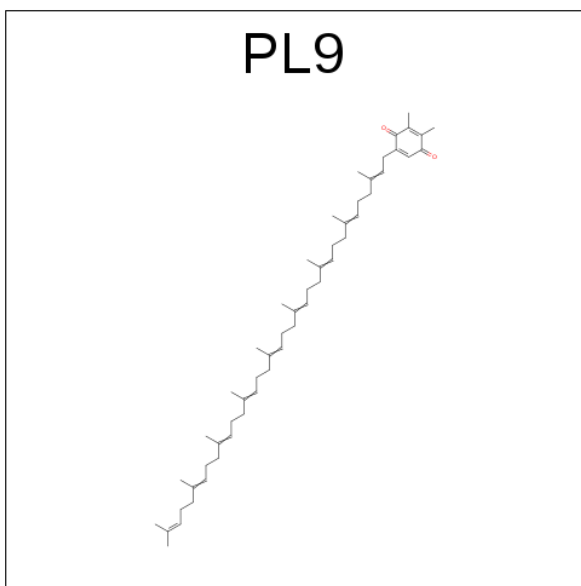
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



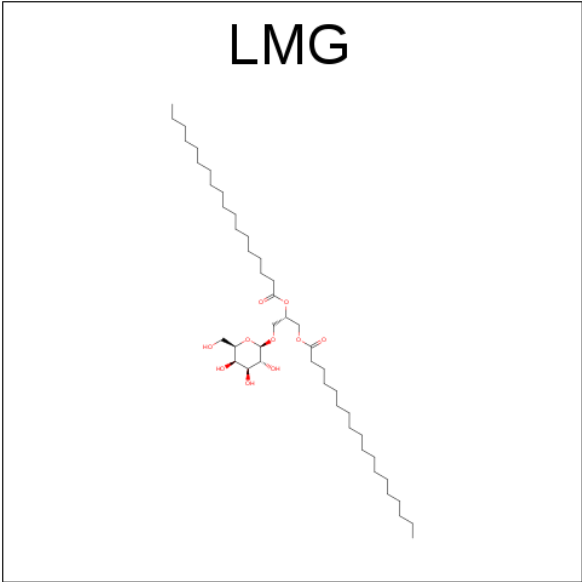
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	y	1	Total C 40 40	0	0

- Molecule 28 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
28	A	1	Total	C	O	0	0
			55	53	2		
28	D	1	Total	C	O	0	0
			55	53	2		
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C		0	0
			9	9			
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		

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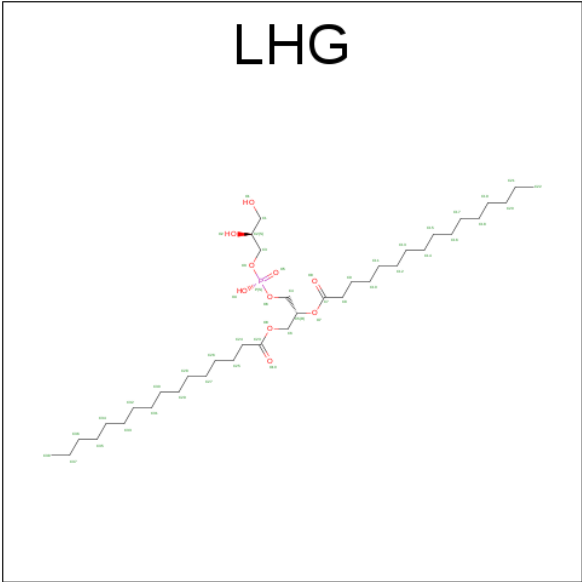
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	d	1	Total	C	O	0	0
			42	32	10		
29	d	1	Total	C	O	0	0
			40	35	5		

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

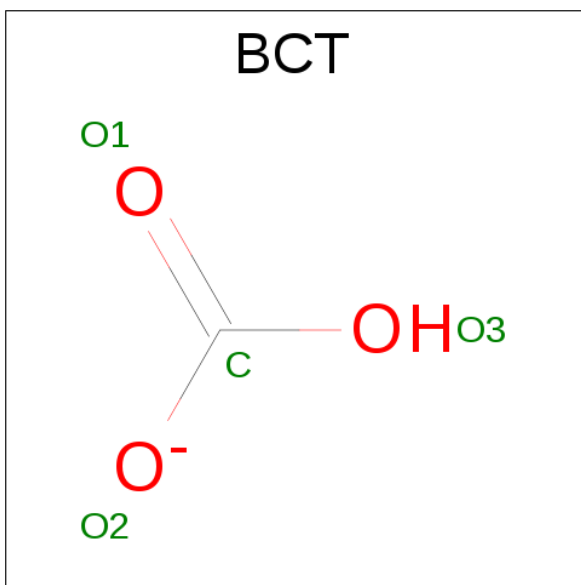
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	j	1	Total	C		0	0
			9	9			
30	d	1	Total	C		0	0
			22	22			
30	H	1	Total	C		0	0
			8	8			
30	B	3	Total	C		0	0
			28	28			
30	i	1	Total	C		0	0
			12	12			
30	C	1	Total	C		0	0
			9	9			
30	z	1	Total	C		0	0
			11	11			
30	A	1	Total	C		0	0
			7	7			
30	t	1	Total	C		0	0
			10	10			
30	m	2	Total	C		0	0
			21	21			
30	b	2	Total	C		0	0
			26	26			
30	M	2	Total	C		0	0
			23	23			

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



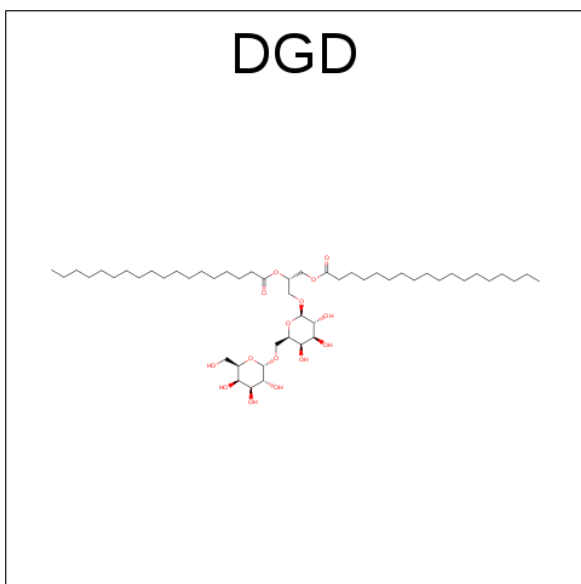
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			35	24	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



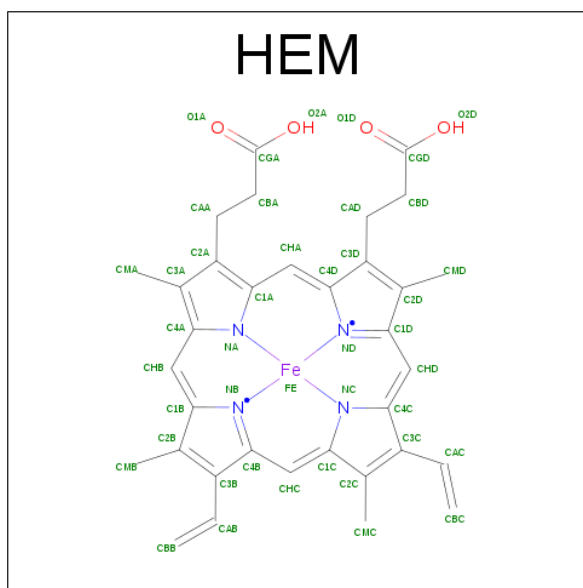
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

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



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	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

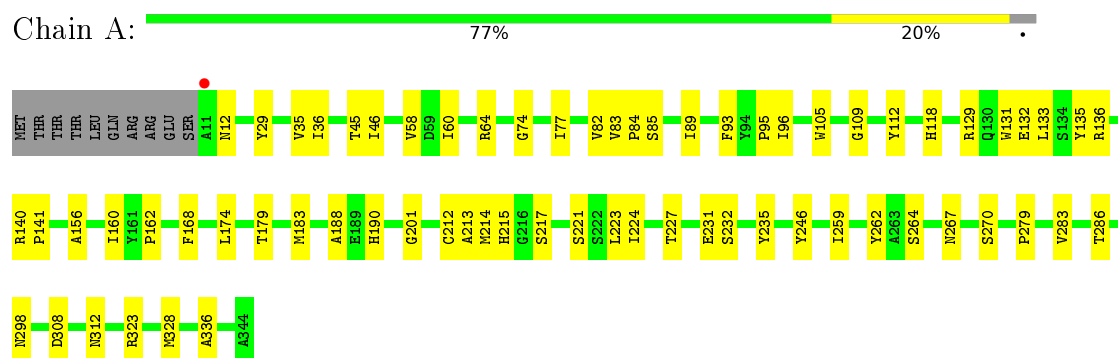
- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	10	Total O 10 10	0	0
35	B	17	Total O 17 17	0	0
35	C	11	Total O 11 11	0	0
35	D	9	Total O 9 9	0	0
35	E	3	Total O 3 3	0	0
35	L	2	Total O 2 2	0	0
35	M	2	Total O 2 2	0	0
35	O	5	Total O 5 5	0	0
35	T	1	Total O 1 1	0	0
35	V	2	Total O 2 2	0	0
35	X	1	Total O 1 1	0	0
35	Z	1	Total O 1 1	0	0
35	a	11	Total O 11 11	0	0
35	b	12	Total O 12 12	0	0
35	c	11	Total O 11 11	0	0
35	d	9	Total O 9 9	0	0
35	i	1	Total O 1 1	0	0
35	l	2	Total O 2 2	0	0
35	o	9	Total O 9 9	0	0
35	u	2	Total O 2 2	0	0
35	v	3	Total O 3 3	0	0

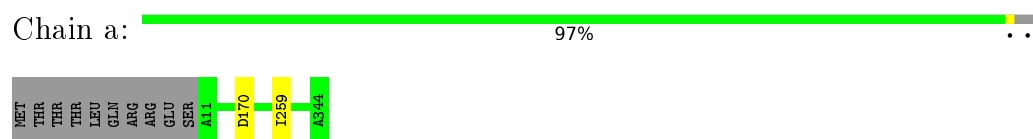
3 Residue-property plots [i](#)

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

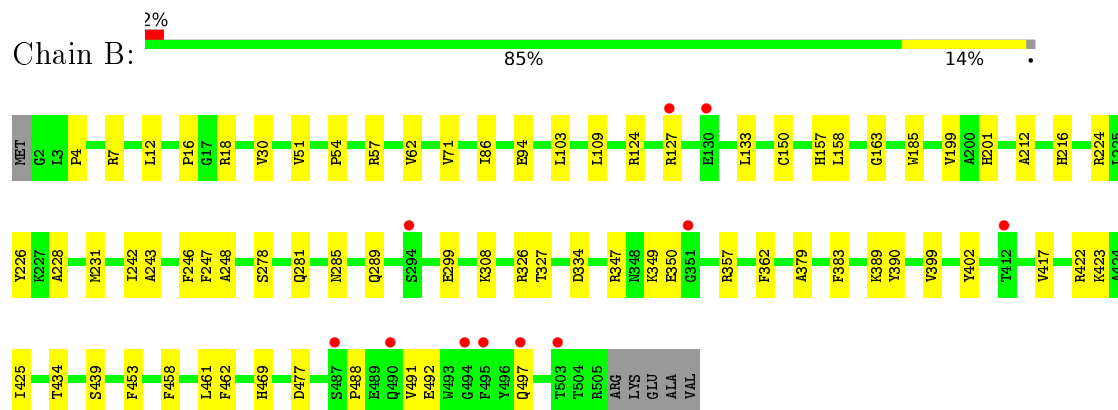
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

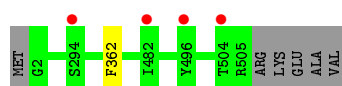


- Molecule 2: Photosystem II CP47 reaction center protein

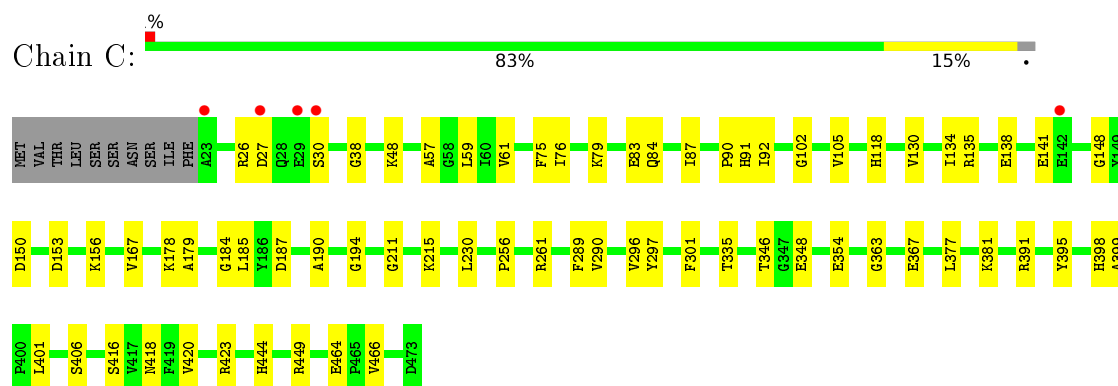


- Molecule 2: Photosystem II CP47 reaction center protein

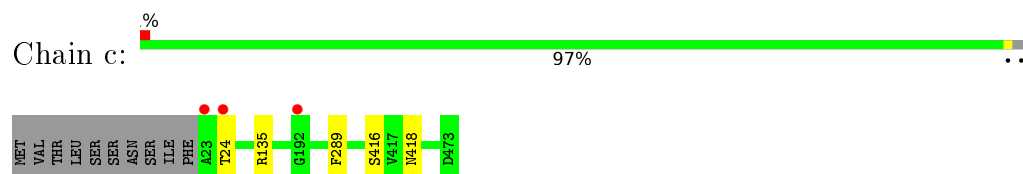




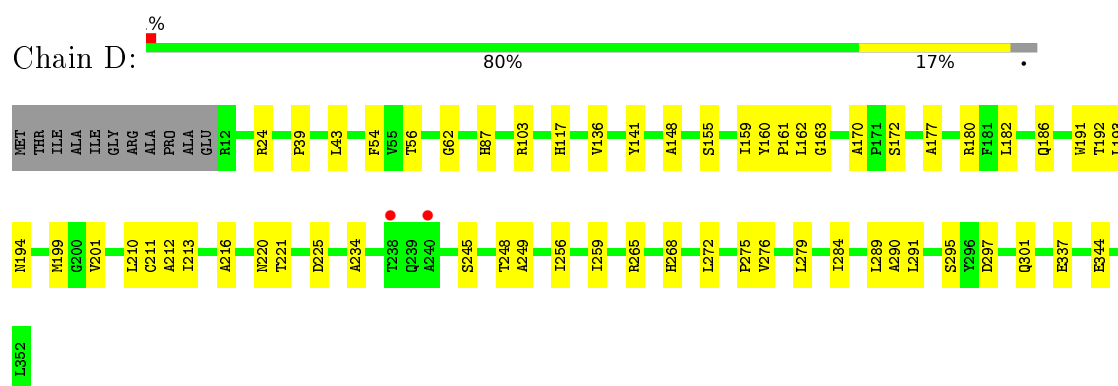
- Molecule 3: Photosystem II CP43 reaction center protein



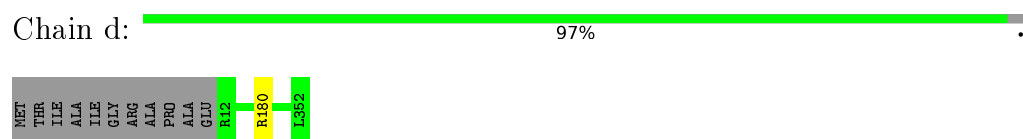
- Molecule 3: Photosystem II CP43 reaction center protein



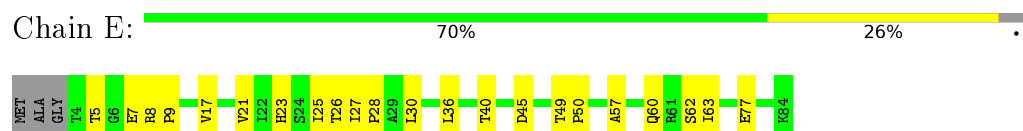
- Molecule 4: Photosystem II D2 protein



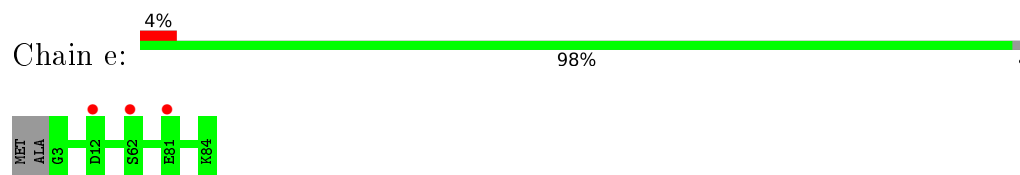
- Molecule 4: Photosystem II D2 protein



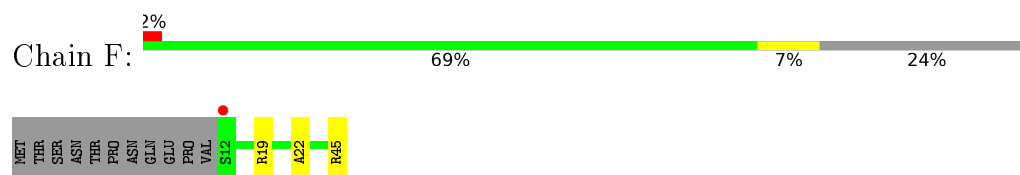
- Molecule 5: Cytochrome b559 subunit alpha



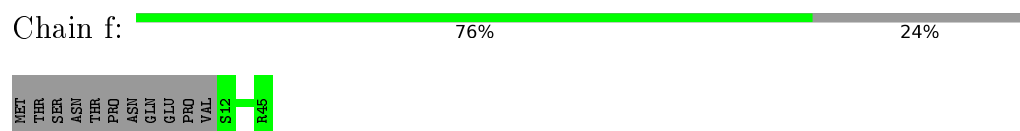
- Molecule 5: Cytochrome b559 subunit alpha



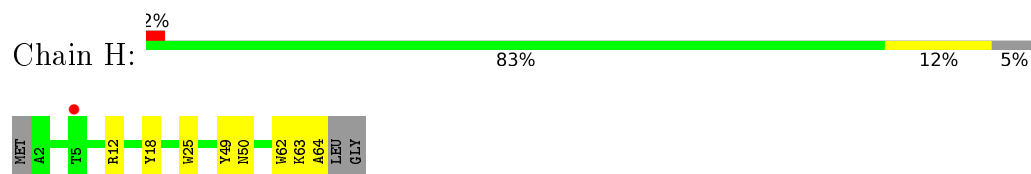
- Molecule 6: Cytochrome b559 subunit beta



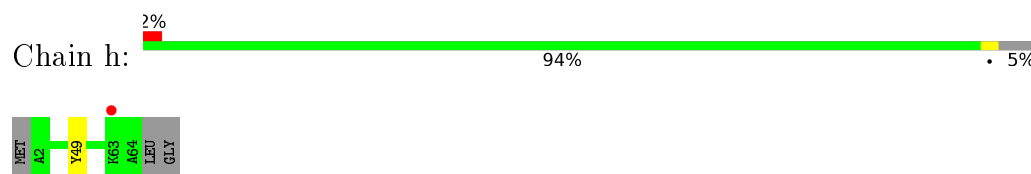
- Molecule 6: Cytochrome b559 subunit beta



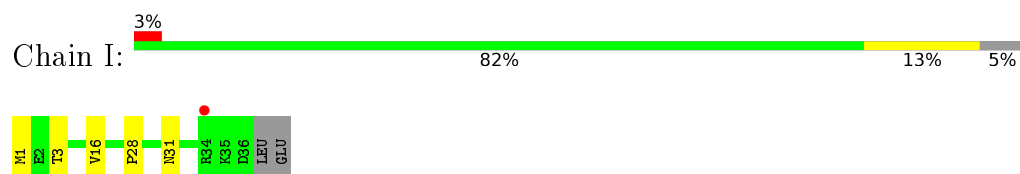
- Molecule 7: Photosystem II reaction center protein H



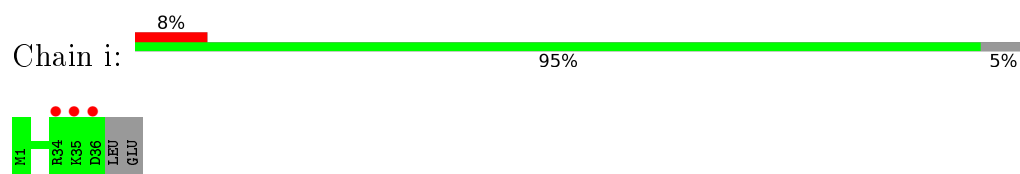
- Molecule 7: Photosystem II reaction center protein H




- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

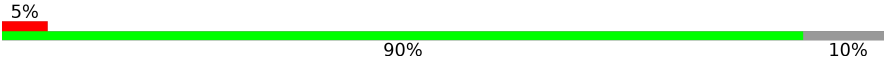


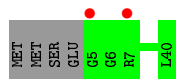
- Molecule 9: Photosystem II reaction center protein J

Chain J:  83% 8% 10%



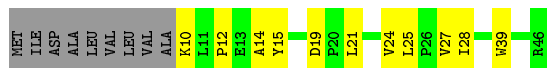
- Molecule 9: Photosystem II reaction center protein J

Chain j:  5% 90% 10%




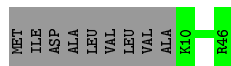
- Molecule 10: Photosystem II reaction center protein K

Chain K:  57% 24% 20%




- Molecule 10: Photosystem II reaction center protein K

Chain k:  80% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  3% 81% 19%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  3% 100%

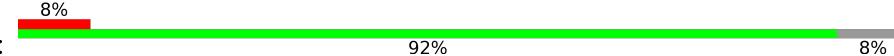


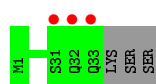
- Molecule 12: Photosystem II reaction center protein M

Chain M:  6% 75% 17% 8%

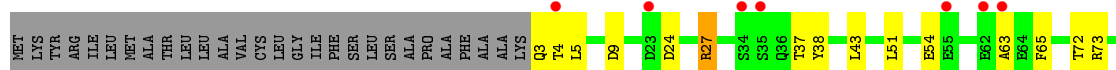
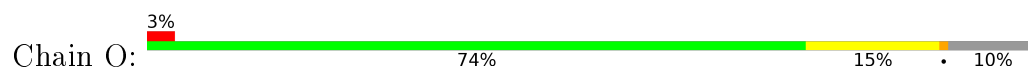


- Molecule 12: Photosystem II reaction center protein M

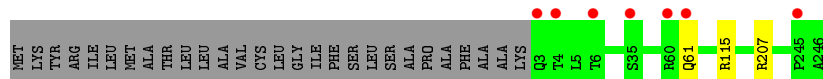
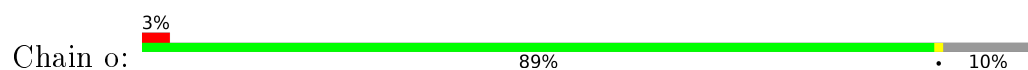
Chain m:  8% 92% 8%



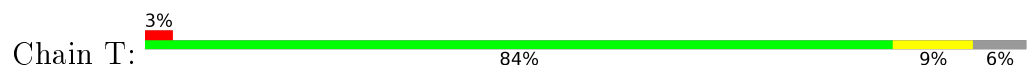
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



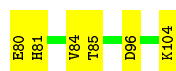
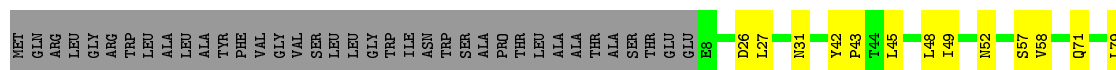
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

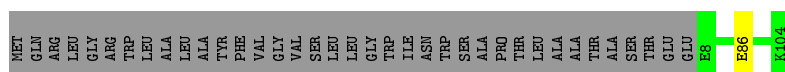


- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

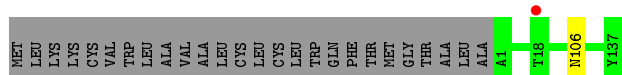
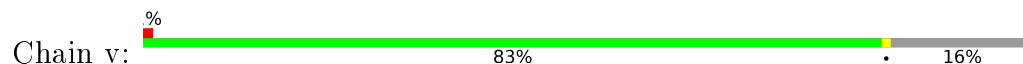




• Molecule 16: Cytochrome c-550



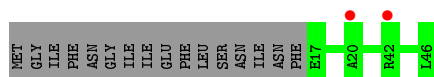
• Molecule 16: Cytochrome c-550



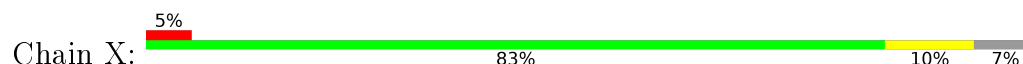
• Molecule 17: Photosystem II reaction center protein Ycf12



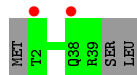
• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 18: Photosystem II reaction center X protein

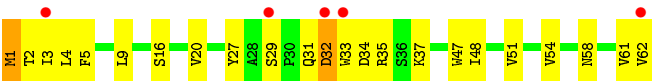


• Molecule 18: Photosystem II reaction center X protein

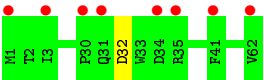


• Molecule 19: Photosystem II reaction center protein Z





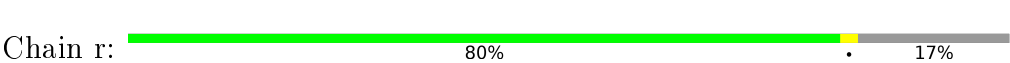
• Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.73Å 223.81Å 330.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 3.00 43.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.12-3.00) 86.3 (43.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_2411)	Depositor
R, R_{free}	0.264 , 0.303 0.267 , 0.306	Depositor DCC
R_{free} test set	1446 reflections (0.97%)	DCC
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50162	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, OEX, PHO, DGD, CL, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2703	0.39	0/3687
1	a	0.24	0/2698	0.39	0/3681
2	B	0.25	0/4093	0.39	0/5580
2	b	0.25	0/4103	0.39	0/5593
3	C	0.24	0/3599	0.39	0/4900
3	c	0.24	0/3599	0.38	0/4900
4	D	0.25	0/2811	0.39	0/3830
4	d	0.25	0/2804	0.39	0/3821
5	E	0.30	0/676	0.39	0/924
5	e	0.23	0/684	0.39	0/933
6	F	0.24	0/283	0.37	0/386
6	f	0.24	0/283	0.37	0/386
7	H	0.24	0/511	0.41	0/697
7	h	0.24	0/511	0.40	0/697
8	I	0.24	0/293	0.37	0/396
8	i	0.25	0/293	0.38	0/396
9	J	0.24	0/263	0.37	0/356
9	j	0.24	0/263	0.38	0/356
10	K	0.25	0/303	0.40	0/416
10	k	0.25	0/303	0.37	0/416
11	L	0.24	0/308	0.37	0/419
11	l	0.23	0/308	0.36	0/419
12	M	0.24	0/249	0.35	0/341
12	m	0.24	0/249	0.35	0/341
13	O	0.24	0/1876	0.45	0/2549
13	o	0.24	0/1884	0.45	0/2557
14	T	0.26	0/257	0.35	0/349
14	t	0.26	0/257	0.36	0/349
15	U	0.23	0/785	0.40	0/1064
15	u	0.24	0/785	0.41	0/1064
16	V	0.23	0/1085	0.40	0/1473
16	v	0.22	0/1085	0.41	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.27	0/225	0.54	0/301
17	y	0.24	0/225	0.37	0/301
18	X	0.23	0/282	0.35	0/381
18	x	0.24	0/284	0.37	0/384
19	Z	0.23	0/490	0.34	0/669
19	z	0.24	0/490	0.36	0/669
20	R	0.21	0/279	0.36	0/383
20	r	0.22	0/279	0.39	0/383
All	All	0.24	0/42758	0.39	0/58220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2618	0	2515	55	0
1	a	2613	0	2506	0	0
2	B	3953	0	3802	69	0
2	b	3960	0	3811	0	0
3	C	3486	0	3407	49	0
3	c	3486	0	3407	0	0
4	D	2716	0	2621	50	0
4	d	2709	0	2612	0	0
5	E	657	0	637	21	0
5	e	665	0	651	0	0
6	F	274	0	279	4	0
6	f	274	0	279	0	0
7	H	498	0	518	5	0
7	h	498	0	518	0	0
8	I	296	0	311	3	0
8	i	296	0	311	0	0
9	J	257	0	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	257	0	268	0	0
10	K	293	0	305	10	0
10	k	293	0	305	0	0
11	L	301	0	309	8	0
11	l	301	0	309	0	0
12	M	256	0	269	5	0
12	m	256	0	269	0	0
13	O	1845	0	1793	25	0
13	o	1853	0	1817	0	0
14	T	258	0	261	5	0
14	t	258	0	261	0	0
15	U	774	0	773	10	0
15	u	774	0	773	0	0
16	V	1064	0	1073	11	0
16	v	1064	0	1073	0	0
17	Y	224	0	252	8	0
17	y	224	0	252	0	0
18	X	279	0	307	3	0
18	x	281	0	312	0	0
19	Z	479	0	516	15	0
19	z	479	0	516	0	0
20	R	273	0	305	10	0
20	r	273	0	305	0	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	92	0	138	3	0
23	B	54	0	78	7	0
23	D	90	0	111	1	0
23	I	40	0	67	0	0
23	b	54	0	77	0	0
23	c	54	0	78	0	0
23	f	43	0	53	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	252	0	269	17	0
25	B	1040	0	1152	63	0
25	C	845	0	936	50	0
25	D	130	0	144	11	0
25	a	254	0	274	0	0
25	b	1040	0	1152	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	c	838	0	919	0	0
25	d	130	0	144	0	0
26	A	64	0	74	2	0
26	D	64	0	74	7	0
26	a	64	0	74	0	0
26	d	64	0	74	0	0
27	A	40	0	56	5	0
27	B	160	0	224	11	0
27	C	80	0	112	4	0
27	D	40	0	56	3	0
27	H	40	0	56	4	0
27	K	40	0	56	3	0
27	T	40	0	56	6	0
27	Y	40	0	56	4	0
27	a	40	0	56	0	0
27	b	120	0	168	0	0
27	c	80	0	112	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	k	40	0	56	0	0
27	y	40	0	56	0	0
28	A	55	0	80	7	0
28	D	55	0	80	2	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	102	0	144	2	0
29	B	153	0	216	4	0
29	C	102	0	144	3	0
29	D	51	0	72	2	0
29	b	111	0	158	0	0
29	c	153	0	216	0	0
29	d	82	0	115	0	0
30	A	7	0	0	0	0
30	B	28	0	0	0	0
30	C	9	0	0	0	0
30	H	8	0	0	0	0
30	M	23	0	0	0	0
30	b	26	0	0	0	0
30	d	22	0	0	0	0
30	i	12	0	0	0	0
30	j	9	0	0	0	0
30	m	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	t	10	0	0	0	0
30	z	11	0	0	0	0
31	A	147	0	222	12	0
31	D	49	0	74	1	0
31	L	49	0	74	7	0
31	a	126	0	171	0	0
31	d	49	0	74	0	0
31	l	49	0	74	0	0
32	A	4	0	1	1	0
32	a	4	0	1	0	0
33	C	186	0	246	5	0
33	H	62	0	82	2	0
33	c	186	0	246	0	0
33	h	62	0	82	0	0
34	E	43	0	30	4	0
34	V	43	0	30	2	0
34	e	43	0	30	0	0
34	v	43	0	30	0	0
35	A	10	0	0	0	0
35	B	17	0	0	0	0
35	C	11	0	0	0	0
35	D	9	0	0	0	0
35	E	3	0	0	0	0
35	L	2	0	0	0	0
35	M	2	0	0	0	0
35	O	5	0	0	0	0
35	T	1	0	0	0	0
35	V	2	0	0	0	0
35	X	1	0	0	0	0
35	Z	1	0	0	0	0
35	a	11	0	0	0	0
35	b	12	0	0	0	0
35	c	11	0	0	0	0
35	d	9	0	0	0	0
35	i	1	0	0	0	0
35	l	2	0	0	0	0
35	o	9	0	0	0	0
35	u	2	0	0	0	0
35	v	3	0	0	0	0
All	All	50162	0	51048	448	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (448) 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:B:157:HIS:HE1	25:B:606:CLA:NA	1.76	0.83
31:A:618:LHG:HC31	5:E:9:PRO:HB3	1.61	0.81
31:A:616:LHG:O4	4:D:141:TYR:OH	1.98	0.80
25:A:607:CLA:HAB	25:D:403:CLA:H72	28.85	0.74
29:C:519:LMG:H191	10:K:27:VAL:HG11	1.70	0.74
25:B:607:CLA:HAC2	27:B:627:BCR:H272	1.71	0.72
3:C:48:LYS:HE3	3:C:138:GLU:HG2	1.70	0.72
34:V:201:HEM:HHO	34:V:201:HEM:HBC2	1.72	0.72
25:B:612:CLA:H171	25:B:613:CLA:HBB2	1.73	0.70
25:C:505:CLA:H172	25:C:512:CLA:HBB2	38.63	0.69
2:B:124:ARG:O	7:H:12:ARG:NH2	7.36	0.69
14:T:15:ALA:HB2	27:T:101:BCR:H14C	1.73	0.69
4:D:279:LEU:HD22	26:D:401:PHO:HBC3	1.72	0.69
1:A:217:SER:O	1:A:221:SER:OG	4.31	0.69
13:O:27:ARG:NH1	13:O:202:ALA:O	2.25	0.68
1:A:201:GLY:HA3	1:A:286:THR:HB	1.94	0.66
12:M:24:ILE:HG12	12:M:24:ILE:HG12	0.00	0.66
1:A:227:THR:HB	1:A:231:GLU:HG3	1.96	0.66
5:E:40:THR:HB	20:R:4:ARG:HG2	2.07	0.65
20:R:2:ASP:OD2	20:R:4:ARG:NH1	2.78	0.65
2:B:469:HIS:HE1	25:B:611:CLA:NA	1.94	0.64
26:D:401:PHO:HMB2	25:D:403:CLA:H101	32.64	0.64
19:Z:32:ASP:HB2	19:Z:35:ARG:HE	1.63	0.64
13:O:24:ASP:OD1	13:O:203:LYS:NZ	2.31	0.63
4:D:192:THR:HG23	25:D:403:CLA:HBC2	41.28	0.63
1:A:224:ILE:O	4:D:265:ARG:NH2	2.32	0.63
5:E:26:THR:HA	20:R:15:ALA:HB1	2.12	0.63
23:A:603:SQD:H251	31:A:617:LHG:H131	1.81	0.62
31:A:617:LHG:H192	25:C:504:CLA:H202	1.80	0.62
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.33	0.62
2:B:12:LEU:HB2	25:B:615:CLA:HMC2	18.43	0.62
4:D:192:THR:HG23	25:D:402:CLA:HBC2	1.81	0.61
2:B:127:ARG:NH2	7:H:18:TYR:O	2.30	0.61
2:B:103:LEU:HD21	25:B:605:CLA:HMC3	1.81	0.61
25:B:604:CLA:H121	25:B:615:CLA:H42	1.82	0.61
3:C:27:ASP:OD1	3:C:30:SER:OG	2.31	0.61
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	40.31	0.60
25:A:609:CLA:H143	25:C:507:CLA:H192	14.24	0.60
10:K:10:LYS:NZ	10:K:19:ASP:OD2	2.34	0.60
11:L:23:LEU:HD22	31:L:101:LHG:H122	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:616:LHG:H223	25:B:613:CLA:H192	1.84	0.60
19:Z:34:ASP:HA	19:Z:37:LYS:HD3	4.93	0.60
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.83	0.60
16:V:66:ARG:NH2	16:V:80:THR:OG1	3.23	0.60
2:B:150:CYS:HB2	25:B:603:CLA:HMC3	1.83	0.59
25:B:610:CLA:HAC2	27:T:101:BCR:H272	60.44	0.59
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.95	0.59
5:E:30:LEU:HD11	34:E:101:HEM:HAB	1.95	0.59
5:E:5:THR:OG1	5:E:7:GLU:OE1	2.50	0.59
3:C:26:ARG:NH2	17:Y:45:ASN:OD1	2.36	0.59
13:O:51:LEU:HB2	13:O:234:LYS:HB3	2.20	0.59
13:O:158:ASP:OD1	13:O:162:ARG:N	2.27	0.59
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.84	0.59
25:C:504:CLA:H42	33:C:517:DGD:HB42	1.85	0.58
31:A:617:LHG:H371	25:C:508:CLA:H92	1.84	0.58
25:C:503:CLA:H151	25:C:509:CLA:HMB3	13.41	0.58
3:C:38:GLY:HA3	25:C:511:CLA:HMD3	1.85	0.58
34:E:101:HEM:HBC2	34:E:101:HEM:HMC2	3.41	0.58
25:A:606:CLA:HMB1	25:A:606:CLA:HBB1	1.86	0.57
25:A:609:CLA:H171	25:C:508:CLA:H121	33.99	0.57
5:E:36:LEU:HD13	20:R:7:VAL:HG12	5.73	0.57
4:D:259:ILE:HD13	31:D:406:LHG:H262	1.86	0.57
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.86	0.57
25:C:501:CLA:H71	25:C:501:CLA:HBB1	1.86	0.57
2:B:497:GLN:NE2	18:X:38:GLN:O	2.38	0.57
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.33	0.57
34:E:101:HEM:HMB2	34:E:101:HEM:HBB2	1.87	0.57
8:I:28:PRO:O	8:I:31:ASN:ND2	2.56	0.57
3:C:444:HIS:CE1	25:C:510:CLA:NA	11.70	0.56
25:C:511:CLA:H171	19:Z:20:VAL:HA	1.86	0.56
2:B:150:CYS:HB2	25:B:606:CLA:HMC3	8.40	0.56
4:D:216:ALA:O	4:D:220:ASN:ND2	2.45	0.56
34:V:201:HEM:HBB2	34:V:201:HEM:HMB2	1.91	0.56
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.88	0.56
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.01	0.56
1:A:217:SER:HA	4:D:272:LEU:HD12	1.98	0.56
25:B:602:CLA:H172	33:H:103:DGD:HAT1	1.87	0.56
23:A:619:SQD:H102	2:B:94:GLU:HG2	56.18	0.55
2:B:469:HIS:CE1	25:B:614:CLA:NA	14.70	0.55
34:E:101:HEM:HMC1	34:E:101:HEM:HBC2	1.88	0.55
25:B:604:CLA:HBB1	25:B:607:CLA:HAB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:LYS:NZ	3:C:184:GLY:O	2.47	0.55
3:C:87:ILE:O	3:C:91:HIS:ND1	2.37	0.55
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.89	0.55
28:A:611:PL9:H403	6:F:22:ALA:HB2	1.89	0.55
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	1.88	0.55
4:D:221:THR:HG21	4:D:249:ALA:HB2	1.93	0.54
31:A:617:LHG:H352	31:A:617:LHG:H151	1.87	0.54
16:V:87:GLU:OE1	16:V:96:ARG:NH1	2.55	0.54
5:E:60:GLN:NE2	5:E:62:SER:O	2.40	0.54
1:A:183:MET:HA	25:A:606:CLA:HMD2	1.90	0.54
3:C:135:ARG:HG2	19:Z:27:TYR:CG	3.62	0.54
25:C:503:CLA:H172	25:C:510:CLA:HBB2	1.89	0.54
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.90	0.54
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.54
1:A:131:TRP:CH2	25:C:505:CLA:HAA2	2.44	0.53
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.53
1:A:64:ARG:NH1	13:O:105:PRO:O	2.65	0.53
2:B:327:THR:HG22	25:B:610:CLA:H12	29.46	0.53
13:O:118:LEU:HD22	13:O:233:VAL:HG11	2.99	0.53
19:Z:16:SER:HG	19:Z:47:TRP:HE1	1.52	0.53
13:O:103:PHE:HB3	13:O:123:LYS:HE2	1.89	0.53
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.02	0.52
25:B:614:CLA:H121	23:B:626:SQD:H381	1.91	0.52
3:C:297:TYR:O	3:C:423:ARG:NH2	2.60	0.52
4:D:54:PHE:O	5:E:49:THR:OG1	2.25	0.52
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.01	0.52
3:C:92:ILE:HD11	25:C:503:CLA:HED2	1.91	0.52
4:D:186:GLN:HB2	25:D:402:CLA:HBC1	1.91	0.52
2:B:228:ALA:HB1	29:B:625:LMG:H111	52.25	0.52
13:O:3:GLN:N	13:O:4:THR:HA	2.25	0.52
13:O:189:ARG:NH1	13:O:226:GLY:O	2.43	0.52
2:B:103:LEU:HD21	25:B:608:CLA:HMC3	30.79	0.52
3:C:444:HIS:CE1	25:C:508:CLA:NA	2.77	0.52
25:C:501:CLA:H193	25:C:507:CLA:HBB1	1.91	0.52
1:A:283:VAL:HA	1:A:286:THR:HG22	1.96	0.52
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.91	0.52
3:C:167:VAL:HG13	25:C:512:CLA:H102	1.92	0.52
2:B:157:HIS:HA	2:B:163:GLY:HA3	2.01	0.51
3:C:75:PHE:HZ	3:C:105:VAL:HG21	2.09	0.51
11:L:12:LEU:HD12	31:L:101:LHG:HC11	1.93	0.51
3:C:59:LEU:HD13	25:C:512:CLA:HMD2	15.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:GLY:HA3	5:E:63:ILE:HD13	1.92	0.51
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.75	0.51
17:Y:42:ARG:HH21	19:Z:29:SER:HB3	4.26	0.51
13:O:54:GLU:HG2	13:O:63:ALA:HB1	3.11	0.51
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.91	0.51
1:A:232:SER:OG	31:L:101:LHG:O5	2.80	0.51
23:B:626:SQD:H371	23:B:626:SQD:H162	1.93	0.51
1:A:308:ASP:OD1	1:A:312:ASN:N	2.42	0.51
25:C:501:CLA:C3D	25:C:503:CLA:H2	2.40	0.51
1:A:156:ALA:HA	1:A:160:ILE:HB	2.09	0.50
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.24	0.50
3:C:148:GLY:O	3:C:156:LYS:NZ	2.45	0.50
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.93	0.50
27:B:627:BCR:H14C	14:T:15:ALA:HB2	36.42	0.50
19:Z:3:ILE:HG23	19:Z:4:LEU:HD22	5.22	0.50
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.50
2:B:4:PRO:HD2	2:B:7:ARG:HD2	2.14	0.50
19:Z:31:GLN:O	19:Z:33:TRP:N	2.45	0.50
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.93	0.50
2:B:248:ALA:HA	25:B:603:CLA:H42	1.94	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.46	0.50
17:Y:17:GLU:HB3	17:Y:19:ILE:N	2.26	0.50
1:A:286:THR:OG1	25:A:606:CLA:O1D	2.23	0.49
31:A:617:LHG:H211	33:C:518:DGD:HBN2	1.93	0.49
2:B:285:ASN:O	2:B:289:GLN:HG2	2.70	0.49
4:D:117:HIS:CE1	25:D:403:CLA:NA	2.80	0.49
4:D:199:MET:HG2	28:D:407:PL9:H321	1.95	0.49
2:B:71:VAL:HG23	25:B:606:CLA:HMA2	1.94	0.49
25:B:608:CLA:H193	25:D:403:CLA:HAA2	1.93	0.49
25:C:502:CLA:H61	25:C:512:CLA:H42	1.94	0.49
1:A:118:HIS:CE1	25:A:609:CLA:NA	2.80	0.49
23:B:626:SQD:H361	27:B:627:BCR:H362	1.94	0.49
3:C:406:SER:HA	3:C:420:VAL:HG23	1.95	0.49
29:C:520:LMG:H171	29:C:520:LMG:H331	1.95	0.49
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.04	0.49
25:B:614:CLA:H71	31:L:101:LHG:H322	10.40	0.49
26:D:401:PHO:HBA2	25:D:402:CLA:H142	1.95	0.49
16:V:13:ASN:HD21	16:V:17:LYS:HD2	2.80	0.49
25:C:503:CLA:H71	25:C:503:CLA:HBB1	11.94	0.49
3:C:57:ALA:O	3:C:61:VAL:HG23	2.17	0.49
15:U:27:LEU:HD22	15:U:49:ILE:HG21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:104:LYS:HE3	16:V:45:ILE:HG22	2.04	0.48
19:Z:61:VAL:HG23	19:Z:62:VAL:HG23	1.94	0.48
1:A:262:TYR:CD2	31:A:618:LHG:HC42	2.48	0.48
2:B:18:ARG:NH2	23:B:626:SQD:O7	2.36	0.48
3:C:38:GLY:HA3	25:C:513:CLA:HMD3	24.43	0.48
2:B:423:LYS:NZ	13:O:175:PRO:O	3.16	0.48
5:E:60:GLN:HG2	5:E:62:SER:H	1.79	0.48
2:B:185:TRP:HD1	29:B:621:LMG:HC2	1.79	0.48
25:B:614:CLA:H41	25:B:614:CLA:H62	1.59	0.48
2:B:71:VAL:HG23	25:B:609:CLA:HMA2	34.91	0.48
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.78	0.48
3:C:90:PRO:HB3	3:C:301:PHE:HB3	1.95	0.48
9:J:9:PRO:HD2	9:J:12:ILE:HD12	1.95	0.48
13:O:162:ARG:NH1	13:O:186:ASN:OD1	2.69	0.48
25:B:601:CLA:H92	27:H:102:BCR:H402	1.96	0.48
4:D:87:HIS:O	7:H:50:ASN:ND2	2.63	0.47
11:L:23:LEU:HD13	31:L:101:LHG:H171	1.96	0.47
1:A:132:GLU:O	1:A:136:ARG:HG2	2.13	0.47
2:B:201:HIS:HE2	25:B:606:CLA:C2B	14.07	0.47
25:A:609:CLA:H193	25:C:505:CLA:H13	1.96	0.47
3:C:76:ILE:O	3:C:84:GLN:NE2	2.44	0.47
5:E:57:ALA:HB3	5:E:60:GLN:HB3	2.21	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.47
29:A:613:LMG:H422	27:T:101:BCR:HC7	1.97	0.47
2:B:477:ASP:N	2:B:477:ASP:OD1	2.46	0.47
4:D:155:SER:HA	4:D:159:ILE:HB	1.98	0.47
25:B:605:CLA:H101	25:B:612:CLA:H18	6.25	0.47
28:A:611:PL9:H251	28:A:611:PL9:H272	2.37	0.47
25:B:616:CLA:H141	25:B:616:CLA:H161	1.70	0.47
29:C:520:LMG:HC71	29:C:520:LMG:O2	2.15	0.47
4:D:225:ASP:HB2	4:D:234:ALA:HB1	1.97	0.47
27:D:404:BCR:H383	29:D:405:LMG:H161	1.95	0.47
20:R:16:ALA:O	20:R:20:VAL:HG23	2.26	0.47
2:B:109:LEU:HD13	29:B:625:LMG:H311	1.97	0.47
25:A:607:CLA:HMD3	4:D:182:LEU:HD11	2.01	0.47
19:Z:1:MET:N	19:Z:1:MET:SD	2.81	0.47
3:C:363:GLY:O	3:C:367:GLU:HG2	2.15	0.46
25:A:609:CLA:H202	25:C:508:CLA:H102	33.21	0.46
2:B:458:PHE:HB3	25:B:607:CLA:HBC2	15.76	0.46
3:C:187:ASP:HB3	3:C:190:ALA:HB2	2.33	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:37:THR:OG1	13:O:246:ALA:OXT	2.31	0.46
23:A:619:SQD:H292	23:A:619:SQD:H262	1.65	0.46
3:C:377:LEU:HG	3:C:381:LYS:HE2	1.97	0.46
3:C:466:VAL:HG21	4:D:248:THR:HG23	1.98	0.46
32:A:620:BCT:O1	4:D:268:HIS:CE1	2.67	0.46
15:U:57:SER:HA	15:U:84:VAL:HG21	2.13	0.46
1:A:223:LEU:HD23	1:A:246:TYR:HB3	1.98	0.46
25:A:607:CLA:HED1	33:C:518:DGD:HAT1	1.98	0.46
2:B:248:ALA:HA	25:B:606:CLA:H42	23.62	0.46
25:B:615:CLA:H162	25:B:615:CLA:H122	3.52	0.46
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.52	0.46
27:B:627:BCR:HC8	14:T:18:PHE:HB2	45.67	0.46
10:K:15:TYR:OH	19:Z:58:ASN:OD1	2.23	0.46
1:A:267:ASN:HB3	1:A:270:SER:HB3	1.98	0.46
27:H:102:BCR:H24C	27:H:102:BCR:H371	1.79	0.46
1:A:131:TRP:CH2	25:C:507:CLA:HAA2	21.73	0.46
2:B:334:ASP:N	2:B:334:ASP:OD1	2.55	0.46
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.97	0.46
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.97	0.46
15:U:31:ASN:ND2	15:U:96:ASP:O	2.60	0.46
2:B:16:PRO:HB3	2:B:133:LEU:HD11	2.16	0.46
25:B:606:CLA:H112	25:B:606:CLA:H91	1.77	0.46
10:K:24:VAL:HG11	17:Y:25:ILE:HB	1.98	0.46
2:B:278:SER:HB3	2:B:281:GLN:HB3	2.06	0.45
2:B:51:VAL:HG13	2:B:308:LYS:HB2	2.13	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
27:H:102:BCR:H20C	27:H:102:BCR:H361	1.80	0.45
25:C:503:CLA:H191	25:C:503:CLA:HMD2	1.98	0.45
1:A:96:ILE:HD12	25:A:609:CLA:HMD1	2.14	0.45
5:E:36:LEU:O	5:E:40:THR:OG1	2.39	0.45
3:C:59:LEU:HD13	25:C:510:CLA:HMD2	1.97	0.45
4:D:201:VAL:HG22	25:D:403:CLA:C1B	33.84	0.45
20:R:10:LEU:HB3	20:R:11:PRO:HD3	2.55	0.45
1:A:190:HIS:O	1:A:298:ASN:HB3	2.16	0.45
1:A:46:ILE:HD12	27:A:610:BCR:H15C	1.99	0.45
25:B:602:CLA:H62	25:B:602:CLA:H41	1.79	0.45
3:C:102:GLY:N	3:C:194:GLY:O	2.44	0.45
25:C:503:CLA:H142	25:C:503:CLA:H112	3.55	0.45
25:A:609:CLA:H91	25:A:609:CLA:H111	2.03	0.45
31:A:617:LHG:H361	31:A:617:LHG:H331	1.69	0.45
25:C:505:CLA:H141	8:I:16:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:101:BCR:H20C	27:Y:101:BCR:H361	1.84	0.45
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.13	0.45
25:B:613:CLA:H142	25:B:615:CLA:H2	28.03	0.45
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.98	0.45
25:C:505:CLA:H111	25:C:505:CLA:H93	1.73	0.45
1:A:214:MET:HB3	28:A:611:PL9:H103	1.99	0.45
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.98	0.45
10:K:25:LEU:HD22	27:Y:101:BCR:H332	1.99	0.45
2:B:347:ARG:NH2	2:B:402:TYR:OH	3.01	0.45
25:C:504:CLA:H151	25:C:508:CLA:H143	1.99	0.45
27:D:404:BCR:H361	27:D:404:BCR:H20C	1.81	0.45
27:T:101:BCR:H351	27:T:101:BCR:H15C	1.81	0.45
1:A:29:TYR:O	1:A:129:ARG:NH2	2.54	0.44
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.50	0.44
1:A:131:TRP:HD1	1:A:141:PRO:HB2	1.83	0.44
1:A:74:GLY:O	4:D:301:GLN:NE2	2.77	0.44
27:B:618:BCR:H361	27:B:618:BCR:H20C	1.85	0.44
26:D:401:PHO:HBB1	26:D:401:PHO:HMB1	2.04	0.44
2:B:228:ALA:HB1	23:D:408:SQD:H262	1.98	0.44
1:A:35:VAL:HG13	27:A:610:BCR:HC31	2.51	0.44
5:E:8:ARG:O	6:F:19:ARG:NH2	3.04	0.44
5:E:25:ILE:HD11	20:R:18:TRP:HB3	1.99	0.44
25:C:505:CLA:H43	27:C:515:BCR:HC7	1.99	0.44
25:C:513:CLA:HMC2	27:C:514:BCR:H372	2.00	0.44
26:D:401:PHO:H3A	26:D:401:PHO:HBA2	1.79	0.44
15:U:42:TYR:HA	15:U:43:PRO:HA	1.79	0.44
25:B:615:CLA:HBA1	25:B:615:CLA:H3A	1.99	0.44
3:C:256:PRO:O	3:C:261:ARG:NH1	2.68	0.44
33:C:516:DGD:HAH1	33:C:516:DGD:HAT2	1.80	0.44
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.52	0.44
1:A:133:LEU:HD23	4:D:256:ILE:HG12	2.14	0.44
25:C:503:CLA:H203	25:C:509:CLA:H111	12.07	0.44
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.05	0.44
1:A:45:THR:HG21	29:A:613:LMG:H241	1.98	0.44
31:A:617:LHG:H132	31:A:617:LHG:H372	2.00	0.44
25:B:610:CLA:H161	25:B:610:CLA:H202	1.83	0.44
25:B:616:CLA:H11	25:B:616:CLA:H51	1.74	0.44
25:C:503:CLA:H203	25:C:509:CLA:H13	14.05	0.44
13:O:224:ASP:HB3	13:O:227:ALA:HB3	2.41	0.44
20:R:23:ILE:O	20:R:27:ALA:N	2.66	0.44
25:B:614:CLA:H141	25:B:614:CLA:H162	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:503:CLA:C2D	25:C:505:CLA:H2	30.63	0.44
25:C:509:CLA:HBB1	25:C:509:CLA:HMB1	2.00	0.44
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.82	0.44
26:D:401:PHO:H112	26:D:401:PHO:H72	1.86	0.44
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.03	0.44
26:D:401:PHO:HBA2	25:D:403:CLA:H142	31.68	0.44
29:D:405:LMG:H382	29:D:405:LMG:H351	1.72	0.44
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.20	0.44
18:X:24:THR:O	18:X:28:LEU:HD12	3.52	0.43
1:A:58:VAL:HB	1:A:83:VAL:HB	2.01	0.43
2:B:399:VAL:HG12	2:B:417:VAL:HG22	2.11	0.43
3:C:211:GLY:O	3:C:215:LYS:HG3	2.18	0.43
10:K:12:PRO:HB2	10:K:15:TYR:HD1	1.83	0.43
27:A:610:BCR:H24C	27:A:610:BCR:H371	1.80	0.43
3:C:141:GLU:HA	3:C:148:GLY:HA3	2.58	0.43
4:D:39:PRO:O	4:D:43:LEU:HG	2.30	0.43
5:E:23:HIS:HA	5:E:26:THR:OG1	2.18	0.43
13:O:38:TYR:HD1	13:O:245:PRO:HA	2.32	0.43
1:A:336:ALA:O	3:C:354:GLU:HG3	2.37	0.43
3:C:335:THR:O	13:O:152:ARG:NH2	2.95	0.43
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.54	0.43
27:A:610:BCR:H361	27:A:610:BCR:H20C	1.84	0.43
1:A:264:SER:OG	28:A:611:PL9:O2	2.72	0.43
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.15	0.43
25:B:611:CLA:H161	25:B:611:CLA:H141	4.18	0.43
28:D:407:PL9:H371	28:D:407:PL9:H351	1.67	0.43
2:B:299:GLU:HG2	2:B:402:TYR:HD2	1.84	0.43
2:B:30:VAL:HG11	25:B:612:CLA:H112	1.99	0.43
6:F:45:ARG:NH2	9:J:40:LEU:OXT	2.46	0.43
17:Y:42:ARG:NH2	19:Z:31:GLN:HB2	5.08	0.43
26:A:608:PHO:H2	26:A:608:PHO:H61	1.74	0.43
25:C:506:CLA:H112	25:C:506:CLA:H93	1.77	0.43
25:C:513:CLA:H162	25:C:513:CLA:H141	1.80	0.43
13:O:72:THR:HG23	13:O:107:THR:HB	2.01	0.43
15:U:48:LEU:O	15:U:52:ASN:ND2	2.38	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.19	0.43
25:B:608:CLA:H62	25:B:609:CLA:H112	2.01	0.43
27:K:101:BCR:H15C	27:K:101:BCR:H351	1.85	0.43
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.24	0.43
25:B:610:CLA:H142	25:B:612:CLA:H2	2.01	0.43
25:C:509:CLA:H93	25:C:509:CLA:HBA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:62:TRP:O	7:H:64:ALA:N	2.52	0.43
12:M:27:VAL:HG12	12:M:28:GLN:HB3	4.74	0.43
16:V:45:ILE:HG13	16:V:45:ILE:H	1.71	0.43
2:B:469:HIS:HE1	25:B:611:CLA:C1A	2.32	0.42
25:B:602:CLA:H92	25:B:602:CLA:H61	1.76	0.42
23:B:626:SQD:H242	23:B:626:SQD:H111	2.01	0.42
2:B:242:ILE:HG23	2:B:462:PHE:HD2	1.93	0.42
25:B:602:CLA:H151	25:B:602:CLA:H111	1.86	0.42
25:B:615:CLA:H13	25:B:616:CLA:HAB	7.23	0.42
12:M:17:VAL:HB	12:M:18:PRO:HD3	2.26	0.42
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.60	0.42
2:B:357:ARG:NH2	4:D:337:GLU:O	2.77	0.42
2:B:389:LYS:HB2	2:B:389:LYS:HE3	4.59	0.42
27:B:617:BCR:H351	27:B:617:BCR:H15C	1.84	0.42
3:C:179:ALA:HA	3:C:184:GLY:HA2	2.09	0.42
2:B:383:PHE:N	4:D:344:GLU:O	2.39	0.42
8:I:1:FME:O1	8:I:3:THR:N	2.52	0.42
1:A:179:THR:O	1:A:183:MET:HG3	2.23	0.42
2:B:212:ALA:HB2	25:B:612:CLA:HMC3	28.23	0.42
25:B:609:CLA:H62	25:B:609:CLA:H92	1.81	0.42
1:A:12:ASN:N	1:A:12:ASN:OD1	2.52	0.42
2:B:247:PHE:HB2	25:B:608:CLA:HBC1	2.01	0.42
3:C:79:LYS:HB2	3:C:84:GLN:NE2	2.34	0.42
2:B:349:LYS:HG3	2:B:350:GLU:HG3	2.01	0.42
4:D:194:ASN:HA	4:D:295:SER:HB2	2.01	0.42
3:C:79:LYS:HD2	16:V:35:TYR:HE1	1.83	0.42
16:V:81:THR:OG1	16:V:83:ASP:OD1	2.68	0.42
19:Z:48:ILE:O	19:Z:51:VAL:HG12	4.51	0.42
31:A:618:LHG:H141	31:A:618:LHG:H112	1.92	0.42
3:C:290:VAL:O	3:C:423:ARG:NH1	2.54	0.42
2:B:212:ALA:HB2	25:B:609:CLA:HMC3	2.01	0.42
27:B:617:BCR:H383	23:B:626:SQD:H91	2.01	0.42
25:C:501:CLA:H151	25:C:507:CLA:HMB3	2.00	0.42
3:C:296:VAL:HG11	25:C:501:CLA:HMA2	2.02	0.42
27:C:515:BCR:H351	27:C:515:BCR:H15C	1.85	0.42
13:O:99:ASP:OD1	13:O:100:GLY:N	2.53	0.42
28:A:611:PL9:HC8	28:A:611:PL9:HC2	1.81	0.42
25:B:615:CLA:H102	25:B:615:CLA:H61	4.41	0.42
11:L:22:LEU:HG	31:L:101:LHG:H181	2.50	0.42
13:O:5:LEU:HD22	13:O:9:ASP:HB3	2.47	0.42
15:U:80:GLU:HG3	15:U:81:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:59:LEU:HD13	16:V:72:LEU:HD21	2.02	0.42
25:B:614:CLA:H142	23:B:626:SQD:H372	2.01	0.42
10:K:28:ILE:HD13	27:Y:101:BCR:HC8	2.11	0.42
12:M:20:VAL:HG11	12:M:20:VAL:HG22	2.97	0.42
25:B:605:CLA:H41	25:B:605:CLA:H62	1.89	0.41
3:C:61:VAL:HG12	3:C:118:HIS:O	2.23	0.41
5:E:17:VAL:O	5:E:21:VAL:HG23	2.20	0.41
27:K:101:BCR:H361	27:K:101:BCR:H20C	1.86	0.41
11:L:7:ARG:HE	11:L:7:ARG:HB3	1.99	0.41
13:O:214:THR:HA	13:O:238:VAL:HA	2.00	0.41
25:B:607:CLA:H41	25:B:607:CLA:H62	2.06	0.41
27:B:618:BCR:H371	27:B:618:BCR:H24C	1.86	0.41
2:B:216:HIS:HE1	25:B:612:CLA:CHA	18.75	0.41
25:C:501:CLA:H203	25:C:507:CLA:H111	2.02	0.41
25:C:505:CLA:H62	25:C:505:CLA:H101	3.61	0.41
27:D:404:BCR:H351	27:D:404:BCR:H15C	1.87	0.41
5:E:25:ILE:HG13	5:E:26:THR:N	2.34	0.41
1:A:235:TYR:OH	11:L:11:GLU:OE1	2.67	0.41
16:V:34:GLN:HA	16:V:38:ALA:HB2	2.01	0.41
2:B:30:VAL:HG12	25:B:608:CLA:HHD	23.86	0.41
27:B:619:BCR:H351	27:B:619:BCR:H15C	1.87	0.41
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.09	0.41
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.62	0.41
2:B:216:HIS:HE1	25:B:612:CLA:C1A	20.06	0.41
13:O:188:LYS:HB3	13:O:225:MET:HB3	2.03	0.41
17:Y:18:VAL:O	17:Y:21:GLN:N	2.53	0.41
25:A:615:CLA:HMA1	25:A:615:CLA:H121	2.03	0.41
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.84	0.41
27:B:619:BCR:H361	27:B:619:BCR:H20C	1.83	0.41
3:C:444:HIS:HE1	25:C:510:CLA:C1A	11.11	0.41
25:A:609:CLA:H122	25:A:609:CLA:H161	3.25	0.41
2:B:216:HIS:HE1	25:B:609:CLA:NA	2.12	0.41
2:B:453:PHE:HB2	4:D:291:LEU:HD12	2.03	0.41
27:B:627:BCR:H341	27:B:627:BCR:H11C	1.94	0.41
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.01	0.41
33:C:517:DGD:HBN1	33:C:517:DGD:HBW1	1.81	0.41
4:D:193:LEU:O	11:L:34:TYR:OH	2.84	0.41
17:Y:17:GLU:HA	17:Y:18:VAL:HB	2.03	0.41
1:A:36:ILE:HG23	25:A:609:CLA:HBB1	2.01	0.41
27:A:610:BCR:H341	27:A:610:BCR:H11C	1.96	0.41
2:B:488:PRO:O	2:B:492:GLU:HB2	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:NH1	16:V:137:TYR:OXT	2.60	0.41
3:C:346:THR:OG1	3:C:348:GLU:OE2	2.32	0.41
4:D:87:HIS:HB2	33:H:103:DGD:HG11	2.03	0.41
20:R:8:VAL:O	20:R:11:PRO:HD2	2.21	0.41
27:Y:101:BCR:H24C	27:Y:101:BCR:H371	1.98	0.41
10:K:39:TRP:NE1	17:Y:46:LEU:O	2.80	0.41
1:A:174:LEU:HD22	26:A:608:PHO:H151	2.41	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.93	0.41
3:C:130:VAL:O	3:C:134:ILE:HG12	2.21	0.41
25:A:609:CLA:H51	25:A:609:CLA:H8	1.86	0.41
2:B:62:VAL:HB	25:B:608:CLA:HED3	35.07	0.41
29:B:620:LMG:H401	12:M:17:VAL:HG21	2.03	0.41
3:C:135:ARG:HA	3:C:135:ARG:HD2	2.04	0.41
1:A:308:ASP:O	6:F:45:ARG:HD2	2.21	0.41
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.64	0.41
16:V:64:PRO:HD2	16:V:66:ARG:NH2	2.64	0.41
28:A:611:PL9:H121	28:A:611:PL9:HC8	1.67	0.40
3:C:399:ALA:O	3:C:401:LEU:N	2.57	0.40
1:A:135:TYR:CE1	3:C:449:ARG:HB3	2.56	0.40
25:C:503:CLA:H62	25:C:503:CLA:H101	1.81	0.40
25:C:511:CLA:H2A	25:C:511:CLA:O1A	4.75	0.40
10:K:21:LEU:O	10:K:25:LEU:HG	2.21	0.40
27:T:101:BCR:H361	27:T:101:BCR:H20C	1.82	0.40
1:A:215:HIS:ND1	28:A:611:PL9:O1	2.85	0.40
25:B:601:CLA:H111	25:B:601:CLA:H93	1.75	0.40
25:B:605:CLA:H92	25:B:605:CLA:H61	2.79	0.40
25:C:509:CLA:H141	25:C:509:CLA:H162	3.73	0.40
10:K:14:ALA:HB1	19:Z:5:PHE:CE2	3.10	0.40
2:B:462:PHE:CZ	25:B:613:CLA:HMB3	2.56	0.40
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.57	0.40
25:C:506:CLA:H192	25:C:506:CLA:H161	1.83	0.40
27:K:101:BCR:H341	27:K:101:BCR:H11C	1.99	0.40
2:B:434:THR:HG22	2:B:439:SER:HB2	2.02	0.40
3:C:464:GLU:OE2	4:D:245:SER:OG	2.35	0.40
25:C:508:CLA:H122	25:C:508:CLA:H162	1.86	0.40
4:D:163:GLY:HA3	4:D:290:ALA:HB1	2.29	0.40
27:H:102:BCR:H15C	27:H:102:BCR:H351	1.86	0.40
11:L:26:VAL:HG11	31:L:101:LHG:H201	2.38	0.40
14:T:15:ALA:HA	27:T:101:BCR:H12C	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	46	84
1	a	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	46	84
2	B	502/510 (98%)	483 (96%)	19 (4%)	0	100	100
2	b	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
3	C	449/461 (97%)	436 (97%)	12 (3%)	1 (0%)	52	88
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	39	80
4	D	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
4	d	339/352 (96%)	324 (96%)	15 (4%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	12	48
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	242/272 (89%)	228 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	232 (96%)	9 (4%)	1 (0%)	39	80
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	90 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	4	24
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	36/41 (88%)	32 (89%)	4 (11%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	5	26
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	32 (100%)	0	0	100	100
All	All	5240/5700 (92%)	5040 (96%)	190 (4%)	10 (0%)	52	88

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Y	18	VAL
19	Z	32	ASP
13	o	61	GLN
3	C	416	SER
7	H	63	LYS
3	c	24	THR
3	c	416	SER
19	Z	2	THR
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	269 (100%)	0	100	100
1	a	268/280 (96%)	267 (100%)	1 (0%)	93	98
2	B	398/407 (98%)	397 (100%)	1 (0%)	94	98
2	b	400/407 (98%)	399 (100%)	1 (0%)	94	98
3	C	352/362 (97%)	350 (99%)	2 (1%)	90	97
3	c	352/362 (97%)	349 (99%)	3 (1%)	84	95
4	D	276/283 (98%)	275 (100%)	1 (0%)	93	98
4	d	274/283 (97%)	273 (100%)	1 (0%)	93	98
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	52 (98%)	1 (2%)	65	90
7	h	53/55 (96%)	52 (98%)	1 (2%)	65	90
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	200/228 (88%)	198 (99%)	2 (1%)	82	95
13	o	202/228 (89%)	200 (99%)	2 (1%)	82	95
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	78	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	116 (99%)	1 (1%)	84	95
17	Y	23/37 (62%)	23 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	90
19	z	52/52 (100%)	51 (98%)	1 (2%)	65	90
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	29/33 (88%)	28 (97%)	1 (3%)	44	81
All	All	4313/4654 (93%)	4292 (100%)	21 (0%)	92	98

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
3	C	289	PHE
3	C	418	ASN
4	D	180	ARG
7	H	49	TYR
13	O	27	ARG
13	O	118	LEU
19	Z	1	MET
1	a	170	ASP
2	b	362	PHE
3	c	135	ARG
3	c	289	PHE
3	c	418	ASN
4	d	180	ARG
7	h	49	TYR
13	o	115	ARG
13	o	207	ARG
15	u	86	GLU
16	v	106	ASN
19	z	32	ASP
20	r	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	216	HIS
2	B	223	GLN
2	B	289	GLN
4	D	332	GLN
13	O	196	GLN
19	Z	31	GLN
2	b	216	HIS
2	b	289	GLN
2	b	374	ASN
4	d	332	GLN
12	m	5	GLN
13	o	104	GLN
16	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.79	0	5,9,11	0.88	0
12	FME	M	1	12	8,9,10	0.87	0	5,9,11	0.82	0
14	FME	T	1	14	8,9,10	0.86	0	5,9,11	0.92	0
8	FME	i	1	8	8,9,10	0.86	0	5,9,11	0.88	0
12	FME	m	1	12	8,9,10	0.86	0	5,9,11	0.92	0
14	FME	t	1	14	8,9,10	0.87	0	5,9,11	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 17 are unknown and 6 are monoatomic - leaving 151 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	OEX	A	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
23	SQD	A	603	-	51,52,54	0.96	4 (7%)	60,63,65	1.93	11 (18%)
25	CLA	A	606	-	57,73,73	1.13	5 (8%)	61,113,113	1.17	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	607	35	49,65,73	1.23	5 (10%)	51,103,113	1.18	5 (9%)
26	PHO	A	608	-	67,69,69	1.24	9 (13%)	86,99,99	1.06	7 (8%)
25	CLA	A	609	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
27	BCR	A	610	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	A	611	-	54,55,55	0.86	2 (3%)	68,69,69	1.45	14 (20%)
29	LMG	A	612	-	51,51,55	0.71	0	59,59,63	1.31	6 (10%)
29	LMG	A	613	-	51,51,55	0.70	0	59,59,63	1.51	8 (13%)
25	CLA	A	615	35	57,73,73	1.14	4 (7%)	61,113,113	1.10	4 (6%)
31	LHG	A	616	-	48,48,48	0.61	0	49,54,54	1.28	6 (12%)
31	LHG	A	617	-	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
31	LHG	A	618	-	48,48,48	0.65	1 (2%)	49,54,54	1.25	7 (14%)
23	SQD	A	619	-	39,39,54	0.86	2 (5%)	41,41,65	1.17	2 (4%)
32	BCT	A	620	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	B	601	35	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	B	602	-	57,73,73	1.14	5 (8%)	61,113,113	1.08	5 (8%)
25	CLA	B	603	-	57,73,73	1.14	5 (8%)	61,113,113	1.10	6 (9%)
25	CLA	B	604	-	57,73,73	1.14	4 (7%)	61,113,113	1.17	7 (11%)
25	CLA	B	605	-	57,73,73	1.15	5 (8%)	61,113,113	1.09	5 (8%)
25	CLA	B	606	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	7 (11%)
25	CLA	B	607	35	57,73,73	1.13	5 (8%)	61,113,113	1.09	5 (8%)
25	CLA	B	608	-	57,73,73	1.13	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	B	609	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	7 (11%)
25	CLA	B	610	35	57,73,73	1.14	4 (7%)	61,113,113	1.08	5 (8%)
25	CLA	B	611	-	57,73,73	1.14	4 (7%)	61,113,113	1.13	7 (11%)
25	CLA	B	612	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	B	613	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	B	614	-	57,73,73	1.13	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	B	615	-	57,73,73	1.15	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	B	616	-	57,73,73	1.13	6 (10%)	61,113,113	1.16	6 (9%)
27	BCR	B	617	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
27	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
27	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	8 (14%)
29	LMG	B	620	-	51,51,55	0.72	0	59,59,63	1.34	7 (11%)
29	LMG	B	621	-	51,51,55	0.72	1 (1%)	59,59,63	1.39	8 (13%)
29	LMG	B	625	-	51,51,55	0.82	2 (3%)	59,59,63	1.42	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	SQD	B	626	-	53,54,54	0.94	4 (7%)	62,65,65	1.93	12 (19%)
27	BCR	B	627	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
25	CLA	C	501	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	C	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	C	503	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	C	504	35	57,73,73	1.13	5 (8%)	61,113,113	1.11	6 (9%)
25	CLA	C	505	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	C	506	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	7 (11%)
25	CLA	C	507	35	57,73,73	1.13	4 (7%)	61,113,113	1.14	7 (11%)
25	CLA	C	508	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	C	509	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	C	510	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	5 (8%)
25	CLA	C	511	3	57,73,73	1.14	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	C	512	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	7 (11%)
25	CLA	C	513	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
27	BCR	C	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	7 (12%)
27	BCR	C	515	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
33	DGD	C	516	-	63,63,67	0.84	1 (1%)	77,77,81	1.43	7 (9%)
33	DGD	C	517	-	63,63,67	0.89	1 (1%)	77,77,81	1.37	8 (10%)
33	DGD	C	518	-	63,63,67	0.85	1 (1%)	77,77,81	1.41	9 (11%)
29	LMG	C	519	-	51,51,55	0.71	0	59,59,63	1.33	6 (10%)
29	LMG	C	520	-	51,51,55	0.77	1 (1%)	59,59,63	1.35	6 (10%)
26	PHO	D	401	-	67,69,69	1.24	7 (10%)	86,99,99	1.07	7 (8%)
25	CLA	D	402	-	57,73,73	1.14	4 (7%)	61,113,113	1.08	6 (9%)
25	CLA	D	403	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
27	BCR	D	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	7 (12%)
29	LMG	D	405	-	51,51,55	0.72	0	59,59,63	1.32	7 (11%)
31	LHG	D	406	-	48,48,48	0.61	0	49,54,54	1.25	6 (12%)
28	PL9	D	407	-	54,55,55	0.85	3 (5%)	68,69,69	1.45	16 (23%)
23	SQD	D	408	-	46,47,54	1.00	4 (8%)	55,58,65	2.02	12 (21%)
23	SQD	D	409	-	42,43,54	1.06	5 (11%)	51,54,65	2.00	10 (19%)
34	HEM	E	101	5,6	24,50,50	1.94	5 (20%)	16,82,82	1.39	3 (18%)
27	BCR	H	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	7 (12%)
33	DGD	H	103	-	63,63,67	0.86	1 (1%)	77,77,81	1.36	9 (11%)
23	SQD	I	101	-	39,39,54	0.84	2 (5%)	41,41,65	1.20	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	8 (14%)
31	LHG	L	101	-	48,48,48	0.62	0	49,54,54	1.25	6 (12%)
27	BCR	T	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	7 (12%)
34	HEM	V	201	16	24,50,50	2.02	5 (20%)	16,82,82	1.35	3 (18%)
27	BCR	Y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	3 (5%)
21	OEX	a	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
32	BCT	a	605	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	a	606	-	57,73,73	1.13	5 (8%)	61,113,113	1.14	5 (8%)
25	CLA	a	607	35	51,67,73	1.21	5 (9%)	53,105,113	1.16	4 (7%)
26	PHO	a	608	-	67,69,69	1.23	7 (10%)	86,99,99	1.05	8 (9%)
25	CLA	a	609	-	57,73,73	1.13	4 (7%)	61,113,113	1.10	5 (8%)
27	BCR	a	610	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	a	611	-	54,55,55	0.81	2 (3%)	68,69,69	1.42	13 (19%)
25	CLA	a	612	35	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
31	LHG	a	613	-	48,48,48	0.61	0	49,54,54	1.29	6 (12%)
31	LHG	a	614	-	34,34,48	0.72	0	35,40,54	1.20	3 (8%)
31	LHG	a	615	-	41,41,48	0.67	0	42,47,54	1.31	6 (14%)
23	SQD	b	601	-	53,54,54	0.95	5 (9%)	62,65,65	1.76	9 (14%)
25	CLA	b	604	35	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	b	605	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	b	606	-	57,73,73	1.13	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	b	607	-	57,73,73	1.13	4 (7%)	61,113,113	1.19	7 (11%)
25	CLA	b	608	-	57,73,73	1.15	4 (7%)	61,113,113	1.10	5 (8%)
25	CLA	b	609	-	57,73,73	1.13	5 (8%)	61,113,113	1.14	6 (9%)
25	CLA	b	610	35	57,73,73	1.13	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	b	611	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	b	612	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	7 (11%)
25	CLA	b	613	35	57,73,73	1.14	4 (7%)	61,113,113	1.08	5 (8%)
25	CLA	b	614	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	7 (11%)
25	CLA	b	615	-	57,73,73	1.14	5 (8%)	61,113,113	1.14	6 (9%)
25	CLA	b	616	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	b	617	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	7 (11%)
25	CLA	b	618	-	57,73,73	1.14	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	b	619	-	57,73,73	1.13	5 (8%)	61,113,113	1.16	5 (8%)
27	BCR	b	620	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	b	621	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	3 (5%)
27	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	5 (8%)
29	LMG	b	623	-	51,51,55	0.71	0	59,59,63	1.36	7 (11%)
29	LMG	b	624	-	51,51,55	0.74	0	59,59,63	1.31	7 (11%)
29	LMG	b	625	-	8,8,55	0.15	0	7,7,63	0.91	0
23	SQD	c	501	-	53,54,54	0.95	5 (9%)	62,65,65	1.83	9 (14%)
29	LMG	c	502	-	51,51,55	0.75	0	59,59,63	1.33	6 (10%)
25	CLA	c	503	-	57,73,73	1.13	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	c	504	-	57,73,73	1.15	5 (8%)	61,113,113	1.10	6 (9%)
25	CLA	c	505	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	c	506	35	57,73,73	1.13	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	c	507	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	c	508	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	6 (9%)
25	CLA	c	509	35	57,73,73	1.13	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	510	-	50,66,73	1.21	4 (8%)	52,104,113	1.20	7 (13%)
25	CLA	c	511	-	57,73,73	1.14	5 (8%)	61,113,113	1.13	7 (11%)
25	CLA	c	512	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	c	513	3	57,73,73	1.13	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	c	514	-	57,73,73	1.12	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	c	515	-	57,73,73	1.13	4 (7%)	61,113,113	1.11	7 (11%)
27	BCR	c	516	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	6 (10%)
27	BCR	c	517	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)
33	DGD	c	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.43	10 (12%)
33	DGD	c	519	-	63,63,67	0.88	2 (3%)	77,77,81	1.39	10 (12%)
33	DGD	c	520	-	63,63,67	0.86	1 (1%)	77,77,81	1.41	11 (14%)
29	LMG	c	521	-	51,51,55	0.70	0	59,59,63	1.33	6 (10%)
29	LMG	c	522	-	51,51,55	0.78	1 (1%)	59,59,63	1.36	7 (11%)
26	PHO	d	401	-	67,69,69	1.24	8 (11%)	86,99,99	1.08	8 (9%)
25	CLA	d	403	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	7 (11%)
25	CLA	d	404	-	57,73,73	1.12	4 (7%)	61,113,113	1.15	6 (9%)
27	BCR	d	405	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	4 (7%)
29	LMG	d	406	-	42,42,55	0.78	0	50,50,63	1.32	8 (16%)
31	LHG	d	407	-	48,48,48	0.61	0	49,54,54	1.26	6 (12%)
28	PL9	d	408	-	54,55,55	0.86	3 (5%)	68,69,69	1.43	13 (19%)
29	LMG	d	409	-	39,39,55	0.56	0	41,41,63	1.27	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	e	101	5,6	24,50,50	1.93	4 (16%)	16,82,82	1.35	1 (6%)
23	SQD	f	101	-	42,43,54	1.06	4 (9%)	51,54,65	2.01	11 (21%)
27	BCR	h	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	7 (12%)
33	DGD	h	102	-	63,63,67	0.85	0	77,77,81	1.33	8 (10%)
27	BCR	k	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	4 (7%)
31	LHG	l	101	-	48,48,48	0.61	1 (2%)	49,54,54	1.24	6 (12%)
34	HEM	v	201	16	24,50,50	2.03	5 (20%)	16,82,82	1.36	1 (6%)
27	BCR	y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	4 (7%)

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	OEX	A	601	1,3,35	-	0/0/68/68	0/0/6/6
23	SQD	A	603	-	-	0/47/67/69	0/1/1/1
25	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	607	35	3/3/18/25	0/28/126/135	0/0/9/9
26	PHO	A	608	-	-	0/53/103/103	0/1/6/6
25	CLA	A	609	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
28	PL9	A	611	-	-	0/53/73/73	0/1/1/1
29	LMG	A	612	-	-	0/46/66/70	0/1/1/1
29	LMG	A	613	-	-	0/46/66/70	0/1/1/1
25	CLA	A	615	35	3/3/20/25	0/37/135/135	0/0/9/9
31	LHG	A	616	-	-	0/53/53/53	0/0/0/0
31	LHG	A	617	-	-	0/53/53/53	0/0/0/0
31	LHG	A	618	-	-	0/53/53/53	0/0/0/0
23	SQD	A	619	-	-	0/41/41/69	0/0/0/1
32	BCT	A	620	22	-	0/0/0/0	0/0/0/0
25	CLA	B	601	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	605	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	607	35	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	609	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMG	B	620	-	-	0/46/66/70	0/1/1/1
29	LMG	B	621	-	-	0/46/66/70	0/1/1/1
29	LMG	B	625	-	-	0/46/66/70	0/1/1/1
23	SQD	B	626	-	-	2/49/69/69	0/1/1/1
27	BCR	B	627	-	-	0/29/63/63	0/2/2/2
25	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	502	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	504	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	505	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	507	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
33	DGD	C	516	-	-	0/51/91/95	0/2/2/2
33	DGD	C	517	-	-	0/51/91/95	0/2/2/2
33	DGD	C	518	-	-	0/51/91/95	0/2/2/2
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
29	LMG	C	520	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	D	401	-	-	0/53/103/103	0/1/6/6
25	CLA	D	402	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	D	404	-	-	0/29/63/63	0/2/2/2
29	LMG	D	405	-	-	0/46/66/70	0/1/1/1
31	LHG	D	406	-	-	0/53/53/53	0/0/0/0
28	PL9	D	407	-	-	0/53/73/73	0/1/1/1
23	SQD	D	408	-	-	0/42/62/69	0/1/1/1
23	SQD	D	409	-	-	0/38/58/69	0/1/1/1
34	HEM	E	101	5,6	-	0/6/54/54	0/0/8/8
27	BCR	H	102	-	-	0/29/63/63	0/2/2/2
33	DGD	H	103	-	-	0/51/91/95	0/2/2/2
23	SQD	I	101	-	-	0/41/41/69	0/0/0/1
27	BCR	K	101	-	-	0/29/63/63	0/2/2/2
31	LHG	L	101	-	-	0/53/53/53	0/0/0/0
27	BCR	T	101	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
27	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
21	OEX	a	601	1,3,35	-	0/0/68/68	0/0/6/6
32	BCT	a	605	22	-	0/0/0/0	0/0/0/0
25	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	607	35	3/3/18/25	0/30/128/135	0/0/9/9
26	PHO	a	608	-	-	0/53/103/103	0/1/6/6
25	CLA	a	609	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	a	610	-	-	0/29/63/63	0/2/2/2
28	PL9	a	611	-	-	0/53/73/73	0/1/1/1
25	CLA	a	612	35	3/3/20/25	0/37/135/135	0/0/9/9
31	LHG	a	613	-	-	0/53/53/53	0/0/0/0
31	LHG	a	614	-	-	0/39/39/53	0/0/0/0
31	LHG	a	615	-	-	0/46/46/53	0/0/0/0
23	SQD	b	601	-	-	0/49/69/69	0/1/1/1
25	CLA	b	604	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	608	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	610	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	b	613	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	b	620	-	-	0/29/63/63	0/2/2/2
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	BCR	b	622	-	-	0/29/63/63	0/2/2/2
29	LMG	b	623	-	-	0/46/66/70	0/1/1/1
29	LMG	b	624	-	-	0/46/66/70	0/1/1/1
29	LMG	b	625	-	-	0/6/6/70	0/0/0/1
23	SQD	c	501	-	-	0/49/69/69	0/1/1/1
29	LMG	c	502	-	-	0/46/66/70	0/1/1/1
25	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	507	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	509	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	510	-	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	513	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	514	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	515	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	516	-	-	0/29/63/63	0/2/2/2
27	BCR	c	517	-	-	0/29/63/63	0/2/2/2
33	DGD	c	518	-	-	0/51/91/95	0/2/2/2
33	DGD	c	519	-	-	0/51/91/95	0/2/2/2
33	DGD	c	520	-	-	0/51/91/95	0/2/2/2
29	LMG	c	521	-	-	0/46/66/70	0/1/1/1
29	LMG	c	522	-	-	0/46/66/70	0/1/1/1
26	PHO	d	401	-	-	0/53/103/103	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	d	405	-	-	0/29/63/63	0/2/2/2
29	LMG	d	406	-	-	0/37/57/70	0/1/1/1
31	LHG	d	407	-	-	0/53/53/53	0/0/0/0
28	PL9	d	408	-	-	0/53/73/73	0/1/1/1
29	LMG	d	409	-	-	1/41/41/70	0/0/0/1
34	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
23	SQD	f	101	-	-	0/38/58/69	0/1/1/1
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
33	DGD	h	102	-	-	0/51/91/95	0/2/2/2
27	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LHG	l	101	-	-	0/53/53/53	0/0/0/0
34	HEM	v	201	16	-	0/6/54/54	0/0/8/8
27	BCR	y	101	-	-	0/29/63/63	0/2/2/2

All (457) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3C-C2C	-4.96	1.34	1.40
34	V	201	HEM	C3C-C2C	-4.91	1.34	1.40
34	E	101	HEM	C3B-C2B	-4.11	1.35	1.40
34	v	201	HEM	C3B-C2B	-4.04	1.35	1.40
34	E	101	HEM	C3C-C2C	-4.03	1.35	1.40
34	e	101	HEM	C3C-C2C	-4.01	1.35	1.40
34	e	101	HEM	C3B-C2B	-4.00	1.35	1.40
34	V	201	HEM	C3B-C2B	-3.95	1.35	1.40
27	B	627	BCR	C1-C6	-3.61	1.48	1.53
27	C	515	BCR	C1-C6	-3.54	1.49	1.53
27	C	514	BCR	C1-C6	-3.53	1.49	1.53
27	B	617	BCR	C1-C6	-3.52	1.49	1.53
27	T	101	BCR	C1-C6	-3.51	1.49	1.53
27	D	404	BCR	C1-C6	-3.50	1.49	1.53
27	b	620	BCR	C1-C6	-3.47	1.49	1.53
27	y	101	BCR	C1-C6	-3.47	1.49	1.53
27	c	517	BCR	C1-C6	-3.42	1.49	1.53
27	B	618	BCR	C1-C6	-3.42	1.49	1.53
27	b	621	BCR	C1-C6	-3.37	1.49	1.53
27	a	610	BCR	C1-C6	-3.35	1.49	1.53
27	B	617	BCR	C30-C25	-3.35	1.49	1.53
27	A	610	BCR	C1-C6	-3.34	1.49	1.53
27	b	620	BCR	C30-C25	-3.33	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y	101	BCR	C1-C6	-3.32	1.49	1.53
27	B	619	BCR	C1-C6	-3.29	1.49	1.53
27	k	101	BCR	C1-C6	-3.28	1.49	1.53
27	B	619	BCR	C30-C25	-3.28	1.49	1.53
27	K	101	BCR	C30-C25	-3.22	1.49	1.53
27	y	101	BCR	C30-C25	-3.19	1.49	1.53
27	c	516	BCR	C30-C25	-3.17	1.49	1.53
27	b	621	BCR	C30-C25	-3.17	1.49	1.53
27	b	622	BCR	C30-C25	-3.16	1.49	1.53
27	c	517	BCR	C30-C25	-3.16	1.49	1.53
27	Y	101	BCR	C30-C25	-3.13	1.49	1.53
27	c	516	BCR	C1-C6	-3.13	1.49	1.53
27	d	405	BCR	C1-C6	-3.12	1.49	1.53
27	C	514	BCR	C30-C25	-3.12	1.49	1.53
27	h	101	BCR	C30-C25	-3.11	1.49	1.53
27	A	610	BCR	C30-C25	-3.11	1.49	1.53
27	C	515	BCR	C30-C25	-3.11	1.49	1.53
27	K	101	BCR	C1-C6	-3.11	1.49	1.53
27	D	404	BCR	C30-C25	-3.10	1.49	1.53
27	h	101	BCR	C1-C6	-3.10	1.49	1.53
27	d	405	BCR	C30-C25	-3.10	1.49	1.53
27	b	622	BCR	C1-C6	-3.09	1.49	1.53
27	B	618	BCR	C30-C25	-3.09	1.49	1.53
27	a	610	BCR	C30-C25	-3.03	1.49	1.53
27	B	627	BCR	C30-C25	-3.00	1.49	1.53
27	H	102	BCR	C1-C6	-2.98	1.49	1.53
27	k	101	BCR	C30-C25	-2.98	1.49	1.53
27	H	102	BCR	C30-C25	-2.98	1.49	1.53
27	T	101	BCR	C30-C25	-2.89	1.49	1.53
25	c	508	CLA	CMB-C2B	-2.65	1.46	1.51
25	C	506	CLA	CMB-C2B	-2.65	1.46	1.51
28	d	408	PL9	C3-C4	-2.65	1.45	1.49
28	D	407	PL9	C3-C4	-2.62	1.45	1.49
28	A	611	PL9	C3-C4	-2.61	1.45	1.49
25	b	614	CLA	CMB-C2B	-2.56	1.46	1.51
25	B	611	CLA	CMB-C2B	-2.53	1.46	1.51
25	c	504	CLA	CMB-C2B	-2.51	1.46	1.51
25	B	604	CLA	CMB-C2B	-2.51	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.51	1.46	1.51
25	b	604	CLA	CMB-C2B	-2.51	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.50	1.46	1.51
25	A	615	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	CMB-C2B	-2.49	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.49	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.48	1.46	1.51
25	C	507	CLA	CMB-C2B	-2.48	1.46	1.51
25	a	609	CLA	CMB-C2B	-2.48	1.46	1.51
25	b	618	CLA	CMB-C2B	-2.48	1.46	1.51
25	C	505	CLA	CMD-C2D	-2.48	1.46	1.51
25	c	506	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	608	CLA	CMB-C2B	-2.47	1.46	1.51
25	a	607	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	609	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.47	1.46	1.51
25	C	504	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	612	CLA	CMB-C2B	-2.47	1.46	1.51
25	c	507	CLA	CMD-C2D	-2.46	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	608	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	601	CLA	CMB-C2B	-2.45	1.46	1.51
25	a	612	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	508	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	606	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	605	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.45	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.44	1.46	1.51
25	A	607	CLA	CMB-C2B	-2.44	1.46	1.51
25	D	402	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.44	1.46	1.51
25	b	617	CLA	CMB-C2B	-2.44	1.46	1.51
25	d	403	CLA	CMB-C2B	-2.44	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.44	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	615	CLA	CMB-C2B	-2.44	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.44	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.44	1.46	1.51
25	b	605	CLA	CMB-C2B	-2.44	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	CMB-C2B	-2.44	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.43	1.46	1.51
25	A	609	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.43	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	501	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	613	CLA	CMB-C2B	-2.42	1.46	1.51
25	a	606	CLA	CMB-C2B	-2.42	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.42	1.46	1.51
25	C	502	CLA	CMB-C2B	-2.42	1.46	1.51
28	a	611	PL9	C3-C4	-2.41	1.45	1.49
25	c	515	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	514	CLA	CMB-C2B	-2.39	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.39	1.46	1.51
25	A	606	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	606	CLA	CMD-C2D	-2.37	1.46	1.51
25	d	404	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	619	CLA	CMB-C2B	-2.36	1.46	1.51
25	D	402	CLA	CMD-C2D	-2.36	1.46	1.51
25	B	612	CLA	CMD-C2D	-2.33	1.46	1.51
25	C	503	CLA	CMD-C2D	-2.32	1.46	1.51
25	B	603	CLA	CMD-C2D	-2.32	1.46	1.51
25	A	607	CLA	CMD-C2D	-2.32	1.46	1.51
25	B	614	CLA	CMD-C2D	-2.32	1.46	1.51
25	a	607	CLA	CMD-C2D	-2.31	1.46	1.51
25	C	512	CLA	CMD-C2D	-2.31	1.46	1.51
25	b	607	CLA	CMD-C2D	-2.31	1.46	1.51
25	a	606	CLA	CMD-C2D	-2.31	1.46	1.51
25	B	605	CLA	CMD-C2D	-2.31	1.46	1.51
25	b	615	CLA	CMD-C2D	-2.31	1.46	1.51
25	b	617	CLA	CMD-C2D	-2.31	1.46	1.51
25	C	510	CLA	CMD-C2D	-2.30	1.46	1.51
25	b	608	CLA	CMD-C2D	-2.30	1.46	1.51
25	C	509	CLA	CMD-C2D	-2.30	1.46	1.51
25	B	607	CLA	CMD-C2D	-2.30	1.46	1.51
25	b	619	CLA	CMD-C2D	-2.30	1.46	1.51
25	B	604	CLA	CMD-C2D	-2.29	1.46	1.51
25	A	606	CLA	CMD-C2D	-2.29	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	515	CLA	CMD-C2D	-2.29	1.46	1.51
25	C	504	CLA	CMD-C2D	-2.29	1.46	1.51
25	c	505	CLA	CMD-C2D	-2.28	1.46	1.51
25	c	504	CLA	CMD-C2D	-2.27	1.46	1.51
25	B	608	CLA	CMD-C2D	-2.27	1.46	1.51
25	b	609	CLA	CMD-C2D	-2.27	1.46	1.51
25	c	514	CLA	CMD-C2D	-2.27	1.46	1.51
25	d	403	CLA	CMD-C2D	-2.27	1.46	1.51
25	B	611	CLA	CMD-C2D	-2.27	1.46	1.51
25	D	403	CLA	CMD-C2D	-2.27	1.46	1.51
25	A	609	CLA	CMD-C2D	-2.27	1.46	1.51
25	a	612	CLA	CMD-C2D	-2.27	1.46	1.51
25	a	609	CLA	CMD-C2D	-2.26	1.46	1.51
25	b	616	CLA	CMD-C2D	-2.26	1.46	1.51
25	C	502	CLA	CMD-C2D	-2.26	1.46	1.51
25	b	618	CLA	CMD-C2D	-2.26	1.46	1.51
25	b	605	CLA	CMD-C2D	-2.26	1.46	1.51
25	B	613	CLA	CMD-C2D	-2.26	1.46	1.51
25	B	602	CLA	CMD-C2D	-2.26	1.46	1.51
25	c	512	CLA	CMD-C2D	-2.26	1.46	1.51
25	B	601	CLA	CMD-C2D	-2.26	1.46	1.51
25	B	616	CLA	CMD-C2D	-2.26	1.46	1.51
25	c	503	CLA	CMD-C2D	-2.25	1.46	1.51
25	c	506	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	612	CLA	CMD-C2D	-2.25	1.46	1.51
33	C	516	DGD	O1G-C1G	-2.25	1.40	1.45
25	A	615	CLA	CMD-C2D	-2.25	1.46	1.51
25	B	610	CLA	CMD-C2D	-2.25	1.46	1.51
25	c	510	CLA	CMD-C2D	-2.25	1.46	1.51
25	B	615	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	611	CLA	CMD-C2D	-2.25	1.46	1.51
25	C	513	CLA	CMD-C2D	-2.25	1.46	1.51
33	C	517	DGD	O1G-C1G	-2.24	1.40	1.45
25	C	508	CLA	CMD-C2D	-2.24	1.46	1.51
25	b	613	CLA	CMD-C2D	-2.24	1.46	1.51
25	c	509	CLA	CMD-C2D	-2.24	1.46	1.51
26	D	401	PHO	C1C-NC	-2.24	1.33	1.38
25	C	506	CLA	CMD-C2D	-2.24	1.46	1.51
33	c	519	DGD	O1G-C1G	-2.24	1.40	1.45
25	C	501	CLA	CMD-C2D	-2.24	1.46	1.51
25	b	610	CLA	CMD-C2D	-2.24	1.46	1.51
25	B	606	CLA	CMD-C2D	-2.24	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	625	LMG	O6-C5	-2.23	1.38	1.44
33	c	518	DGD	O1G-C1G	-2.23	1.40	1.45
25	b	604	CLA	CMD-C2D	-2.23	1.46	1.51
25	d	404	CLA	CMD-C2D	-2.23	1.46	1.51
25	c	508	CLA	CMD-C2D	-2.23	1.46	1.51
25	b	614	CLA	CMD-C2D	-2.23	1.46	1.51
25	c	513	CLA	CMD-C2D	-2.23	1.46	1.51
25	B	609	CLA	CMD-C2D	-2.22	1.46	1.51
26	A	608	PHO	C1C-NC	-2.21	1.33	1.38
25	C	511	CLA	CMD-C2D	-2.21	1.46	1.51
25	C	507	CLA	CMD-C2D	-2.21	1.46	1.51
25	c	511	CLA	CMD-C2D	-2.21	1.46	1.51
26	d	401	PHO	C1C-NC	-2.21	1.33	1.38
33	c	520	DGD	O1G-C1G	-2.20	1.40	1.45
23	c	501	SQD	O2-C2	-2.20	1.37	1.43
26	a	608	PHO	C1C-NC	-2.19	1.33	1.38
23	A	603	SQD	O2-C2	-2.17	1.37	1.43
23	f	101	SQD	O2-C2	-2.17	1.37	1.43
23	D	409	SQD	O2-C2	-2.17	1.37	1.43
33	C	518	DGD	O1G-C1G	-2.16	1.40	1.45
23	B	626	SQD	O2-C2	-2.15	1.37	1.43
25	b	619	CLA	CMC-C2C	-2.14	1.46	1.50
23	b	601	SQD	O2-C2	-2.12	1.38	1.43
28	d	408	PL9	C53-C6	-2.11	1.46	1.50
25	B	616	CLA	CMC-C2C	-2.11	1.46	1.50
28	a	611	PL9	C53-C6	-2.08	1.46	1.50
28	A	611	PL9	C53-C6	-2.08	1.46	1.50
23	D	408	SQD	O2-C2	-2.08	1.38	1.43
28	D	407	PL9	C6-C1	-2.08	1.44	1.48
31	l	101	LHG	O7-C5	-2.07	1.41	1.46
33	c	518	DGD	O2G-C2G	-2.07	1.41	1.46
28	d	408	PL9	C6-C1	-2.07	1.44	1.48
23	c	501	SQD	O3-C3	-2.05	1.38	1.43
28	D	407	PL9	C53-C6	-2.05	1.46	1.50
23	b	601	SQD	O3-C3	-2.05	1.38	1.43
23	b	601	SQD	O4-C4	-2.05	1.38	1.43
23	D	409	SQD	O4-C4	-2.04	1.38	1.43
25	b	615	CLA	CMC-C2C	-2.04	1.46	1.50
23	D	409	SQD	O3-C3	-2.04	1.38	1.43
33	c	519	DGD	O2G-C2G	-2.03	1.41	1.46
23	D	408	SQD	O3-C3	-2.02	1.38	1.43
23	A	603	SQD	O3-C3	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	H	103	DGD	O1G-C1G	-2.01	1.40	1.45
23	f	101	SQD	O3-C3	-2.01	1.38	1.43
23	B	626	SQD	O3-C3	-2.00	1.38	1.43
23	c	501	SQD	O4-C4	-2.00	1.38	1.43
26	A	608	PHO	CMC-C2C	-2.00	1.46	1.50
25	C	502	CLA	C4C-NC	2.00	1.40	1.37
25	C	508	CLA	C4C-NC	2.00	1.40	1.37
25	b	606	CLA	C4C-NC	2.00	1.40	1.37
25	C	504	CLA	C4C-NC	2.00	1.40	1.37
25	c	504	CLA	C4C-NC	2.01	1.40	1.37
25	B	603	CLA	C4C-NC	2.01	1.40	1.37
25	b	611	CLA	C4C-NC	2.01	1.40	1.37
25	A	607	CLA	C4C-NC	2.02	1.40	1.37
25	c	511	CLA	C4C-NC	2.02	1.40	1.37
25	b	604	CLA	C4C-NC	2.02	1.40	1.37
25	b	609	CLA	C4C-NC	2.02	1.40	1.37
34	v	201	HEM	CAD-C3D	2.02	1.54	1.52
26	d	401	PHO	C4B-NB	2.02	1.41	1.36
25	a	606	CLA	C4C-NC	2.02	1.40	1.37
25	B	616	CLA	C4C-NC	2.02	1.40	1.37
31	A	618	LHG	P-O6	2.03	1.67	1.59
26	A	608	PHO	C4B-NB	2.03	1.41	1.36
25	B	602	CLA	C4C-NC	2.04	1.40	1.37
25	A	609	CLA	C4C-NC	2.04	1.40	1.37
29	B	621	LMG	C7-C8	2.04	1.56	1.50
25	B	607	CLA	C4C-NC	2.04	1.40	1.37
25	B	605	CLA	C4C-NC	2.05	1.40	1.37
25	A	606	CLA	C4C-NC	2.07	1.40	1.37
25	a	607	CLA	C4C-NC	2.08	1.40	1.37
29	B	625	LMG	C3-C2	2.10	1.57	1.52
34	E	101	HEM	CAD-C3D	2.15	1.55	1.52
34	V	201	HEM	CAD-C3D	2.22	1.55	1.52
26	A	608	PHO	CHD-C1D	2.24	1.43	1.38
26	d	401	PHO	CHD-C1D	2.26	1.43	1.38
26	a	608	PHO	CHD-C1D	2.27	1.43	1.38
26	a	608	PHO	C4C-C3C	2.30	1.49	1.45
26	d	401	PHO	C4C-C3C	2.31	1.49	1.45
26	D	401	PHO	C4C-C3C	2.32	1.49	1.45
26	D	401	PHO	CHD-C1D	2.32	1.43	1.38
26	A	608	PHO	C4C-C3C	2.33	1.49	1.45
29	C	520	LMG	C1-C2	2.36	1.59	1.52
29	c	522	LMG	C1-C2	2.43	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	C1A-NA	2.52	1.42	1.37
26	a	608	PHO	C1A-NA	2.53	1.42	1.37
26	d	401	PHO	C1A-NA	2.53	1.42	1.37
26	D	401	PHO	C1A-NA	2.53	1.42	1.37
25	C	507	CLA	CHC-C1C	2.59	1.42	1.35
25	c	509	CLA	CHC-C1C	2.60	1.42	1.35
25	C	512	CLA	CHC-C1C	2.60	1.42	1.35
25	b	619	CLA	CHC-C1C	2.61	1.43	1.35
26	d	401	PHO	C4C-NC	2.61	1.42	1.36
26	A	608	PHO	C4C-NC	2.61	1.42	1.36
25	c	508	CLA	CHC-C1C	2.61	1.43	1.35
25	b	607	CLA	CHC-C1C	2.62	1.43	1.35
25	B	616	CLA	CHC-C1C	2.62	1.43	1.35
25	b	618	CLA	CHC-C1C	2.62	1.43	1.35
25	a	612	CLA	CHC-C1C	2.62	1.43	1.35
25	C	506	CLA	CHC-C1C	2.62	1.43	1.35
25	b	604	CLA	CHC-C1C	2.63	1.43	1.35
25	C	505	CLA	CHC-C1C	2.63	1.43	1.35
25	c	507	CLA	CHC-C1C	2.63	1.43	1.35
25	c	504	CLA	CHC-C1C	2.64	1.43	1.35
25	B	601	CLA	CHC-C1C	2.64	1.43	1.35
25	B	604	CLA	CHC-C1C	2.64	1.43	1.35
25	C	509	CLA	CHC-C1C	2.65	1.43	1.35
25	D	403	CLA	CHC-C1C	2.65	1.43	1.35
25	c	514	CLA	CHC-C1C	2.65	1.43	1.35
25	B	609	CLA	CHC-C1C	2.65	1.43	1.35
25	a	609	CLA	CHC-C1C	2.65	1.43	1.35
26	a	608	PHO	C4C-NC	2.65	1.43	1.36
25	b	614	CLA	CHC-C1C	2.65	1.43	1.35
25	B	611	CLA	CHC-C1C	2.65	1.43	1.35
25	b	612	CLA	CHC-C1C	2.65	1.43	1.35
25	b	616	CLA	CHC-C1C	2.65	1.43	1.35
25	B	613	CLA	CHC-C1C	2.65	1.43	1.35
25	D	402	CLA	CHC-C1C	2.65	1.43	1.35
25	b	609	CLA	CHC-C1C	2.65	1.43	1.35
25	C	501	CLA	CHC-C1C	2.66	1.43	1.35
25	B	610	CLA	CHC-C1C	2.66	1.43	1.35
25	A	615	CLA	CHC-C1C	2.66	1.43	1.35
25	C	502	CLA	CHC-C1C	2.66	1.43	1.35
26	D	401	PHO	C4C-NC	2.66	1.43	1.36
25	A	607	CLA	CHC-C1C	2.66	1.43	1.35
25	c	503	CLA	CHC-C1C	2.66	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	CHC-C1C	2.67	1.43	1.35
25	B	605	CLA	CHC-C1C	2.67	1.43	1.35
25	c	511	CLA	CHC-C1C	2.67	1.43	1.35
25	b	608	CLA	CHC-C1C	2.67	1.43	1.35
25	B	614	CLA	CHC-C1C	2.67	1.43	1.35
25	B	608	CLA	CHC-C1C	2.67	1.43	1.35
25	b	610	CLA	CHC-C1C	2.67	1.43	1.35
25	A	606	CLA	CHC-C1C	2.67	1.43	1.35
25	B	607	CLA	CHC-C1C	2.67	1.43	1.35
25	b	605	CLA	CHC-C1C	2.67	1.43	1.35
25	c	506	CLA	CHC-C1C	2.67	1.43	1.35
25	c	505	CLA	CHC-C1C	2.67	1.43	1.35
25	c	513	CLA	CHC-C1C	2.67	1.43	1.35
25	B	606	CLA	CHC-C1C	2.68	1.43	1.35
25	C	504	CLA	CHC-C1C	2.68	1.43	1.35
25	B	602	CLA	CHC-C1C	2.68	1.43	1.35
25	C	503	CLA	CHC-C1C	2.68	1.43	1.35
25	b	606	CLA	CHC-C1C	2.68	1.43	1.35
25	b	611	CLA	CHC-C1C	2.68	1.43	1.35
25	d	404	CLA	CHC-C1C	2.68	1.43	1.35
25	C	511	CLA	CHC-C1C	2.68	1.43	1.35
25	b	613	CLA	CHC-C1C	2.68	1.43	1.35
25	d	403	CLA	CHC-C1C	2.68	1.43	1.35
25	B	615	CLA	CHC-C1C	2.68	1.43	1.35
25	B	612	CLA	CHC-C1C	2.68	1.43	1.35
23	b	601	SQD	O47-C7	2.69	1.42	1.34
25	b	615	CLA	CHC-C1C	2.69	1.43	1.35
25	a	607	CLA	CHC-C1C	2.69	1.43	1.35
25	c	510	CLA	CHC-C1C	2.69	1.43	1.35
25	a	606	CLA	CHC-C1C	2.69	1.43	1.35
25	C	513	CLA	CHC-C1C	2.69	1.43	1.35
25	C	510	CLA	CHC-C1C	2.69	1.43	1.35
25	C	508	CLA	CHC-C1C	2.70	1.43	1.35
25	c	512	CLA	CHC-C1C	2.71	1.43	1.35
25	b	617	CLA	CHC-C1C	2.71	1.43	1.35
23	f	101	SQD	O47-C7	2.73	1.42	1.34
25	c	515	CLA	CHC-C1C	2.73	1.43	1.35
23	A	603	SQD	O47-C7	2.73	1.42	1.34
23	c	501	SQD	O47-C7	2.73	1.42	1.34
25	A	609	CLA	CHC-C1C	2.73	1.43	1.35
23	I	101	SQD	O47-C7	2.74	1.42	1.34
23	D	409	SQD	O47-C7	2.77	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	626	SQD	O47-C7	2.79	1.42	1.34
23	D	408	SQD	O47-C7	2.79	1.42	1.34
23	A	619	SQD	O47-C7	2.85	1.42	1.34
26	a	608	PHO	CHC-C1C	2.90	1.44	1.38
26	d	401	PHO	CHC-C1C	2.91	1.44	1.38
26	A	608	PHO	CHC-C1C	2.91	1.44	1.38
26	D	401	PHO	CHC-C1C	2.94	1.44	1.38
23	D	408	SQD	O48-C23	3.05	1.42	1.33
23	b	601	SQD	O48-C23	3.06	1.42	1.33
23	A	603	SQD	O48-C23	3.10	1.42	1.33
23	D	409	SQD	O48-C23	3.10	1.42	1.33
23	f	101	SQD	O48-C23	3.11	1.42	1.33
23	B	626	SQD	O48-C23	3.11	1.42	1.33
23	c	501	SQD	O48-C23	3.12	1.42	1.33
23	I	101	SQD	O48-C23	3.16	1.42	1.33
23	A	619	SQD	O48-C23	3.22	1.42	1.33
26	A	608	PHO	C3B-C4B	3.50	1.50	1.43
26	a	608	PHO	C3B-C4B	3.51	1.50	1.43
26	d	401	PHO	C3B-C4B	3.53	1.50	1.43
26	D	401	PHO	C3B-C4B	3.53	1.50	1.43
34	E	101	HEM	C3B-CAB	3.68	1.55	1.47
34	V	201	HEM	C3B-CAB	3.70	1.55	1.47
34	v	201	HEM	C3C-CAC	3.70	1.55	1.47
34	V	201	HEM	C3C-CAC	3.70	1.55	1.47
34	e	101	HEM	C3B-CAB	3.73	1.55	1.47
34	v	201	HEM	C3B-CAB	3.75	1.55	1.47
25	b	611	CLA	CHB-C4A	3.77	1.38	1.33
34	e	101	HEM	C3C-CAC	3.78	1.55	1.47
25	b	610	CLA	CHB-C4A	3.79	1.38	1.33
25	B	607	CLA	CHB-C4A	3.79	1.38	1.33
25	A	609	CLA	CHB-C4A	3.79	1.38	1.33
34	E	101	HEM	C3C-CAC	3.79	1.55	1.47
25	b	606	CLA	CHB-C4A	3.79	1.38	1.33
25	c	509	CLA	CHB-C4A	3.80	1.38	1.33
25	C	512	CLA	CHB-C4A	3.83	1.38	1.33
25	a	609	CLA	CHB-C4A	3.83	1.38	1.33
25	D	402	CLA	CHB-C4A	3.84	1.38	1.33
25	d	403	CLA	CHB-C4A	3.85	1.38	1.33
25	a	607	CLA	CHB-C4A	3.89	1.38	1.33
25	B	608	CLA	CHB-C4A	3.89	1.38	1.33
25	C	505	CLA	CHB-C4A	3.89	1.38	1.33
25	C	504	CLA	CHB-C4A	3.90	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	CHB-C4A	3.90	1.38	1.33
25	C	501	CLA	CHB-C4A	3.90	1.38	1.33
25	C	510	CLA	CHB-C4A	3.90	1.38	1.33
25	b	609	CLA	CHB-C4A	3.90	1.38	1.33
25	B	603	CLA	CHB-C4A	3.90	1.38	1.33
25	b	608	CLA	CHB-C4A	3.90	1.38	1.33
25	c	510	CLA	CHB-C4A	3.91	1.38	1.33
25	C	506	CLA	CHB-C4A	3.91	1.38	1.33
25	c	508	CLA	CHB-C4A	3.91	1.38	1.33
25	c	507	CLA	CHB-C4A	3.91	1.38	1.33
25	d	404	CLA	CHB-C4A	3.91	1.38	1.33
25	a	606	CLA	CHB-C4A	3.92	1.38	1.33
25	D	403	CLA	CHB-C4A	3.92	1.38	1.33
25	b	605	CLA	CHB-C4A	3.92	1.38	1.33
25	A	615	CLA	CHB-C4A	3.92	1.38	1.33
25	B	616	CLA	CHB-C4A	3.92	1.38	1.33
25	A	607	CLA	CHB-C4A	3.92	1.38	1.33
25	B	606	CLA	CHB-C4A	3.93	1.38	1.33
25	c	515	CLA	CHB-C4A	3.93	1.38	1.33
25	c	511	CLA	CHB-C4A	3.93	1.38	1.33
25	c	506	CLA	CHB-C4A	3.93	1.38	1.33
25	C	513	CLA	CHB-C4A	3.94	1.38	1.33
25	B	602	CLA	CHB-C4A	3.94	1.38	1.33
25	C	507	CLA	CHB-C4A	3.94	1.38	1.33
25	c	503	CLA	CHB-C4A	3.94	1.38	1.33
25	B	614	CLA	CHB-C4A	3.94	1.38	1.33
25	b	613	CLA	CHB-C4A	3.94	1.38	1.33
25	a	612	CLA	CHB-C4A	3.95	1.38	1.33
25	B	610	CLA	CHB-C4A	3.95	1.38	1.33
25	b	612	CLA	CHB-C4A	3.95	1.38	1.33
25	B	613	CLA	CHB-C4A	3.95	1.38	1.33
25	B	605	CLA	CHB-C4A	3.95	1.38	1.33
25	C	502	CLA	CHB-C4A	3.96	1.38	1.33
25	b	614	CLA	CHB-C4A	3.96	1.38	1.33
25	A	606	CLA	CHB-C4A	3.96	1.38	1.33
25	b	616	CLA	CHB-C4A	3.96	1.38	1.33
25	b	607	CLA	CHB-C4A	3.96	1.38	1.33
25	b	604	CLA	CHB-C4A	3.96	1.38	1.33
25	b	619	CLA	CHB-C4A	3.96	1.38	1.33
25	b	618	CLA	CHB-C4A	3.97	1.38	1.33
25	c	505	CLA	CHB-C4A	3.98	1.38	1.33
25	B	611	CLA	CHB-C4A	3.98	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	CHB-C4A	3.98	1.38	1.33
25	B	615	CLA	CHB-C4A	3.98	1.38	1.33
25	b	617	CLA	CHB-C4A	3.98	1.38	1.33
25	c	512	CLA	CHB-C4A	3.99	1.38	1.33
25	C	511	CLA	CHB-C4A	4.00	1.38	1.33
25	c	514	CLA	CHB-C4A	4.00	1.38	1.33
25	C	503	CLA	CHB-C4A	4.00	1.38	1.33
25	c	513	CLA	CHB-C4A	4.01	1.38	1.33
25	B	609	CLA	CHB-C4A	4.01	1.38	1.33
25	C	509	CLA	CHB-C4A	4.02	1.38	1.33
25	b	615	CLA	CHB-C4A	4.03	1.38	1.33
25	c	504	CLA	CHB-C4A	4.04	1.38	1.33
25	B	604	CLA	CHB-C4A	4.04	1.38	1.33
25	B	601	CLA	CHB-C4A	4.05	1.39	1.33

All (950) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	603	SQD	O9-S-O7	-4.66	100.79	113.96
29	A	613	LMG	O1-C1-C2	-4.65	102.28	108.00
33	c	518	DGD	O3G-C3G-C2G	-4.56	100.14	110.99
23	D	408	SQD	O9-S-O7	-4.56	101.08	113.96
23	B	626	SQD	O9-S-O7	-4.55	101.11	113.96
33	C	516	DGD	O3G-C3G-C2G	-4.53	100.21	110.99
23	f	101	SQD	O9-S-O7	-4.51	101.22	113.96
23	D	409	SQD	O9-S-O7	-4.50	101.24	113.96
23	c	501	SQD	O9-S-O7	-4.48	101.31	113.96
23	b	601	SQD	O9-S-O7	-4.45	101.40	113.96
33	C	518	DGD	O3G-C3G-C2G	-4.34	100.66	110.99
33	c	520	DGD	O3G-C3G-C2G	-4.33	100.69	110.99
33	c	519	DGD	O3G-C3G-C2G	-4.26	100.85	110.99
33	H	103	DGD	O3G-C3G-C2G	-3.92	101.66	110.99
29	c	522	LMG	O6-C1-O1	-3.80	100.88	109.99
33	C	517	DGD	O3G-C3G-C2G	-3.80	101.95	110.99
33	h	102	DGD	O3G-C3G-C2G	-3.79	101.96	110.99
29	C	520	LMG	O6-C1-O1	-3.79	100.90	109.99
25	A	606	CLA	CMB-C2B-C1B	-3.74	121.95	128.31
25	c	514	CLA	CMB-C2B-C1B	-3.73	121.96	128.31
25	d	404	CLA	CMB-C2B-C1B	-3.57	122.23	128.31
25	b	619	CLA	CMB-C2B-C1B	-3.57	122.23	128.31
25	a	606	CLA	CMB-C2B-C1B	-3.56	122.26	128.31
29	B	621	LMG	O6-C1-O1	-3.55	101.48	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	509	CLA	CMB-C2B-C1B	-3.52	122.33	128.31
25	B	616	CLA	CMB-C2B-C1B	-3.43	122.48	128.31
33	C	517	DGD	O6D-C1D-O3G	-3.41	101.82	109.99
33	c	518	DGD	O6D-C1D-O3G	-3.40	101.83	109.99
25	B	612	CLA	CMB-C2B-C1B	-3.39	122.55	128.31
25	c	512	CLA	CMB-C2B-C1B	-3.38	122.56	128.31
33	c	520	DGD	O6D-C1D-O3G	-3.36	101.92	109.99
33	C	516	DGD	O6D-C1D-O3G	-3.35	101.94	109.99
33	C	518	DGD	O6D-C1D-O3G	-3.35	101.96	109.99
29	A	613	LMG	O6-C1-O1	-3.33	101.99	109.99
25	B	613	CLA	CMB-C2B-C1B	-3.31	122.68	128.31
25	c	508	CLA	CMB-C2B-C1B	-3.30	122.69	128.31
33	c	519	DGD	O6D-C1D-O3G	-3.27	102.14	109.99
25	C	508	CLA	CMB-C2B-C1B	-3.27	122.75	128.31
25	A	609	CLA	CMB-C2B-C1B	-3.26	122.78	128.31
25	b	615	CLA	CMB-C2B-C1B	-3.25	122.78	128.31
25	c	510	CLA	CMB-C2B-C1B	-3.23	122.82	128.31
25	C	510	CLA	CMB-C2B-C1B	-3.21	122.86	128.31
25	B	611	CLA	CMB-C2B-C1B	-3.20	122.88	128.31
25	D	403	CLA	CMB-C2B-C1B	-3.20	122.88	128.31
25	B	607	CLA	CMB-C2B-C1B	-3.19	122.88	128.31
25	b	614	CLA	CMB-C2B-C1B	-3.19	122.89	128.31
25	C	504	CLA	CMB-C2B-C1B	-3.19	122.89	128.31
25	b	606	CLA	CMB-C2B-C1B	-3.19	122.89	128.31
29	A	613	LMG	O1-C7-C8	-3.17	103.45	110.99
28	d	408	PL9	C22-C23-C24	-3.16	120.78	127.75
25	c	506	CLA	CMB-C2B-C1B	-3.14	122.98	128.31
25	c	515	CLA	CMB-C2B-C1B	-3.13	122.98	128.31
33	H	103	DGD	O6D-C1D-O3G	-3.13	102.47	109.99
25	c	513	CLA	CMB-C2B-C1B	-3.13	122.98	128.31
27	T	101	BCR	C33-C5-C6	-3.12	121.30	124.62
25	c	511	CLA	CMB-C2B-C1B	-3.10	123.03	128.31
27	B	627	BCR	C33-C5-C6	-3.09	121.33	124.62
25	B	603	CLA	CMB-C2B-C1B	-3.08	123.07	128.31
25	b	611	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
25	B	614	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
25	B	606	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
25	b	616	CLA	CMB-C2B-C1B	-3.07	123.09	128.31
25	b	609	CLA	CMB-C2B-C1B	-3.07	123.09	128.31
25	a	607	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
25	b	607	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
25	c	503	CLA	CMB-C2B-C1B	-3.05	123.12	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	610	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
25	C	512	CLA	CMB-C2B-C1B	-3.03	123.15	128.31
25	B	608	CLA	CMB-C2B-C1B	-3.03	123.15	128.31
25	d	403	CLA	CMB-C2B-C1B	-3.03	123.17	128.31
25	c	505	CLA	CMB-C2B-C1B	-3.02	123.17	128.31
25	C	513	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
33	h	102	DGD	O6D-C1D-O3G	-3.01	102.77	109.99
25	c	509	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
25	b	617	CLA	CMB-C2B-C1B	-3.01	123.20	128.31
25	C	511	CLA	CMB-C2B-C1B	-3.00	123.20	128.31
25	C	501	CLA	CMB-C2B-C1B	-3.00	123.21	128.31
25	C	505	CLA	CMB-C2B-C1B	-2.99	123.23	128.31
25	C	507	CLA	CMB-C2B-C1B	-2.98	123.24	128.31
27	b	620	BCR	C33-C5-C6	-2.98	121.45	124.62
25	b	605	CLA	CMB-C2B-C1B	-2.97	123.25	128.31
25	A	607	CLA	CMB-C2B-C1B	-2.97	123.26	128.31
29	B	625	LMG	O1-C1-C2	-2.96	104.35	108.00
25	A	615	CLA	CMB-C2B-C1B	-2.96	123.28	128.31
25	B	605	CLA	CMB-C2B-C1B	-2.96	123.28	128.31
29	B	625	LMG	O6-C1-O1	-2.96	102.90	109.99
25	b	613	CLA	CMB-C2B-C1B	-2.95	123.29	128.31
27	B	617	BCR	C33-C5-C6	-2.95	121.47	124.62
25	a	609	CLA	CMB-C2B-C1B	-2.95	123.29	128.31
25	C	503	CLA	CMB-C2B-C1B	-2.94	123.30	128.31
27	C	514	BCR	C33-C5-C6	-2.94	121.48	124.62
25	b	608	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
25	C	506	CLA	CMB-C2B-C1B	-2.94	123.32	128.31
25	B	610	CLA	CMB-C2B-C1B	-2.93	123.32	128.31
28	A	611	PL9	C22-C23-C24	-2.93	121.30	127.75
29	b	624	LMG	O6-C1-O1	-2.92	102.98	109.99
25	B	604	CLA	CMB-C2B-C1B	-2.92	123.34	128.31
25	B	601	CLA	CMB-C2B-C1B	-2.92	123.35	128.31
25	D	402	CLA	CMB-C2B-C1B	-2.91	123.37	128.31
25	C	502	CLA	CMB-C2B-C1B	-2.91	123.37	128.31
29	B	621	LMG	O1-C7-C8	-2.90	104.09	110.99
25	c	507	CLA	CMB-C2B-C1B	-2.89	123.39	128.31
25	B	602	CLA	CMB-C2B-C1B	-2.88	123.41	128.31
27	h	101	BCR	C24-C23-C22	-2.86	121.89	126.21
25	a	612	CLA	CMB-C2B-C1B	-2.86	123.45	128.31
25	b	607	CLA	O2D-CGD-O1D	-2.85	117.77	123.77
25	B	615	CLA	CMB-C2B-C1B	-2.85	123.47	128.31
25	b	604	CLA	CMB-C2B-C1B	-2.84	123.47	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	CLA	CMB-C2B-C1B	-2.82	123.51	128.31
27	D	404	BCR	C33-C5-C6	-2.82	121.61	124.62
25	B	609	CLA	CMB-C2B-C1B	-2.81	123.53	128.31
25	b	612	CLA	CMB-C2B-C1B	-2.81	123.54	128.31
27	B	627	BCR	C15-C14-C13	-2.81	123.14	127.22
27	B	619	BCR	C33-C5-C6	-2.80	121.64	124.62
28	a	611	PL9	C22-C23-C24	-2.80	121.57	127.75
28	a	611	PL9	C7-C3-C2	-2.80	118.59	122.66
25	b	617	CLA	O2D-CGD-O1D	-2.80	117.89	123.77
29	b	623	LMG	O6-C1-O1	-2.79	103.30	109.99
25	c	504	CLA	CMB-C2B-C1B	-2.79	123.57	128.31
27	y	101	BCR	C33-C5-C6	-2.78	121.66	124.62
28	A	611	PL9	C27-C28-C29	-2.78	121.62	127.75
25	b	609	CLA	O2D-CGD-O1D	-2.78	117.93	123.77
33	C	517	DGD	O5D-C6D-C5D	-2.77	104.21	109.14
25	B	606	CLA	O2D-CGD-O1D	-2.77	117.94	123.77
28	D	407	PL9	C22-C23-C24	-2.76	121.66	127.75
28	D	407	PL9	C7-C3-C2	-2.76	118.64	122.66
28	A	611	PL9	C7-C3-C2	-2.76	118.65	122.66
27	c	516	BCR	C15-C16-C17	-2.75	117.30	123.23
33	h	102	DGD	CDB-CCB-CBB	-2.75	100.25	114.54
25	c	510	CLA	O2D-CGD-O1D	-2.75	117.98	123.77
33	C	518	DGD	C3G-C2G-C1G	-2.75	105.68	112.08
28	d	408	PL9	C31-C32-C33	-2.74	104.41	111.61
25	b	604	CLA	O2D-CGD-O1D	-2.74	118.01	123.77
33	C	518	DGD	CDB-CCB-CBB	-2.73	100.34	114.54
28	d	408	PL9	C27-C28-C29	-2.73	121.72	127.75
25	d	404	CLA	O2D-CGD-O1D	-2.73	118.02	123.77
33	c	518	DGD	CDB-CCB-CBB	-2.73	100.36	114.54
25	B	601	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
33	c	519	DGD	O5D-C6D-C5D	-2.72	104.30	109.14
27	K	101	BCR	C24-C23-C22	-2.72	122.10	126.21
25	c	509	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
29	B	625	LMG	O2-C2-C1	-2.71	103.99	110.01
25	B	603	CLA	O2D-CGD-O1D	-2.71	118.07	123.77
33	c	519	DGD	CDB-CCB-CBB	-2.71	100.48	114.54
25	b	619	CLA	O2D-CGD-O1D	-2.70	118.08	123.77
27	T	101	BCR	C15-C14-C13	-2.70	123.29	127.22
28	a	611	PL9	C27-C28-C29	-2.70	121.80	127.75
28	d	408	PL9	C7-C3-C2	-2.70	118.74	122.66
25	B	604	CLA	O2D-CGD-O1D	-2.70	118.10	123.77
29	B	625	LMG	O1-C7-C8	-2.70	104.58	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	516	DGD	O5D-C6D-C5D	-2.69	104.35	109.14
25	C	507	CLA	O2D-CGD-O1D	-2.69	118.11	123.77
33	H	103	DGD	CDB-CCB-CBB	-2.69	100.57	114.54
25	b	606	CLA	O2D-CGD-O1D	-2.69	118.11	123.77
25	B	614	CLA	O2D-CGD-O1D	-2.69	118.11	123.77
33	c	520	DGD	O5D-C6D-C5D	-2.69	104.36	109.14
29	C	519	LMG	O6-C1-O1	-2.69	103.55	109.99
33	c	520	DGD	CDB-CCB-CBB	-2.69	100.59	114.54
25	C	505	CLA	O2D-CGD-O1D	-2.68	118.13	123.77
28	A	611	PL9	C7-C8-C9	-2.68	122.15	126.70
25	b	618	CLA	O2D-CGD-O1D	-2.67	118.14	123.77
27	C	515	BCR	C33-C5-C6	-2.67	121.77	124.62
25	c	506	CLA	O2D-CGD-O1D	-2.67	118.14	123.77
25	C	508	CLA	O2D-CGD-O1D	-2.67	118.14	123.77
25	C	504	CLA	O2D-CGD-O1D	-2.67	118.15	123.77
25	c	503	CLA	O2D-CGD-O1D	-2.67	118.16	123.77
28	D	407	PL9	C27-C28-C29	-2.66	121.87	127.75
25	c	505	CLA	O2D-CGD-O1D	-2.66	118.17	123.77
27	c	517	BCR	C33-C5-C6	-2.66	121.79	124.62
27	C	515	BCR	C15-C16-C17	-2.66	117.50	123.23
25	B	602	CLA	O2D-CGD-O1D	-2.66	118.18	123.77
27	c	516	BCR	C15-C14-C13	-2.65	123.37	127.22
25	b	605	CLA	O2D-CGD-O1D	-2.65	118.19	123.77
25	B	613	CLA	O2D-CGD-O1D	-2.65	118.20	123.77
27	B	618	BCR	C33-C5-C6	-2.64	121.81	124.62
25	B	610	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
25	c	507	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
27	B	619	BCR	C24-C23-C22	-2.63	122.23	126.21
25	B	615	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
27	a	610	BCR	C33-C5-C6	-2.63	121.82	124.62
25	b	610	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
26	D	401	PHO	CBD-CHA-C4D	-2.63	105.58	108.54
25	a	612	CLA	O2D-CGD-O1D	-2.63	118.24	123.77
27	k	101	BCR	C33-C5-C6	-2.62	121.83	124.62
25	b	615	CLA	O2D-CGD-O1D	-2.62	118.26	123.77
25	A	607	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
25	B	616	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
27	b	621	BCR	C33-C5-C6	-2.61	121.84	124.62
25	c	515	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
33	C	517	DGD	CDB-CCB-CBB	-2.61	100.99	114.54
25	b	614	CLA	O2D-CGD-O1D	-2.61	118.28	123.77
25	B	612	CLA	O2D-CGD-O1D	-2.61	118.28	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	401	PHO	CBD-CHA-C4D	-2.60	105.61	108.54
25	A	609	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
25	b	616	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
25	C	502	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
27	Y	101	BCR	C33-C5-C6	-2.60	121.85	124.62
25	C	501	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
33	C	516	DGD	C3G-C2G-C1G	-2.60	106.03	112.08
29	B	625	LMG	O3-C3-C2	-2.60	104.50	110.36
33	c	518	DGD	O5D-C6D-C5D	-2.60	104.52	109.14
25	c	504	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
28	d	408	PL9	C36-C34-C33	-2.59	116.15	120.98
27	B	617	BCR	C15-C16-C17	-2.59	117.64	123.23
25	C	506	CLA	O2D-CGD-O1D	-2.59	118.32	123.77
27	C	514	BCR	C15-C14-C13	-2.59	123.46	127.22
25	C	510	CLA	O2D-CGD-O1D	-2.59	118.32	123.77
25	c	508	CLA	O2D-CGD-O1D	-2.59	118.32	123.77
27	C	514	BCR	C15-C16-C17	-2.58	117.66	123.23
25	a	609	CLA	O2D-CGD-O1D	-2.58	118.34	123.77
26	A	608	PHO	CBD-CHA-C4D	-2.58	105.63	108.54
27	A	610	BCR	C33-C5-C6	-2.58	121.87	124.62
26	D	401	PHO	O2D-CGD-O1D	-2.58	118.34	123.77
25	B	607	CLA	O2D-CGD-O1D	-2.58	118.34	123.77
26	a	608	PHO	CBD-CHA-C4D	-2.58	105.64	108.54
25	c	512	CLA	O2D-CGD-O1D	-2.57	118.35	123.77
25	C	509	CLA	O2D-CGD-O1D	-2.57	118.35	123.77
29	B	620	LMG	O6-C1-O1	-2.57	103.81	109.99
25	C	512	CLA	O2D-CGD-O1D	-2.56	118.37	123.77
25	B	611	CLA	O2D-CGD-O1D	-2.56	118.37	123.77
29	A	612	LMG	O6-C1-O1	-2.56	103.84	109.99
33	C	516	DGD	CDB-CCB-CBB	-2.56	101.23	114.54
25	a	607	CLA	O2D-CGD-O1D	-2.56	118.38	123.77
25	C	513	CLA	O2D-CGD-O1D	-2.56	118.38	123.77
25	c	514	CLA	O2D-CGD-O1D	-2.56	118.39	123.77
27	B	617	BCR	C24-C23-C22	-2.56	122.35	126.21
27	B	627	BCR	C24-C23-C22	-2.56	122.35	126.21
26	A	608	PHO	O2D-CGD-O1D	-2.55	118.39	123.77
29	A	613	LMG	C40-C39-C38	-2.55	101.27	114.54
27	c	517	BCR	C15-C16-C17	-2.55	117.72	123.23
25	D	403	CLA	O2D-CGD-O1D	-2.55	118.39	123.77
25	b	612	CLA	O2D-CGD-O1D	-2.55	118.40	123.77
26	d	401	PHO	O2D-CGD-O1D	-2.55	118.40	123.77
29	c	521	LMG	O6-C1-O1	-2.55	103.87	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	406	LMG	O6-C1-O1	-2.55	103.87	109.99
33	c	520	DGD	C3G-C2G-C1G	-2.55	106.14	112.08
33	h	102	DGD	C3G-C2G-C1G	-2.55	106.15	112.08
25	A	615	CLA	O2D-CGD-O1D	-2.55	118.41	123.77
33	C	518	DGD	O5D-C6D-C5D	-2.55	104.61	109.14
33	c	518	DGD	C3G-C2G-C1G	-2.54	106.15	112.08
27	C	515	BCR	C15-C14-C13	-2.54	123.53	127.22
31	A	616	LHG	C11-C10-C9	-2.54	101.34	114.54
25	b	611	CLA	O2D-CGD-O1D	-2.54	118.42	123.77
25	c	513	CLA	O2D-CGD-O1D	-2.54	118.42	123.77
25	B	609	CLA	O2D-CGD-O1D	-2.54	118.43	123.77
28	A	611	PL9	C37-C38-C39	-2.54	122.16	127.75
27	K	101	BCR	C15-C16-C17	-2.53	117.77	123.23
27	d	405	BCR	C33-C5-C6	-2.52	121.93	124.62
25	c	511	CLA	O2D-CGD-O1D	-2.52	118.46	123.77
29	A	613	LMG	C3-C4-C5	-2.52	105.73	110.23
31	a	613	LHG	C11-C10-C9	-2.52	101.48	114.54
27	B	627	BCR	C15-C16-C17	-2.51	117.81	123.23
27	b	620	BCR	C15-C16-C17	-2.50	117.84	123.23
27	T	101	BCR	C24-C23-C22	-2.50	122.43	126.21
25	C	503	CLA	O2D-CGD-O1D	-2.50	118.51	123.77
25	C	511	CLA	O2D-CGD-O1D	-2.49	118.52	123.77
27	c	517	BCR	C15-C14-C13	-2.49	123.60	127.22
33	H	103	DGD	C3G-C2G-C1G	-2.49	106.29	112.08
25	b	613	CLA	O2D-CGD-O1D	-2.48	118.54	123.77
31	a	613	LHG	C20-C19-C18	-2.48	101.67	114.54
29	B	625	LMG	C40-C39-C38	-2.48	101.68	114.54
25	A	606	CLA	O2D-CGD-O1D	-2.48	118.56	123.77
27	k	101	BCR	C24-C23-C22	-2.48	122.47	126.21
29	B	620	LMG	C40-C39-C38	-2.47	101.69	114.54
31	l	101	LHG	C11-C10-C9	-2.47	101.73	114.54
25	d	403	CLA	O2D-CGD-O1D	-2.47	118.58	123.77
31	a	615	LHG	C11-C10-C9	-2.46	101.74	114.54
27	b	620	BCR	C15-C14-C13	-2.46	123.64	127.22
28	a	611	PL9	C37-C38-C39	-2.46	122.33	127.75
33	c	519	DGD	C3G-C2G-C1G	-2.46	106.35	112.08
25	a	606	CLA	O2D-CGD-O1D	-2.46	118.60	123.77
29	c	502	LMG	O6-C1-O1	-2.45	104.11	109.99
25	b	608	CLA	O2D-CGD-O1D	-2.45	118.61	123.77
27	K	101	BCR	C33-C5-C6	-2.45	122.01	124.62
28	d	408	PL9	C7-C8-C9	-2.45	122.54	126.70
25	D	402	CLA	O2D-CGD-O1D	-2.44	118.62	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	617	BCR	C15-C14-C13	-2.44	123.67	127.22
34	v	201	HEM	CBD-CAD-C3D	-2.44	108.19	112.47
25	B	608	CLA	O2D-CGD-O1D	-2.44	118.64	123.77
26	a	608	PHO	O2D-CGD-O1D	-2.44	118.64	123.77
29	b	623	LMG	O1-C7-C8	-2.43	105.20	110.99
27	b	622	BCR	C33-C5-C6	-2.43	122.03	124.62
31	D	406	LHG	C20-C19-C18	-2.43	101.92	114.54
31	L	101	LHG	C11-C10-C9	-2.43	101.93	114.54
25	B	605	CLA	O2D-CGD-O1D	-2.42	118.68	123.77
27	B	617	BCR	C11-C10-C9	-2.42	123.70	127.22
29	b	623	LMG	O1-C1-C2	-2.42	105.03	108.00
26	d	401	PHO	CMB-C2B-C1B	-2.41	121.20	125.06
28	D	407	PL9	C37-C38-C39	-2.41	122.43	127.75
29	D	405	LMG	C40-C39-C38	-2.41	102.02	114.54
29	c	521	LMG	C40-C39-C38	-2.41	102.03	114.54
29	b	623	LMG	C40-C39-C38	-2.41	102.04	114.54
28	A	611	PL9	C31-C32-C33	-2.40	105.30	111.61
29	b	624	LMG	C38-C37-C36	-2.40	102.09	114.54
29	b	623	LMG	C38-C37-C36	-2.40	102.09	114.54
31	A	617	LHG	C11-C10-C9	-2.40	102.10	114.54
29	c	521	LMG	C38-C37-C36	-2.39	102.12	114.54
29	B	620	LMG	C38-C37-C36	-2.39	102.13	114.54
31	d	407	LHG	C20-C19-C18	-2.39	102.13	114.54
31	a	615	LHG	C20-C19-C18	-2.39	102.15	114.54
29	C	520	LMG	C40-C39-C38	-2.38	102.17	114.54
29	C	519	LMG	C38-C37-C36	-2.38	102.17	114.54
29	D	405	LMG	O6-C1-O1	-2.38	104.28	109.99
29	A	612	LMG	C40-C39-C38	-2.38	102.19	114.54
28	D	407	PL9	C7-C8-C9	-2.37	122.67	126.70
31	d	407	LHG	C11-C10-C9	-2.37	102.24	114.54
29	c	502	LMG	C40-C39-C38	-2.37	102.24	114.54
29	C	519	LMG	C40-C39-C38	-2.36	102.26	114.54
28	a	611	PL9	C7-C8-C9	-2.36	122.68	126.70
27	K	101	BCR	C15-C14-C13	-2.36	123.79	127.22
27	C	514	BCR	C11-C10-C9	-2.36	123.79	127.22
31	l	101	LHG	C20-C19-C18	-2.35	102.31	114.54
29	b	623	LMG	O2-C2-C1	-2.35	104.79	110.01
29	b	624	LMG	O1-C1-C2	-2.35	105.11	108.00
29	B	625	LMG	C38-C37-C36	-2.35	102.34	114.54
29	c	502	LMG	C38-C37-C36	-2.35	102.34	114.54
29	B	621	LMG	O3-C3-C2	-2.35	105.06	110.36
29	c	522	LMG	C40-C39-C38	-2.35	102.35	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	408	PL9	C42-C43-C44	-2.35	122.57	127.75
29	A	612	LMG	C38-C37-C36	-2.35	102.36	114.54
28	A	611	PL9	C36-C34-C33	-2.35	116.61	120.98
31	L	101	LHG	C20-C19-C18	-2.34	102.38	114.54
29	B	621	LMG	C40-C39-C38	-2.34	102.40	114.54
29	c	502	LMG	C1-C2-C3	-2.34	105.35	109.98
29	c	521	LMG	O2-C2-C1	-2.33	104.83	110.01
27	y	101	BCR	C24-C23-C22	-2.33	122.68	126.21
31	A	617	LHG	C20-C19-C18	-2.33	102.42	114.54
27	B	618	BCR	C15-C14-C13	-2.33	123.83	127.22
27	h	101	BCR	C33-C5-C6	-2.33	122.14	124.62
29	d	406	LMG	C40-C39-C38	-2.33	102.44	114.54
31	A	616	LHG	C20-C19-C18	-2.33	102.45	114.54
29	b	624	LMG	C40-C39-C38	-2.33	102.46	114.54
31	A	618	LHG	C11-C10-C9	-2.32	102.47	114.54
29	B	625	LMG	C1-O6-C5	-2.32	109.19	113.74
27	B	619	BCR	C15-C16-C17	-2.32	118.23	123.23
29	C	520	LMG	C38-C37-C36	-2.32	102.51	114.54
29	A	613	LMG	O3-C3-C2	-2.31	105.14	110.36
27	A	610	BCR	C15-C14-C13	-2.31	123.86	127.22
27	c	516	BCR	C3-C4-C5	-2.31	110.03	113.87
31	a	613	LHG	C18-C17-C16	-2.31	102.56	114.54
27	T	101	BCR	C15-C16-C17	-2.30	118.27	123.23
29	c	502	LMG	O3-C3-C2	-2.30	105.17	110.36
33	C	517	DGD	C1D-C2D-C3D	-2.30	105.42	109.98
29	C	520	LMG	O3-C3-C2	-2.30	105.17	110.36
26	D	401	PHO	CMB-C2B-C1B	-2.30	121.39	125.06
31	D	406	LHG	C11-C10-C9	-2.30	102.61	114.54
29	c	502	LMG	O2-C2-C1	-2.30	104.91	110.01
27	B	619	BCR	C38-C26-C25	-2.30	122.18	124.62
27	b	620	BCR	C24-C23-C22	-2.29	122.74	126.21
29	c	522	LMG	C38-C37-C36	-2.29	102.63	114.54
27	a	610	BCR	C15-C14-C13	-2.29	123.89	127.22
29	B	620	LMG	O3-C3-C2	-2.29	105.20	110.36
28	D	407	PL9	C32-C33-C34	-2.28	122.72	127.75
29	C	519	LMG	O2-C2-C1	-2.28	104.95	110.01
29	b	624	LMG	O3-C3-C2	-2.27	105.23	110.36
29	c	522	LMG	O3-C3-C2	-2.27	105.23	110.36
29	d	409	LMG	C40-C39-C38	-2.27	102.75	114.54
28	a	611	PL9	C31-C32-C33	-2.27	105.66	111.61
28	D	407	PL9	C31-C32-C33	-2.27	105.66	111.61
31	A	618	LHG	C20-C19-C18	-2.27	102.77	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	515	BCR	C11-C10-C9	-2.27	123.93	127.22
27	H	102	BCR	C24-C23-C22	-2.26	122.79	126.21
27	H	102	BCR	C15-C14-C13	-2.26	123.93	127.22
29	b	623	LMG	O3-C3-C2	-2.26	105.26	110.36
27	A	610	BCR	C15-C16-C17	-2.26	118.36	123.23
29	B	620	LMG	O2-C2-C1	-2.26	105.00	110.01
29	A	612	LMG	O3-C3-C2	-2.26	105.27	110.36
29	d	406	LMG	C38-C37-C36	-2.25	102.83	114.54
27	h	101	BCR	C15-C14-C13	-2.25	123.95	127.22
29	D	405	LMG	C38-C37-C36	-2.25	102.85	114.54
29	d	406	LMG	O1-C7-C8	-2.25	105.64	110.99
27	B	618	BCR	C15-C16-C17	-2.25	118.38	123.23
29	A	613	LMG	O2-C2-C1	-2.25	105.02	110.01
27	c	516	BCR	C11-C10-C9	-2.25	123.95	127.22
33	c	519	DGD	CBB-CAB-C9B	-2.24	102.92	114.54
27	h	101	BCR	C11-C10-C9	-2.24	123.97	127.22
29	D	405	LMG	O2-C2-C1	-2.23	105.06	110.01
27	A	610	BCR	C24-C23-C22	-2.23	122.84	126.21
29	C	519	LMG	O3-C3-C2	-2.23	105.34	110.36
29	c	521	LMG	O3-C3-C2	-2.22	105.34	110.36
27	C	514	BCR	C24-C23-C22	-2.22	122.85	126.21
29	B	621	LMG	C3-C4-C5	-2.22	106.26	110.23
31	A	617	LHG	C27-C26-C25	-2.22	103.00	114.54
27	b	622	BCR	C38-C26-C25	-2.22	122.25	124.62
29	d	409	LMG	C38-C37-C36	-2.22	103.01	114.54
28	A	611	PL9	C32-C33-C34	-2.21	122.87	127.75
29	d	406	LMG	O2-C2-C1	-2.21	105.10	110.01
29	B	621	LMG	C38-C37-C36	-2.21	103.07	114.54
27	H	102	BCR	C11-C10-C9	-2.21	124.01	127.22
29	b	624	LMG	O1-C7-C8	-2.20	105.74	110.99
29	C	520	LMG	O2-C2-C3	-2.20	105.39	110.36
27	D	404	BCR	C24-C23-C22	-2.20	122.88	126.21
27	H	102	BCR	C33-C5-C6	-2.20	122.28	124.62
34	E	101	HEM	CBA-CAA-C2A	-2.20	108.63	112.49
27	D	404	BCR	C11-C10-C9	-2.20	124.03	127.22
29	c	522	LMG	C3-C4-C5	-2.19	106.31	110.23
33	c	520	DGD	O2D-C2D-C1D	-2.19	105.15	110.01
28	D	407	PL9	C46-C47-C48	-2.19	105.86	111.61
29	B	621	LMG	O1-C1-C2	-2.19	105.31	108.00
27	a	610	BCR	C24-C23-C22	-2.19	122.90	126.21
27	a	610	BCR	C15-C16-C17	-2.19	118.52	123.23
29	D	405	LMG	C1-C2-C3	-2.18	105.65	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	408	PL9	C46-C47-C48	-2.18	105.89	111.61
31	d	407	LHG	C27-C26-C25	-2.18	103.22	114.54
31	a	614	LHG	C27-C26-C25	-2.18	103.24	114.54
31	l	101	LHG	C18-C17-C16	-2.17	103.25	114.54
28	a	611	PL9	C36-C34-C33	-2.17	116.93	120.98
31	A	616	LHG	C27-C26-C25	-2.17	103.25	114.54
33	C	516	DGD	CAB-C9B-C8B	-2.17	103.26	114.54
28	a	611	PL9	C32-C33-C34	-2.17	122.96	127.75
31	a	613	LHG	C27-C26-C25	-2.16	103.30	114.54
33	c	518	DGD	O2D-C2D-C1D	-2.16	105.21	110.01
27	K	101	BCR	C38-C26-C25	-2.16	122.32	124.62
33	h	102	DGD	C1D-C2D-C3D	-2.16	105.70	109.98
31	a	615	LHG	C18-C17-C16	-2.16	103.34	114.54
29	A	613	LMG	C38-C37-C36	-2.16	103.34	114.54
26	a	608	PHO	CMB-C2B-C1B	-2.16	121.62	125.06
34	E	101	HEM	CMD-C2D-C1D	-2.15	124.65	128.31
33	C	517	DGD	C3G-C2G-C1G	-2.15	107.06	112.08
33	c	518	DGD	O3G-C1D-C2D	-2.15	105.35	108.00
28	A	611	PL9	C12-C13-C14	-2.15	123.00	127.75
33	c	518	DGD	CBB-CAB-C9B	-2.15	103.36	114.54
28	D	407	PL9	C42-C43-C44	-2.15	123.00	127.75
29	d	406	LMG	O3-C3-C2	-2.15	105.51	110.36
29	c	521	LMG	O1-C7-C8	-2.15	105.87	110.99
28	a	611	PL9	O2-C1-C2	-2.15	116.93	121.78
31	d	407	LHG	C18-C17-C16	-2.15	103.38	114.54
33	H	103	DGD	O2D-C2D-C1D	-2.15	105.25	110.01
29	B	620	LMG	O1-C7-C8	-2.15	105.88	110.99
33	C	518	DGD	CAB-C9B-C8B	-2.15	103.40	114.54
28	D	407	PL9	C36-C37-C38	-2.14	105.98	111.61
28	D	407	PL9	O2-C1-C2	-2.14	116.95	121.78
31	A	618	LHG	C27-C26-C25	-2.14	103.41	114.54
31	A	618	LHG	C5-O7-C7	-2.14	112.62	117.91
31	L	101	LHG	C18-C17-C16	-2.14	103.44	114.54
29	C	519	LMG	O1-C7-C8	-2.13	105.92	110.99
28	a	611	PL9	C46-C47-C48	-2.13	106.02	111.61
28	A	611	PL9	O2-C1-C2	-2.13	116.98	121.78
27	B	617	BCR	C7-C8-C9	-2.13	122.99	126.21
27	b	622	BCR	C24-C23-C22	-2.13	122.99	126.21
27	K	101	BCR	C8-C7-C6	-2.13	121.07	127.24
33	H	103	DGD	CBB-CAB-C9B	-2.12	103.50	114.54
27	C	515	BCR	C24-C23-C22	-2.12	123.00	126.21
25	b	612	CLA	O2A-CGA-O1A	-2.12	117.94	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	519	DGD	O3E-C3E-C2E	-2.12	105.57	110.36
31	a	615	LHG	C27-C26-C25	-2.12	103.52	114.54
29	c	522	LMG	O2-C2-C3	-2.12	105.58	110.36
29	B	621	LMG	O2-C2-C1	-2.12	105.31	110.01
28	D	407	PL9	C36-C34-C33	-2.12	117.04	120.98
29	D	405	LMG	O3-C3-C2	-2.11	105.59	110.36
31	D	406	LHG	C18-C17-C16	-2.11	103.57	114.54
33	c	520	DGD	CBB-CAB-C9B	-2.11	103.59	114.54
33	C	516	DGD	O2D-C2D-C1D	-2.11	105.33	110.01
28	D	407	PL9	C12-C13-C14	-2.11	123.10	127.75
28	d	408	PL9	C11-C12-C13	-2.11	106.08	111.61
25	B	609	CLA	O2A-CGA-O1A	-2.11	117.99	123.51
33	C	517	DGD	O3E-C3E-C2E	-2.10	105.62	110.36
31	A	616	LHG	C18-C17-C16	-2.10	103.63	114.54
33	c	520	DGD	C3D-C4D-C5D	-2.10	106.48	110.23
33	h	102	DGD	CBB-CAB-C9B	-2.10	103.65	114.54
27	D	404	BCR	C7-C8-C9	-2.09	123.04	126.21
33	c	518	DGD	CAB-C9B-C8B	-2.09	103.67	114.54
27	C	514	BCR	C7-C8-C9	-2.09	123.05	126.21
25	c	507	CLA	C4B-CHC-C1C	-2.09	125.19	129.34
27	B	619	BCR	C15-C14-C13	-2.09	124.18	127.22
26	A	608	PHO	C2B-C1B-NB	-2.09	106.70	109.81
28	d	408	PL9	O2-C1-C2	-2.09	117.07	121.78
28	A	611	PL9	C42-C43-C44	-2.09	123.14	127.75
25	c	508	CLA	O2A-CGA-O1A	-2.09	118.04	123.51
29	A	612	LMG	O2-C2-C1	-2.09	105.38	110.01
27	b	621	BCR	C15-C16-C17	-2.08	118.74	123.23
33	c	520	DGD	CAB-C9B-C8B	-2.08	103.72	114.54
31	l	101	LHG	C27-C26-C25	-2.08	103.72	114.54
29	b	624	LMG	O2-C2-C1	-2.08	105.39	110.01
25	c	515	CLA	O2A-CGA-O1A	-2.08	118.06	123.51
31	A	617	LHG	C18-C17-C16	-2.08	103.74	114.54
27	H	102	BCR	C38-C26-C25	-2.08	122.41	124.62
31	D	406	LHG	C27-C26-C25	-2.08	103.75	114.54
29	d	406	LMG	C1-C2-C3	-2.08	105.86	109.98
31	L	101	LHG	C27-C26-C25	-2.08	103.76	114.54
27	B	627	BCR	C35-C13-C14	-2.07	119.87	122.89
27	d	405	BCR	C11-C10-C9	-2.07	124.21	127.22
31	A	618	LHG	C18-C17-C16	-2.07	103.80	114.54
25	C	512	CLA	C4B-CHC-C1C	-2.07	125.23	129.34
29	d	406	LMG	O1-C1-C2	-2.07	105.46	108.00
25	B	603	CLA	O2A-CGA-O1A	-2.06	118.11	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	513	CLA	O2A-CGA-O1A	-2.06	118.11	123.51
27	Y	101	BCR	C8-C7-C6	-2.06	121.26	127.24
33	C	518	DGD	C5B-C4B-C3B	-2.06	103.86	114.54
33	C	517	DGD	CBB-CAB-C9B	-2.06	103.86	114.54
29	C	520	LMG	C3-C4-C5	-2.05	106.57	110.23
27	B	618	BCR	C11-C10-C9	-2.05	124.24	127.22
33	c	519	DGD	O2D-C2D-C1D	-2.05	105.47	110.01
34	V	201	HEM	CMD-C2D-C1D	-2.05	124.83	128.31
33	C	518	DGD	CBB-CAB-C9B	-2.05	103.92	114.54
33	h	102	DGD	C5B-C4B-C3B	-2.05	103.92	114.54
25	a	607	CLA	O2A-CGA-O1A	-2.05	118.15	123.51
25	c	511	CLA	O2A-CGA-O1A	-2.05	118.15	123.51
25	c	510	CLA	O2A-CGA-O1A	-2.04	118.15	123.51
28	A	611	PL9	C46-C47-C48	-2.04	106.25	111.61
25	d	403	CLA	C4B-CHC-C1C	-2.04	125.29	129.34
28	a	611	PL9	C12-C13-C14	-2.04	123.25	127.75
25	B	604	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
33	c	520	DGD	C5B-C4B-C3B	-2.04	103.96	114.54
26	a	608	PHO	C2B-C1B-NB	-2.04	106.78	109.81
27	D	404	BCR	C15-C14-C13	-2.04	124.26	127.22
29	c	522	LMG	O2-C2-C1	-2.04	105.49	110.01
25	a	609	CLA	O2A-CGA-O1A	-2.03	118.19	123.51
27	C	515	BCR	C7-C8-C9	-2.03	123.15	126.21
25	b	614	CLA	O2A-CGA-O1A	-2.03	118.20	123.51
33	c	518	DGD	C5B-C4B-C3B	-2.03	104.02	114.54
27	T	101	BCR	C11-C10-C9	-2.03	124.28	127.22
25	C	506	CLA	C4B-CHC-C1C	-2.03	125.32	129.34
27	B	627	BCR	C11-C10-C9	-2.03	124.28	127.22
27	B	618	BCR	C38-C26-C25	-2.02	122.47	124.62
33	c	519	DGD	C1D-C2D-C3D	-2.02	105.97	109.98
33	H	103	DGD	CAB-C9B-C8B	-2.02	104.05	114.54
34	V	201	HEM	CBA-CAA-C2A	-2.01	108.95	112.49
27	y	101	BCR	C15-C16-C17	-2.01	118.89	123.23
25	C	505	CLA	C4B-CHC-C1C	-2.01	125.34	129.34
26	d	401	PHO	C2B-C1B-NB	-2.01	106.81	109.81
33	C	518	DGD	O2D-C2D-C1D	-2.01	105.55	110.01
29	d	409	LMG	O1-C7-C8	-2.01	105.88	111.65
29	B	620	LMG	C1-C2-C3	-2.01	106.00	109.98
33	h	102	DGD	CAB-C9B-C8B	-2.01	104.11	114.54
25	B	611	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
25	b	611	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
27	B	619	BCR	C8-C7-C6	-2.01	121.42	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	405	LMG	O1-C7-C8	-2.00	106.22	110.99
27	c	517	BCR	C24-C23-C22	-2.00	123.18	126.21
33	c	519	DGD	CAB-C9B-C8B	-2.00	104.13	114.54
25	b	618	CLA	O2A-CGA-O1A	-2.00	118.26	123.51
33	H	103	DGD	O3E-C3E-C2E	-2.00	105.84	110.36
25	B	608	CLA	O2A-CGA-O1A	-2.00	118.26	123.51
33	H	103	DGD	C3D-C4D-C5D	-2.00	106.66	110.23
33	c	520	DGD	O3E-C3E-C2E	-2.00	105.84	110.36
29	A	612	LMG	C1-C2-C3	-2.00	106.01	109.98
27	c	517	BCR	C11-C10-C9	-2.00	124.31	127.22
25	b	607	CLA	O2A-CGA-O1A	-2.00	118.26	123.51
25	b	617	CLA	O1D-CGD-CBD	2.00	127.75	124.64
25	c	515	CLA	C4A-NA-C1A	2.00	108.92	106.38
25	C	507	CLA	O1D-CGD-CBD	2.00	127.75	124.64
25	b	611	CLA	O1D-CGD-CBD	2.00	127.75	124.64
25	B	606	CLA	O1D-CGD-CBD	2.01	127.76	124.64
25	b	608	CLA	O1D-CGD-CBD	2.01	127.76	124.64
25	C	510	CLA	CMD-C2D-C3D	2.01	129.02	125.09
25	c	508	CLA	C4A-NA-C1A	2.01	108.93	106.38
25	c	503	CLA	O1D-CGD-CBD	2.01	127.77	124.64
25	A	606	CLA	CMD-C2D-C3D	2.01	129.03	125.09
25	c	509	CLA	C2A-C1A-CHA	2.01	127.04	123.80
27	D	404	BCR	C4-C5-C6	2.01	124.95	122.73
25	C	503	CLA	O1D-CGD-CBD	2.01	127.77	124.64
23	D	409	SQD	C4-C3-C2	2.02	114.50	110.79
34	V	201	HEM	CMB-C2B-C3B	2.02	129.05	125.09
34	e	101	HEM	CMC-C2C-C3C	2.02	129.05	125.09
25	B	604	CLA	CMD-C2D-C3D	2.03	129.05	125.09
25	C	507	CLA	O2D-CGD-CBD	2.03	114.14	111.22
25	B	602	CLA	O2D-CGD-CBD	2.03	114.14	111.22
25	B	605	CLA	CMD-C2D-C3D	2.03	129.06	125.09
25	c	505	CLA	CMD-C2D-C3D	2.03	129.06	125.09
25	D	403	CLA	O1D-CGD-CBD	2.03	127.80	124.64
23	D	408	SQD	O6-C1-C2	2.03	110.50	108.00
25	b	607	CLA	CMD-C2D-C3D	2.04	129.07	125.09
25	D	402	CLA	O1D-CGD-CBD	2.04	127.81	124.64
25	C	509	CLA	CMD-C2D-C3D	2.04	129.08	125.09
25	C	503	CLA	CMD-C2D-C3D	2.04	129.08	125.09
25	C	513	CLA	O1D-CGD-CBD	2.04	127.81	124.64
25	c	513	CLA	O1D-CGD-CBD	2.04	127.82	124.64
25	a	612	CLA	C4A-NA-C1A	2.05	108.97	106.38
25	b	616	CLA	O2D-CGD-CBD	2.05	114.17	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	607	CLA	O2D-CGD-CBD	2.05	114.18	111.22
25	a	606	CLA	CMD-C2D-C3D	2.06	129.11	125.09
25	b	610	CLA	CMD-C2D-C3D	2.06	129.11	125.09
25	a	612	CLA	CMD-C2D-C3D	2.06	129.12	125.09
25	C	508	CLA	C4A-NA-C1A	2.06	109.00	106.38
25	C	506	CLA	O2D-CGD-CBD	2.06	114.20	111.22
34	E	101	HEM	CMC-C2C-C3C	2.07	129.13	125.09
27	T	101	BCR	C4-C5-C6	2.07	125.00	122.73
25	c	515	CLA	CMD-C2D-C3D	2.07	129.13	125.09
28	d	408	PL9	C35-C34-C36	2.07	118.52	115.37
25	b	605	CLA	O1D-CGD-CBD	2.07	127.85	124.64
25	B	614	CLA	C4A-NA-C1A	2.07	109.01	106.38
25	C	504	CLA	O2D-CGD-CBD	2.07	114.21	111.22
25	b	617	CLA	CMD-C2D-C3D	2.08	129.15	125.09
25	A	609	CLA	C4A-NA-C1A	2.08	109.01	106.38
25	C	504	CLA	C4A-NA-C1A	2.08	109.01	106.38
25	c	512	CLA	CMD-C2D-C3D	2.08	129.15	125.09
25	c	510	CLA	C4A-NA-C1A	2.08	109.02	106.38
25	B	606	CLA	CMD-C2D-C3D	2.08	129.16	125.09
25	c	504	CLA	O1D-CGD-CBD	2.08	127.88	124.64
25	d	403	CLA	O1D-CGD-CBD	2.08	127.88	124.64
25	C	512	CLA	O1D-CGD-CBD	2.08	127.88	124.64
25	d	404	CLA	CMD-C2D-C3D	2.08	129.16	125.09
25	B	607	CLA	CMD-C2D-C3D	2.09	129.17	125.09
23	f	101	SQD	C4-C3-C2	2.09	114.63	110.79
25	a	612	CLA	O2D-CGD-CBD	2.09	114.23	111.22
23	B	626	SQD	C4-C3-C2	2.09	114.63	110.79
25	C	501	CLA	CMD-C2D-C3D	2.09	129.18	125.09
25	c	506	CLA	C4A-NA-C1A	2.09	109.03	106.38
28	D	407	PL9	C35-C34-C36	2.09	118.56	115.37
25	c	514	CLA	O1D-CGD-CBD	2.09	127.89	124.64
25	C	513	CLA	CMD-C2D-C3D	2.09	129.18	125.09
25	B	611	CLA	O1D-CGD-CBD	2.09	127.89	124.64
27	B	627	BCR	C4-C5-C6	2.10	125.04	122.73
25	A	607	CLA	O2D-CGD-CBD	2.10	114.24	111.22
25	b	617	CLA	C4A-NA-C1A	2.10	109.04	106.38
25	b	609	CLA	C4A-NA-C1A	2.10	109.04	106.38
25	A	607	CLA	C4A-NA-C1A	2.10	109.04	106.38
25	b	604	CLA	CMD-C2D-C3D	2.10	129.19	125.09
25	c	507	CLA	CMD-C2D-C3D	2.10	129.20	125.09
23	b	601	SQD	O5-C5-C4	2.10	113.67	109.67
25	b	614	CLA	CMD-C2D-C3D	2.10	129.20	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	B	602	CLA	CMD-C2D-C3D	2.10	129.20	125.09
25	c	503	CLA	C4A-NA-C1A	2.11	109.05	106.38
25	b	609	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	c	506	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	b	608	CLA	C4A-NA-C1A	2.11	109.05	106.38
25	B	615	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	d	403	CLA	CMD-C2D-C3D	2.11	129.22	125.09
25	C	501	CLA	O1D-CGD-CBD	2.12	127.93	124.64
25	D	403	CLA	CMD-C2D-C3D	2.12	129.23	125.09
25	c	503	CLA	CMD-C2D-C3D	2.12	129.23	125.09
25	B	613	CLA	O1D-CGD-CBD	2.12	127.93	124.64
25	C	508	CLA	O2D-CGD-CBD	2.12	114.27	111.22
23	f	101	SQD	O48-C23-C24	2.12	118.37	111.85
25	d	404	CLA	C4A-NA-C1A	2.12	109.07	106.38
25	c	511	CLA	CMD-C2D-C3D	2.12	129.24	125.09
25	b	606	CLA	CMD-C2D-C3D	2.12	129.24	125.09
25	b	618	CLA	CMD-C2D-C3D	2.12	129.24	125.09
25	D	402	CLA	C4A-NA-C1A	2.12	109.07	106.38
25	B	603	CLA	CMD-C2D-C3D	2.13	129.25	125.09
25	c	515	CLA	O1D-CGD-CBD	2.13	127.94	124.64
25	b	614	CLA	O1D-CGD-CBD	2.13	127.95	124.64
25	D	403	CLA	C4A-NA-C1A	2.13	109.08	106.38
25	B	601	CLA	CMD-C2D-C3D	2.13	129.25	125.09
25	A	615	CLA	CMD-C2D-C3D	2.13	129.25	125.09
25	C	511	CLA	O1D-CGD-CBD	2.13	127.95	124.64
25	B	609	CLA	O1D-CGD-CBD	2.13	127.95	124.64
25	b	616	CLA	CMD-C2D-C3D	2.13	129.26	125.09
25	A	609	CLA	CMD-C2D-C3D	2.13	129.26	125.09
25	B	606	CLA	O2D-CGD-CBD	2.14	114.30	111.22
25	C	511	CLA	CMD-C2D-C3D	2.14	129.27	125.09
25	B	610	CLA	CMD-C2D-C3D	2.14	129.27	125.09
25	B	608	CLA	CMD-C2D-C3D	2.14	129.28	125.09
25	C	504	CLA	CMD-C2D-C3D	2.14	129.28	125.09
25	b	619	CLA	CMD-C2D-C3D	2.14	129.28	125.09
25	c	509	CLA	CMD-C2D-C3D	2.15	129.29	125.09
25	b	609	CLA	O1D-CGD-CBD	2.15	127.98	124.64
25	C	509	CLA	O1D-CGD-CBD	2.15	127.98	124.64
25	C	510	CLA	O1D-CGD-CBD	2.15	127.98	124.64
25	B	611	CLA	CMD-C2D-C3D	2.15	129.29	125.09
23	D	408	SQD	O48-C23-C24	2.15	118.48	111.85
25	B	611	CLA	C4A-NA-C1A	2.16	109.11	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	507	CLA	CMD-C2D-C3D	2.16	129.31	125.09
25	c	508	CLA	CMD-C2D-C3D	2.16	129.31	125.09
25	d	403	CLA	C4A-NA-C1A	2.16	109.11	106.38
25	d	404	CLA	O2D-CGD-CBD	2.16	114.33	111.22
25	b	613	CLA	CMD-C2D-C3D	2.16	129.32	125.09
25	b	614	CLA	C4A-NA-C1A	2.16	109.12	106.38
25	b	612	CLA	O1D-CGD-CBD	2.16	128.00	124.64
25	c	513	CLA	CMD-C2D-C3D	2.16	129.32	125.09
25	B	616	CLA	CMD-C2D-C3D	2.16	129.32	125.09
26	a	608	PHO	C1B-NB-C4B	2.17	110.62	106.50
25	a	609	CLA	CMD-C2D-C3D	2.17	129.33	125.09
25	b	610	CLA	O2D-CGD-CBD	2.17	114.34	111.22
25	B	613	CLA	CMD-C2D-C3D	2.17	129.33	125.09
28	d	408	PL9	C20-C19-C21	2.17	118.67	115.37
25	B	615	CLA	O2D-CGD-CBD	2.17	114.35	111.22
25	B	605	CLA	C4A-NA-C1A	2.17	109.13	106.38
25	C	506	CLA	CMD-C2D-C3D	2.17	129.33	125.09
25	c	505	CLA	O2D-CGD-CBD	2.17	114.35	111.22
25	C	505	CLA	CMD-C2D-C3D	2.17	129.34	125.09
25	c	512	CLA	C4A-NA-C1A	2.18	109.14	106.38
25	D	402	CLA	CMD-C2D-C3D	2.18	129.34	125.09
26	d	401	PHO	C1B-NB-C4B	2.18	110.64	106.50
25	B	614	CLA	CMD-C2D-C3D	2.18	129.35	125.09
25	b	617	CLA	O2D-CGD-CBD	2.18	114.36	111.22
23	f	101	SQD	C3-C4-C5	2.18	114.12	110.23
25	c	506	CLA	O2D-CGD-CBD	2.19	114.37	111.22
25	b	615	CLA	C4A-NA-C1A	2.19	109.15	106.38
25	b	612	CLA	CMD-C2D-C3D	2.19	129.37	125.09
23	D	409	SQD	C3-C4-C5	2.19	114.14	110.23
26	D	401	PHO	C1B-NB-C4B	2.20	110.67	106.50
25	b	611	CLA	CMD-C2D-C3D	2.20	129.38	125.09
25	c	514	CLA	CMD-C2D-C3D	2.20	129.38	125.09
25	B	616	CLA	O1D-CGD-CBD	2.20	128.06	124.64
25	C	501	CLA	C4A-NA-C1A	2.20	109.17	106.38
25	a	606	CLA	O1D-CGD-CBD	2.20	128.06	124.64
26	A	608	PHO	C1B-NB-C4B	2.20	110.69	106.50
25	A	609	CLA	O2D-CGD-CBD	2.20	114.40	111.22
25	c	512	CLA	O1D-CGD-CBD	2.21	128.07	124.64
27	K	101	BCR	C2-C1-C6	2.21	113.76	110.48
25	B	606	CLA	C4A-NA-C1A	2.21	109.18	106.38
25	B	609	CLA	CMD-C2D-C3D	2.21	129.41	125.09
25	B	610	CLA	O1D-CGD-CBD	2.21	128.08	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	507	CLA	C4A-NA-C1A	2.23	109.20	106.38
25	B	609	CLA	C4A-NA-C1A	2.23	109.20	106.38
25	B	612	CLA	CMD-C2D-C3D	2.23	129.45	125.09
25	B	608	CLA	O1D-CGD-CBD	2.23	128.11	124.64
25	C	506	CLA	C4A-NA-C1A	2.24	109.21	106.38
25	b	615	CLA	CMD-C2D-C3D	2.24	129.46	125.09
25	B	601	CLA	O2D-CGD-CBD	2.24	114.45	111.22
25	B	603	CLA	O2D-CGD-CBD	2.24	114.45	111.22
25	B	612	CLA	O1D-CGD-CBD	2.25	128.13	124.64
25	b	604	CLA	O2D-CGD-CBD	2.25	114.47	111.22
25	B	612	CLA	C4A-NA-C1A	2.25	109.23	106.38
25	C	505	CLA	C4A-NA-C1A	2.26	109.24	106.38
25	B	616	CLA	C4A-NA-C1A	2.26	109.24	106.38
25	c	511	CLA	O1D-CGD-CBD	2.26	128.15	124.64
25	c	504	CLA	CMB-C2B-C3B	2.26	129.51	125.09
25	b	615	CLA	O1D-CGD-CBD	2.26	128.15	124.64
23	D	408	SQD	O5-C1-C2	2.27	115.01	110.28
25	A	606	CLA	O1D-CGD-CBD	2.28	128.18	124.64
23	A	603	SQD	C44-O6-C1	2.28	118.57	113.81
25	c	510	CLA	CMD-C2D-C3D	2.28	129.55	125.09
25	B	614	CLA	O2D-CGD-CBD	2.28	114.51	111.22
25	c	504	CLA	CMD-C2D-C3D	2.30	129.58	125.09
25	C	508	CLA	CMD-C2D-C3D	2.30	129.59	125.09
25	C	509	CLA	C4A-NA-C1A	2.30	109.30	106.38
25	C	502	CLA	CMD-C2D-C3D	2.30	129.59	125.09
25	C	502	CLA	C4A-NA-C1A	2.31	109.31	106.38
27	B	619	BCR	C2-C1-C6	2.31	113.92	110.48
23	A	603	SQD	C4-C3-C2	2.32	115.05	110.79
25	B	601	CLA	C4A-NA-C1A	2.32	109.32	106.38
25	C	505	CLA	O2D-CGD-CBD	2.32	114.56	111.22
25	C	512	CLA	CMD-C2D-C3D	2.32	129.63	125.09
25	B	613	CLA	C4A-NA-C1A	2.33	109.33	106.38
25	b	604	CLA	CMB-C2B-C3B	2.33	129.64	125.09
25	b	612	CLA	C4A-NA-C1A	2.33	109.34	106.38
25	b	616	CLA	C4A-NA-C1A	2.33	109.34	106.38
25	B	609	CLA	CMB-C2B-C3B	2.34	129.66	125.09
26	A	608	PHO	C3D-C4D-CHA	2.34	112.84	107.14
26	d	401	PHO	C3D-C4D-CHA	2.34	112.84	107.14
27	h	101	BCR	C2-C1-C6	2.35	113.97	110.48
25	b	604	CLA	C4A-NA-C1A	2.35	109.36	106.38
25	b	612	CLA	CMB-C2B-C3B	2.36	129.69	125.09
26	a	608	PHO	C3D-C4D-CHA	2.36	112.88	107.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	CLA	C4A-NA-C1A	2.36	109.37	106.38
25	B	615	CLA	CMB-C2B-C3B	2.36	129.71	125.09
25	c	509	CLA	O1D-CGD-CBD	2.37	128.32	124.64
25	c	511	CLA	C4A-NA-C1A	2.37	109.39	106.38
25	B	615	CLA	C4A-NA-C1A	2.37	109.39	106.38
25	b	613	CLA	O1D-CGD-CBD	2.38	128.34	124.64
25	c	504	CLA	C4A-NA-C1A	2.38	109.40	106.38
25	c	505	CLA	C4A-NA-C1A	2.38	109.40	106.38
25	B	604	CLA	CMB-C2B-C3B	2.38	129.75	125.09
25	b	606	CLA	O2D-CGD-CBD	2.38	114.66	111.22
23	c	501	SQD	O8-S-C6	2.38	109.94	104.99
25	c	509	CLA	C4A-NA-C1A	2.39	109.41	106.38
26	D	401	PHO	C3D-C4D-CHA	2.39	112.97	107.14
25	C	506	CLA	CMB-C2B-C3B	2.40	129.77	125.09
25	c	507	CLA	O2D-CGD-CBD	2.40	114.68	111.22
23	D	409	SQD	O8-S-C6	2.40	109.98	104.99
25	b	618	CLA	CMB-C2B-C3B	2.41	129.80	125.09
25	B	601	CLA	CMB-C2B-C3B	2.41	129.81	125.09
25	a	612	CLA	CMB-C2B-C3B	2.41	129.81	125.09
25	C	511	CLA	C4A-NA-C1A	2.41	109.44	106.38
25	c	514	CLA	C4A-NA-C1A	2.41	109.44	106.38
23	A	603	SQD	O8-S-C6	2.42	110.01	104.99
25	C	502	CLA	CMB-C2B-C3B	2.42	129.81	125.09
25	b	613	CLA	CMB-C2B-C3B	2.42	129.82	125.09
23	c	501	SQD	O48-C23-C24	2.43	119.32	111.85
25	C	503	CLA	CMB-C2B-C3B	2.43	129.84	125.09
23	D	409	SQD	O48-C23-C24	2.44	119.36	111.85
28	a	611	PL9	C20-C19-C21	2.44	119.09	115.37
23	f	101	SQD	O8-S-C6	2.45	110.08	104.99
25	C	512	CLA	C4A-NA-C1A	2.45	109.49	106.38
26	a	608	PHO	CBD-CHA-C1A	2.46	131.03	126.70
25	A	615	CLA	CMB-C2B-C3B	2.46	129.89	125.09
25	B	610	CLA	CMB-C2B-C3B	2.46	129.89	125.09
23	f	101	SQD	C44-O6-C1	2.46	118.95	113.81
25	A	607	CLA	CMB-C2B-C3B	2.46	129.90	125.09
25	b	608	CLA	CMB-C2B-C3B	2.46	129.90	125.09
27	k	101	BCR	C29-C30-C25	2.47	114.15	110.48
25	B	602	CLA	CMB-C2B-C3B	2.47	129.92	125.09
25	c	507	CLA	CMB-C2B-C3B	2.47	129.92	125.09
25	c	513	CLA	C4A-NA-C1A	2.47	109.51	106.38
25	B	605	CLA	CMB-C2B-C3B	2.47	129.92	125.09
26	D	401	PHO	CBD-CHA-C1A	2.48	131.07	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	510	CLA	O2D-CGD-CBD	2.48	114.79	111.22
25	b	607	CLA	C4A-NA-C1A	2.48	109.52	106.38
23	A	603	SQD	O48-C23-C24	2.48	119.49	111.85
25	B	604	CLA	O2D-CGD-CBD	2.48	114.80	111.22
25	B	604	CLA	C4A-NA-C1A	2.48	109.53	106.38
23	A	619	SQD	O48-C23-C24	2.48	119.49	111.85
25	C	503	CLA	C4A-NA-C1A	2.48	109.53	106.38
25	b	618	CLA	O2D-CGD-CBD	2.49	114.81	111.22
31	l	101	LHG	O8-C23-C24	2.49	119.52	111.85
23	c	501	SQD	C44-O6-C1	2.49	119.03	113.81
25	b	619	CLA	O1D-CGD-CBD	2.50	128.52	124.64
25	b	617	CLA	CMB-C2B-C3B	2.50	129.98	125.09
25	C	511	CLA	CMB-C2B-C3B	2.50	129.99	125.09
28	A	611	PL9	C20-C19-C21	2.50	119.19	115.37
25	b	607	CLA	CMB-C2B-C3B	2.51	130.00	125.09
25	D	402	CLA	CMB-C2B-C3B	2.52	130.01	125.09
23	b	601	SQD	O8-S-C6	2.52	110.22	104.99
25	b	605	CLA	CMB-C2B-C3B	2.52	130.01	125.09
25	c	505	CLA	CMB-C2B-C3B	2.52	130.02	125.09
25	C	507	CLA	C4A-NA-C1A	2.52	109.58	106.38
25	C	513	CLA	CMB-C2B-C3B	2.52	130.02	125.09
23	b	601	SQD	O48-C23-C24	2.53	119.62	111.85
25	B	608	CLA	CMB-C2B-C3B	2.53	130.03	125.09
25	a	607	CLA	CMB-C2B-C3B	2.53	130.04	125.09
25	C	501	CLA	CMB-C2B-C3B	2.53	130.04	125.09
25	a	609	CLA	CMB-C2B-C3B	2.53	130.05	125.09
25	B	606	CLA	CMB-C2B-C3B	2.55	130.07	125.09
23	B	626	SQD	C1-O5-C5	2.56	118.76	113.74
25	b	609	CLA	CMB-C2B-C3B	2.56	130.10	125.09
26	d	401	PHO	CBD-CHA-C1A	2.57	131.23	126.70
25	B	611	CLA	CMB-C2B-C3B	2.57	130.11	125.09
25	B	614	CLA	CMB-C2B-C3B	2.57	130.11	125.09
28	D	407	PL9	C20-C19-C21	2.57	119.28	115.37
28	d	408	PL9	C40-C39-C41	2.57	119.28	115.37
25	b	614	CLA	CMB-C2B-C3B	2.57	130.11	125.09
25	c	508	CLA	CMB-C2B-C3B	2.57	130.12	125.09
25	c	503	CLA	CMB-C2B-C3B	2.57	130.12	125.09
25	C	505	CLA	CMB-C2B-C3B	2.58	130.12	125.09
25	c	509	CLA	CMB-C2B-C3B	2.58	130.13	125.09
26	A	608	PHO	CBD-CHA-C1A	2.58	131.25	126.70
23	B	626	SQD	O48-C23-C24	2.58	119.80	111.85
25	C	507	CLA	CMB-C2B-C3B	2.59	130.15	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	403	CLA	CMB-C2B-C3B	2.59	130.16	125.09
25	c	511	CLA	CMB-C2B-C3B	2.59	130.16	125.09
25	c	513	CLA	CMB-C2B-C3B	2.59	130.16	125.09
25	b	610	CLA	CMB-C2B-C3B	2.60	130.16	125.09
25	b	616	CLA	CMB-C2B-C3B	2.60	130.17	125.09
25	B	603	CLA	CMB-C2B-C3B	2.60	130.17	125.09
25	c	515	CLA	CMB-C2B-C3B	2.62	130.20	125.09
25	b	611	CLA	CMB-C2B-C3B	2.62	130.21	125.09
25	c	506	CLA	CMB-C2B-C3B	2.62	130.21	125.09
25	C	512	CLA	CMB-C2B-C3B	2.63	130.24	125.09
23	I	101	SQD	O48-C23-C24	2.64	119.96	111.85
27	h	101	BCR	C27-C26-C25	2.64	125.64	122.73
23	B	626	SQD	C44-O6-C1	2.64	119.34	113.81
25	C	504	CLA	CMB-C2B-C3B	2.65	130.27	125.09
25	C	510	CLA	CMB-C2B-C3B	2.65	130.27	125.09
31	a	615	LHG	O8-C23-C24	2.66	120.02	111.85
25	c	510	CLA	CMB-C2B-C3B	2.66	130.29	125.09
23	D	408	SQD	C44-O6-C1	2.67	119.40	113.81
25	D	403	CLA	CMB-C2B-C3B	2.69	130.35	125.09
31	a	613	LHG	O8-C23-C24	2.69	120.13	111.85
25	b	606	CLA	CMB-C2B-C3B	2.70	130.37	125.09
31	L	101	LHG	O8-C23-C24	2.70	120.17	111.85
25	B	607	CLA	CMB-C2B-C3B	2.71	130.38	125.09
25	C	508	CLA	CMB-C2B-C3B	2.71	130.38	125.09
31	D	406	LHG	O8-C23-C24	2.71	120.19	111.85
25	b	615	CLA	CMB-C2B-C3B	2.73	130.43	125.09
23	D	408	SQD	O8-S-C6	2.74	110.69	104.99
31	A	617	LHG	O8-C23-C24	2.77	120.37	111.85
27	d	405	BCR	C2-C1-C6	2.78	114.61	110.48
25	A	609	CLA	CMB-C2B-C3B	2.78	130.53	125.09
31	d	407	LHG	O8-C23-C24	2.80	120.45	111.85
25	B	613	CLA	CMB-C2B-C3B	2.80	130.56	125.09
23	b	601	SQD	C44-O6-C1	2.81	119.68	113.81
25	c	512	CLA	CMB-C2B-C3B	2.83	130.62	125.09
25	B	612	CLA	CMB-C2B-C3B	2.84	130.64	125.09
31	A	618	LHG	O8-C23-C24	2.84	120.60	111.85
27	T	101	BCR	C27-C26-C25	2.85	125.86	122.73
23	B	626	SQD	O8-S-C6	2.85	110.91	104.99
27	h	101	BCR	C29-C30-C25	2.85	114.72	110.48
31	a	614	LHG	O8-C23-C24	2.86	120.65	111.85
31	A	616	LHG	O8-C23-C24	2.86	120.66	111.85
25	b	607	CLA	O2D-CGD-CBD	2.87	115.36	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	408	SQD	C3-C4-C5	2.88	115.36	110.23
23	A	603	SQD	C3-C4-C5	2.89	115.38	110.23
23	f	101	SQD	O5-C5-C4	2.92	115.23	109.67
28	a	611	PL9	C40-C39-C41	2.92	119.82	115.37
25	B	616	CLA	CMB-C2B-C3B	2.92	130.80	125.09
27	b	622	BCR	C2-C1-C6	2.96	114.89	110.48
28	A	611	PL9	C40-C39-C41	2.99	119.92	115.37
25	C	509	CLA	CMB-C2B-C3B	3.00	130.96	125.09
23	b	601	SQD	O6-C1-C2	3.00	111.70	108.00
27	B	627	BCR	C27-C26-C25	3.01	126.04	122.73
25	d	404	CLA	CMB-C2B-C3B	3.02	130.99	125.09
26	D	401	PHO	O1D-CGD-CBD	3.03	129.35	124.64
27	H	102	BCR	C2-C1-C6	3.03	114.99	110.48
26	d	401	PHO	O1D-CGD-CBD	3.03	129.36	124.64
26	a	608	PHO	O1D-CGD-CBD	3.04	129.36	124.64
25	a	606	CLA	CMB-C2B-C3B	3.04	131.04	125.09
26	A	608	PHO	O1D-CGD-CBD	3.05	129.38	124.64
27	k	101	BCR	C27-C26-C25	3.06	126.10	122.73
27	Y	101	BCR	C27-C26-C25	3.09	126.13	122.73
23	D	409	SQD	O5-C5-C4	3.09	115.57	109.67
25	b	619	CLA	CMB-C2B-C3B	3.12	131.19	125.09
27	A	610	BCR	C27-C26-C25	3.14	126.19	122.73
23	B	626	SQD	C3-C4-C5	3.16	115.86	110.23
27	c	517	BCR	C27-C26-C25	3.16	126.21	122.73
27	C	514	BCR	C27-C26-C25	3.17	126.22	122.73
25	A	606	CLA	CMB-C2B-C3B	3.18	131.30	125.09
27	C	515	BCR	C27-C26-C25	3.19	126.24	122.73
25	c	514	CLA	CMB-C2B-C3B	3.19	131.33	125.09
27	c	516	BCR	C27-C26-C25	3.20	126.25	122.73
27	a	610	BCR	C27-C26-C25	3.20	126.25	122.73
23	c	501	SQD	O5-C5-C4	3.24	115.85	109.67
28	D	407	PL9	C40-C39-C41	3.28	120.36	115.37
27	y	101	BCR	C27-C26-C25	3.30	126.36	122.73
27	b	620	BCR	C27-C26-C25	3.39	126.46	122.73
27	B	617	BCR	C27-C26-C25	3.41	126.48	122.73
23	A	603	SQD	O5-C5-C4	3.48	116.31	109.67
27	H	102	BCR	C27-C26-C25	3.50	126.58	122.73
23	c	501	SQD	O47-C7-C8	3.51	118.92	111.53
27	K	101	BCR	C27-C26-C25	3.51	126.59	122.73
27	b	622	BCR	C27-C26-C25	3.55	126.63	122.73
23	D	409	SQD	O47-C7-C8	3.56	119.02	111.53
27	B	618	BCR	C27-C26-C25	3.61	126.70	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	619	BCR	C27-C26-C25	3.62	126.72	122.73
27	b	621	BCR	C27-C26-C25	3.63	126.73	122.73
23	A	603	SQD	O47-C7-C8	3.65	119.22	111.53
27	d	405	BCR	C27-C26-C25	3.66	126.75	122.73
27	D	404	BCR	C27-C26-C25	3.68	126.77	122.73
27	c	516	BCR	C2-C1-C6	3.69	115.97	110.48
23	D	408	SQD	O47-C7-C8	3.69	119.30	111.53
23	b	601	SQD	O47-C7-C8	3.70	119.33	111.53
23	A	619	SQD	O47-C7-C8	3.75	119.44	111.53
23	I	101	SQD	O47-C7-C8	3.78	119.49	111.53
23	f	101	SQD	O47-C7-C8	3.83	119.60	111.53
31	A	618	LHG	O4-P-O5	3.86	132.66	112.56
31	a	615	LHG	O4-P-O5	3.90	132.86	112.56
31	d	407	LHG	O4-P-O5	3.91	132.93	112.56
31	D	406	LHG	O4-P-O5	3.92	132.93	112.56
31	l	101	LHG	O4-P-O5	3.92	132.95	112.56
31	A	616	LHG	O4-P-O5	3.92	132.96	112.56
31	a	613	LHG	O4-P-O5	3.92	132.97	112.56
31	A	617	LHG	O4-P-O5	3.93	133.01	112.56
31	L	101	LHG	O4-P-O5	3.93	133.02	112.56
31	a	614	LHG	O4-P-O5	3.96	133.16	112.56
23	A	603	SQD	O6-C1-C2	3.98	112.90	108.00
23	c	501	SQD	O6-C1-C2	4.01	112.93	108.00
23	B	626	SQD	O47-C7-C8	4.03	120.02	111.53
23	B	626	SQD	O5-C5-C4	4.05	117.39	109.67
23	D	409	SQD	O6-C1-C2	4.30	113.29	108.00
23	f	101	SQD	O6-C1-C2	4.40	113.41	108.00
23	B	626	SQD	O6-C1-C2	4.53	113.58	108.00
23	D	408	SQD	O5-C5-C4	4.64	118.52	109.67
23	D	408	SQD	C1-O5-C5	4.68	122.92	113.74
23	B	626	SQD	O7-S-C6	5.43	110.75	106.92
23	D	408	SQD	O7-S-C6	5.92	111.09	106.92
23	b	601	SQD	O9-S-C6	6.00	111.15	106.92
23	D	408	SQD	O9-S-C6	6.26	111.33	106.92
23	c	501	SQD	O9-S-C6	6.34	111.39	106.92
23	A	603	SQD	O7-S-C6	6.38	111.42	106.92
23	f	101	SQD	O7-S-C6	6.41	111.44	106.92
23	D	409	SQD	O7-S-C6	6.58	111.56	106.92
23	D	409	SQD	O9-S-C6	6.71	111.64	106.92
23	b	601	SQD	O7-S-C6	6.75	111.68	106.92
23	B	626	SQD	O9-S-C6	6.79	111.70	106.92
23	f	101	SQD	O9-S-C6	6.79	111.71	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	SQD	O7-S-C6	6.80	111.71	106.92
23	A	603	SQD	O9-S-C6	7.08	111.91	106.92

All (198) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	c	515	CLA	NC
25	c	515	CLA	ND
25	c	515	CLA	NA
25	b	614	CLA	NC
25	b	614	CLA	ND
25	b	614	CLA	NA
25	b	606	CLA	NA
25	b	606	CLA	NC
25	b	606	CLA	ND
25	A	615	CLA	NA
25	A	615	CLA	NC
25	A	615	CLA	ND
25	c	510	CLA	NC
25	c	510	CLA	ND
25	c	510	CLA	NA
25	B	608	CLA	NC
25	B	608	CLA	ND
25	B	608	CLA	NA
25	B	607	CLA	NA
25	B	607	CLA	NC
25	B	607	CLA	ND
25	b	605	CLA	NC
25	b	605	CLA	ND
25	b	605	CLA	NA
25	C	511	CLA	NC
25	C	511	CLA	NA
25	B	610	CLA	NA
25	B	610	CLA	NC
25	B	610	CLA	ND
25	B	615	CLA	NC
25	B	615	CLA	ND
25	B	615	CLA	NA
25	a	607	CLA	NA
25	a	607	CLA	NC
25	a	607	CLA	ND
25	C	505	CLA	NC

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Mol	Chain	Res	Type	Atom
25	C	505	CLA	NA
25	B	613	CLA	NC
25	B	613	CLA	NA
25	B	613	CLA	ND
25	C	504	CLA	NC
25	C	504	CLA	ND
25	C	504	CLA	NA
25	B	611	CLA	NC
25	B	611	CLA	ND
25	B	611	CLA	NA
25	c	512	CLA	NC
25	c	512	CLA	ND
25	c	512	CLA	NA
25	B	614	CLA	NC
25	B	614	CLA	ND
25	B	614	CLA	NA
25	D	402	CLA	NC
25	D	402	CLA	NA
25	C	508	CLA	NC
25	C	508	CLA	ND
25	C	508	CLA	NA
25	b	617	CLA	NC
25	b	617	CLA	ND
25	b	617	CLA	NA
25	B	616	CLA	NC
25	B	616	CLA	NA
25	B	616	CLA	ND
25	b	618	CLA	NC
25	b	618	CLA	ND
25	b	618	CLA	NA
25	b	612	CLA	NC
25	b	612	CLA	NA
25	b	611	CLA	NC
25	b	611	CLA	ND
25	b	611	CLA	NA
25	C	512	CLA	NC
25	C	512	CLA	NA
25	C	512	CLA	ND
25	C	513	CLA	NA
25	C	513	CLA	NC
25	C	513	CLA	ND
25	C	501	CLA	NC

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Mol	Chain	Res	Type	Atom
25	C	501	CLA	ND
25	C	501	CLA	NA
25	B	602	CLA	NC
25	B	602	CLA	ND
25	B	602	CLA	NA
25	A	606	CLA	NA
25	A	606	CLA	NC
25	A	606	CLA	ND
25	b	608	CLA	NC
25	b	608	CLA	NA
25	B	609	CLA	NC
25	B	609	CLA	NA
25	b	607	CLA	NC
25	b	607	CLA	ND
25	b	607	CLA	NA
25	c	509	CLA	NC
25	c	509	CLA	ND
25	c	509	CLA	NA
25	c	508	CLA	NC
25	c	508	CLA	ND
25	c	508	CLA	NA
25	c	507	CLA	NC
25	c	507	CLA	NA
25	b	615	CLA	NC
25	b	615	CLA	NA
25	b	615	CLA	ND
25	B	606	CLA	NC
25	B	606	CLA	ND
25	B	606	CLA	NA
25	C	507	CLA	NC
25	C	507	CLA	NA
25	C	507	CLA	ND
25	B	604	CLA	NC
25	B	604	CLA	ND
25	B	604	CLA	NA
25	c	514	CLA	NC
25	c	514	CLA	ND
25	c	514	CLA	NA
25	c	505	CLA	NC
25	c	505	CLA	ND
25	c	505	CLA	NA
25	C	510	CLA	NC

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Mol	Chain	Res	Type	Atom
25	C	510	CLA	NA
25	C	510	CLA	ND
25	B	601	CLA	NC
25	B	601	CLA	ND
25	B	601	CLA	NA
25	a	606	CLA	NC
25	a	606	CLA	ND
25	a	606	CLA	NA
25	c	506	CLA	NC
25	c	506	CLA	ND
25	c	506	CLA	NA
25	b	610	CLA	NA
25	b	610	CLA	NC
25	b	610	CLA	ND
25	a	609	CLA	NC
25	a	609	CLA	ND
25	a	609	CLA	NA
25	C	502	CLA	NC
25	C	502	CLA	NA
25	B	605	CLA	NC
25	B	605	CLA	NA
25	c	511	CLA	NC
25	c	511	CLA	ND
25	c	511	CLA	NA
25	b	616	CLA	NC
25	b	616	CLA	ND
25	b	616	CLA	NA
25	D	403	CLA	NC
25	D	403	CLA	ND
25	D	403	CLA	NA
25	d	404	CLA	NC
25	d	404	CLA	ND
25	d	404	CLA	NA
25	a	612	CLA	NC
25	a	612	CLA	ND
25	a	612	CLA	NA
25	b	604	CLA	NC
25	b	604	CLA	ND
25	b	604	CLA	NA
25	A	607	CLA	NC
25	A	607	CLA	ND
25	A	607	CLA	NA

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Mol	Chain	Res	Type	Atom
25	A	609	CLA	NC
25	A	609	CLA	ND
25	A	609	CLA	NA
25	c	504	CLA	NC
25	c	504	CLA	NA
25	b	619	CLA	NA
25	b	619	CLA	NC
25	b	619	CLA	ND
25	c	503	CLA	NC
25	c	503	CLA	ND
25	c	503	CLA	NA
25	b	609	CLA	NC
25	b	609	CLA	ND
25	b	609	CLA	NA
25	B	612	CLA	NC
25	B	612	CLA	ND
25	B	612	CLA	NA
25	C	509	CLA	NC
25	C	509	CLA	ND
25	C	509	CLA	NA
25	C	503	CLA	NC
25	C	503	CLA	ND
25	C	503	CLA	NA
25	C	506	CLA	NC
25	C	506	CLA	NA
25	B	603	CLA	NC
25	B	603	CLA	ND
25	B	603	CLA	NA
25	b	613	CLA	NA
25	b	613	CLA	NC
25	b	613	CLA	ND
25	d	403	CLA	NC
25	d	403	CLA	NA
25	c	513	CLA	NC
25	c	513	CLA	ND
25	c	513	CLA	NA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	d	409	LMG	C8-O7-C10-C11
23	B	626	SQD	C45-O47-C7-O49

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Mol	Chain	Res	Type	Atoms
23	B	626	SQD	C45-O47-C7-C8

There are no ring outliers.

74 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	603	SQD	1	0
25	A	606	CLA	3	0
25	A	607	CLA	3	0
26	A	608	PHO	2	0
25	A	609	CLA	10	0
27	A	610	BCR	5	0
28	A	611	PL9	7	0
29	A	613	LMG	2	0
25	A	615	CLA	1	0
31	A	616	LHG	2	0
31	A	617	LHG	7	0
31	A	618	LHG	3	0
23	A	619	SQD	2	0
32	A	620	BCT	1	0
25	B	601	CLA	3	0
25	B	602	CLA	4	0
25	B	603	CLA	2	0
25	B	604	CLA	2	0
25	B	605	CLA	4	0
25	B	606	CLA	6	0
25	B	607	CLA	4	0
25	B	608	CLA	6	0
25	B	609	CLA	6	0
25	B	610	CLA	4	0
25	B	611	CLA	3	0
25	B	612	CLA	7	0
25	B	613	CLA	4	0
25	B	614	CLA	6	0
25	B	615	CLA	7	0
25	B	616	CLA	3	0
27	B	617	BCR	2	0
27	B	618	BCR	2	0
27	B	619	BCR	2	0
29	B	620	LMG	1	0
29	B	621	LMG	1	0
29	B	625	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	626	SQD	7	0
27	B	627	BCR	5	0
25	C	501	CLA	6	0
25	C	502	CLA	1	0
25	C	503	CLA	11	0
25	C	504	CLA	3	0
25	C	505	CLA	8	0
25	C	506	CLA	2	0
25	C	507	CLA	5	0
25	C	508	CLA	6	0
25	C	509	CLA	6	0
25	C	510	CLA	4	0
25	C	511	CLA	3	0
25	C	512	CLA	4	0
25	C	513	CLA	3	0
27	C	514	BCR	1	0
27	C	515	BCR	3	0
33	C	516	DGD	1	0
33	C	517	DGD	2	0
33	C	518	DGD	2	0
29	C	519	LMG	1	0
29	C	520	LMG	2	0
26	D	401	PHO	7	0
25	D	402	CLA	3	0
25	D	403	CLA	8	0
27	D	404	BCR	3	0
29	D	405	LMG	2	0
31	D	406	LHG	1	0
28	D	407	PL9	2	0
23	D	408	SQD	1	0
34	E	101	HEM	4	0
27	H	102	BCR	4	0
33	H	103	DGD	2	0
27	K	101	BCR	3	0
31	L	101	LHG	7	0
27	T	101	BCR	6	0
34	V	201	HEM	2	0
27	Y	101	BCR	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/344 (97%)	-0.35	1 (0%) 94 84	28, 38, 60, 76	0
1	a	334/344 (97%)	-0.43	0 100 100	28, 38, 60, 76	0
2	B	504/510 (98%)	-0.17	11 (2%) 65 35	27, 41, 66, 86	0
2	b	504/510 (98%)	-0.22	4 (0%) 87 67	29, 42, 67, 85	0
3	C	451/461 (97%)	-0.26	5 (1%) 82 58	30, 45, 61, 75	0
3	c	451/461 (97%)	-0.23	3 (0%) 89 70	31, 46, 63, 93	0
4	D	341/352 (96%)	-0.39	2 (0%) 90 73	28, 39, 56, 67	0
4	d	341/352 (96%)	-0.37	0 100 100	29, 40, 55, 78	0
5	E	81/84 (96%)	-0.05	0 100 100	39, 54, 72, 89	0
5	e	82/84 (97%)	0.24	3 (3%) 45 19	43, 61, 75, 80	0
6	F	34/45 (75%)	-0.35	1 (2%) 55 26	40, 50, 63, 77	0
6	f	34/45 (75%)	-0.42	0 100 100	39, 51, 69, 72	0
7	H	63/66 (95%)	0.03	1 (1%) 74 47	39, 47, 57, 63	0
7	h	63/66 (95%)	-0.10	1 (1%) 74 47	35, 47, 58, 68	0
8	I	35/38 (92%)	0.09	1 (2%) 55 26	29, 44, 71, 73	0
8	i	35/38 (92%)	0.05	3 (8%) 13 4	33, 43, 74, 94	0
9	J	36/40 (90%)	-0.25	0 100 100	44, 58, 68, 75	0
9	j	36/40 (90%)	0.00	2 (5%) 28 11	49, 57, 72, 79	0
10	K	37/46 (80%)	-0.00	0 100 100	45, 59, 75, 89	0
10	k	37/46 (80%)	-0.07	0 100 100	47, 56, 72, 79	0
11	L	37/37 (100%)	-0.34	1 (2%) 58 28	32, 38, 62, 84	0
11	l	37/37 (100%)	-0.35	1 (2%) 58 28	29, 38, 69, 81	0
12	M	32/36 (88%)	-0.14	2 (6%) 23 9	33, 38, 56, 74	0
12	m	32/36 (88%)	0.03	3 (9%) 11 4	31, 41, 59, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.06	8 (3%) 50 22	30, 47, 81, 111	0
13	o	244/272 (89%)	-0.06	7 (2%) 55 26	31, 46, 80, 127	0
14	T	29/32 (90%)	-0.38	1 (3%) 49 21	30, 39, 60, 74	0
14	t	29/32 (90%)	-0.47	0 100 100	31, 36, 63, 66	0
15	U	97/134 (72%)	-0.03	0 100 100	36, 49, 69, 75	0
15	u	97/134 (72%)	-0.27	0 100 100	32, 44, 58, 76	0
16	V	137/163 (84%)	-0.18	0 100 100	34, 47, 59, 74	0
16	v	137/163 (84%)	-0.03	1 (0%) 89 70	34, 54, 67, 81	0
17	Y	30/46 (65%)	0.52	3 (10%) 9 4	60, 73, 84, 87	0
17	y	30/46 (65%)	0.15	2 (6%) 21 7	49, 65, 78, 83	0
18	X	38/41 (92%)	0.14	2 (5%) 30 12	41, 50, 65, 79	0
18	x	38/41 (92%)	0.19	2 (5%) 30 12	46, 55, 74, 76	0
19	Z	62/62 (100%)	0.48	5 (8%) 15 5	52, 69, 88, 98	0
19	z	62/62 (100%)	0.56	8 (12%) 5 2	51, 72, 97, 105	0
20	R	34/41 (82%)	0.88	2 (5%) 26 10	65, 73, 83, 86	0
20	r	34/41 (82%)	0.59	0 100 100	65, 78, 86, 90	0
All	All	5313/5700 (93%)	-0.18	86 (1%) 74 47	27, 45, 72, 127	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	35	SER	6.9
13	o	3	GLN	6.1
12	M	33	GLN	5.2
16	v	18	THR	4.9
12	m	31	SER	4.7
2	B	487	SER	4.2
18	x	2	THR	4.1
13	O	62	GLU	4.0
13	o	4	THR	4.0
12	m	32	GLN	4.0
12	m	33	GLN	3.7
11	l	1	MET	3.6
19	z	34	ASP	3.6
2	B	494	GLY	3.4
3	c	24	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	b	504	THR	3.3
11	L	1	MET	3.3
18	X	38	GLN	3.3
8	i	35	LYS	3.2
8	i	34	ARG	3.2
13	O	4	THR	3.2
19	z	62	VAL	3.2
8	I	34	ARG	3.1
8	i	36	ASP	3.1
3	C	27	ASP	3.0
6	F	12	SER	3.0
13	O	34	SER	3.0
2	B	351	GLY	2.9
13	O	63	ALA	2.9
3	c	192	GLY	2.8
20	R	6	LEU	2.8
19	z	3	ILE	2.8
19	z	1	MET	2.8
2	b	482	ILE	2.7
13	o	35	SER	2.7
2	B	497	GLN	2.7
2	B	294	SER	2.7
17	Y	20	ALA	2.7
13	o	6	THR	2.6
3	C	29	GLU	2.6
13	O	207	ARG	2.6
19	Z	32	ASP	2.6
9	j	7	ARG	2.5
12	M	31	SER	2.5
2	B	127	ARG	2.5
19	Z	33	TRP	2.5
2	B	503	THR	2.4
9	j	5	GLY	2.4
18	x	38	GLN	2.4
3	c	23	ALA	2.4
2	b	496	TYR	2.3
7	h	63	LYS	2.3
3	C	30	SER	2.3
13	O	23	ASP	2.3
17	Y	41	VAL	2.3
18	X	2	THR	2.3
13	O	55	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
19	z	35	ARG	2.2
7	H	5	THR	2.2
19	z	31	GLN	2.2
1	A	11	ALA	2.2
19	z	30	PRO	2.2
3	C	142	GLU	2.2
17	y	42	ARG	2.2
2	B	495	PHE	2.2
2	B	490	GLN	2.1
2	B	130	GLU	2.1
19	Z	62	VAL	2.1
13	o	245	PRO	2.1
19	Z	29	SER	2.1
5	e	81	GLU	2.1
17	y	20	ALA	2.1
19	Z	3	ILE	2.1
4	D	238	THR	2.1
4	D	240	ALA	2.1
13	o	61	GLN	2.1
5	e	62	SER	2.1
17	Y	43	ARG	2.1
2	B	412	THR	2.1
3	C	23	ALA	2.1
2	b	294	SER	2.1
19	z	41	PHE	2.0
20	R	25	PRO	2.0
14	T	30	THR	2.0
13	o	60	ARG	2.0
5	e	12	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
14	FME	T	1	10/11	0.93	0.13	-	44,47,53,54	0
12	FME	M	1	10/11	0.93	0.29	-	30,43,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	FME	I	1	10/11	0.91	0.29	-	43,56,63,71	0
14	FME	t	1	10/11	0.92	0.25	-	39,42,63,72	0
8	FME	i	1	10/11	0.91	0.22	-	35,50,56,61	0
12	FME	m	1	10/11	0.91	0.23	-	26,45,55,64	0

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(\AA^2)	Q<0.9
30	UNL	b	603	13/-	0.77	0.29	6.75	39,48,61,62	0
29	LMG	C	520	51/55	0.74	0.39	4.83	49,62,82,100	0
30	UNL	b	602	13/-	0.87	0.25	4.82	30,36,41,45	0
30	UNL	C	521	9/-	0.84	0.28	4.66	36,42,46,49	0
29	LMG	d	409	40/55	0.79	0.31	4.24	40,55,76,77	0
31	LHG	a	615	42/49	0.77	0.32	4.21	54,78,89,100	0
29	LMG	b	624	51/55	0.76	0.32	4.14	45,64,76,86	0
29	LMG	c	522	51/55	0.80	0.37	4.10	36,68,83,90	0
23	SQD	b	601	54/54	0.81	0.28	3.64	39,60,90,97	0
30	UNL	t	101	10/-	0.76	0.28	3.63	26,41,47,47	0
28	PL9	A	611	55/55	0.74	0.37	3.50	39,58,75,79	0
29	LMG	A	612	51/55	0.80	0.33	3.46	34,59,76,85	0
29	LMG	D	405	51/55	0.89	0.27	3.45	34,53,88,92	0
29	LMG	B	625	51/55	0.81	0.26	3.14	28,52,74,78	0
23	SQD	I	101	40/54	0.70	0.39	3.11	31,52,84,89	0
28	PL9	a	611	55/55	0.84	0.29	3.08	40,59,72,73	0
27	BCR	b	622	40/40	0.87	0.25	3.01	33,43,52,54	0
29	LMG	B	621	51/55	0.80	0.30	2.95	32,56,71,74	0
29	LMG	A	613	51/55	0.80	0.30	2.79	31,53,78,84	0
33	DGD	c	520	62/66	0.87	0.27	2.76	36,47,72,80	0
29	LMG	c	502	51/55	0.78	0.31	2.71	34,57,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	C	504	65/65	0.86	0.27	2.60	33,51,70,78	0
29	LMG	c	521	51/55	0.80	0.32	2.60	33,65,83,88	0
23	SQD	c	501	54/54	0.84	0.32	2.60	38,58,76,77	0
23	SQD	A	619	40/54	0.79	0.28	2.49	25,48,67,69	0
29	LMG	b	623	51/55	0.82	0.30	2.49	29,48,71,74	0
31	LHG	A	617	49/49	0.87	0.33	2.47	33,55,78,82	0
27	BCR	T	101	40/40	0.87	0.28	2.43	31,43,58,62	0
33	DGD	h	102	62/66	0.82	0.29	2.42	35,47,63,73	0
25	CLA	b	604	65/65	0.84	0.28	2.40	44,59,76,88	0
30	UNL	d	402	22/-	0.82	0.31	2.33	26,43,60,78	0
27	BCR	B	627	40/40	0.86	0.26	2.33	30,41,49,53	0
25	CLA	c	505	65/65	0.87	0.27	2.31	32,51,62,68	0
31	LHG	A	618	49/49	0.74	0.29	2.25	41,72,85,94	0
27	BCR	y	101	40/40	0.83	0.29	1.97	50,63,70,74	0
25	CLA	c	504	65/65	0.89	0.26	1.88	32,46,59,65	0
27	BCR	d	405	40/40	0.88	0.23	1.84	29,43,56,62	0
24	CL	a	603	1/1	0.82	0.23	1.67	59,59,59,59	0
28	PL9	D	407	55/55	0.90	0.23	1.67	26,35,45,50	0
33	DGD	H	103	62/66	0.85	0.27	1.67	26,41,53,61	0
27	BCR	Y	101	40/40	0.84	0.26	1.65	46,60,72,76	0
33	DGD	c	519	62/66	0.87	0.26	1.59	37,57,86,95	0
27	BCR	B	618	40/40	0.88	0.25	1.59	28,40,48,52	0
33	DGD	C	518	62/66	0.88	0.25	1.58	33,48,65,74	0
25	CLA	a	609	65/65	0.90	0.25	1.55	19,34,71,81	0
28	PL9	d	408	55/55	0.92	0.21	1.54	21,33,43,45	0
23	SQD	A	603	52/54	0.86	0.29	1.51	38,60,78,82	0
25	CLA	C	512	65/65	0.83	0.30	1.51	42,58,68,79	0
25	CLA	B	601	65/65	0.85	0.29	1.51	41,59,84,96	0
27	BCR	b	620	40/40	0.89	0.23	1.42	33,45,53,54	0
30	UNL	z	101	11/-	0.82	0.28	1.39	31,53,58,60	0
27	BCR	B	619	40/40	0.88	0.21	1.39	33,44,58,60	0
31	LHG	D	406	49/49	0.92	0.24	1.38	25,40,50,59	0
25	CLA	B	608	65/65	0.89	0.28	1.36	29,37,47,52	0
27	BCR	D	404	40/40	0.88	0.25	1.33	28,46,63,67	0
25	CLA	c	511	65/65	0.89	0.24	1.33	38,46,55,57	0
27	BCR	C	514	40/40	0.85	0.29	1.31	45,56,64,66	0
25	CLA	B	606	65/65	0.86	0.28	1.30	29,44,65,84	0
25	CLA	d	404	65/65	0.87	0.24	1.29	32,46,73,91	0
27	BCR	C	515	40/40	0.88	0.23	1.21	32,42,52,53	0
25	CLA	c	510	58/65	0.88	0.24	1.18	34,46,59,67	0
25	CLA	c	514	65/65	0.85	0.27	1.10	45,59,78,83	0
25	CLA	A	615	65/65	0.92	0.22	1.08	22,34,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	c	515	65/65	0.83	0.30	1.06	45,60,78,81	0
31	LHG	d	407	49/49	0.93	0.20	1.06	20,37,47,51	0
25	CLA	C	509	65/65	0.89	0.25	1.04	33,46,59,67	0
25	CLA	b	608	65/65	0.92	0.19	1.02	30,40,46,51	0
29	LMG	d	406	42/55	0.91	0.21	1.01	38,48,63,73	0
25	CLA	D	403	65/65	0.88	0.24	1.00	21,37,63,69	0
25	CLA	b	609	65/65	0.90	0.23	0.99	21,35,59,81	0
25	CLA	B	603	65/65	0.90	0.25	0.98	28,37,45,47	0
27	BCR	c	516	40/40	0.86	0.32	0.96	33,63,70,72	0
23	SQD	B	626	54/54	0.84	0.23	0.96	33,52,85,90	0
23	SQD	D	409	43/54	0.79	0.29	0.95	37,68,89,98	0
25	CLA	A	606	65/65	0.89	0.22	0.92	26,34,45,48	0
25	CLA	C	503	65/65	0.87	0.25	0.92	37,49,58,65	0
25	CLA	A	609	65/65	0.92	0.23	0.91	17,29,79,89	0
25	CLA	C	502	65/65	0.87	0.26	0.87	35,51,62,69	0
29	LMG	C	519	51/55	0.82	0.28	0.86	42,61,73,85	0
33	DGD	C	516	62/66	0.91	0.21	0.85	21,39,63,71	0
27	BCR	K	101	40/40	0.88	0.24	0.83	45,53,60,66	0
27	BCR	B	617	40/40	0.92	0.20	0.81	32,41,49,50	0
26	PHO	d	401	64/64	0.92	0.21	0.81	24,39,45,49	0
25	CLA	D	402	65/65	0.90	0.22	0.80	24,36,48,59	0
30	UNL	m	102	16/-	0.83	0.27	0.80	37,45,51,54	0
27	BCR	k	101	40/40	0.84	0.26	0.80	37,53,59,61	0
31	LHG	L	101	49/49	0.90	0.23	0.79	29,41,51,57	0
23	SQD	D	408	47/54	0.80	0.27	0.76	17,53,103,121	0
29	LMG	B	620	51/55	0.86	0.24	0.76	27,46,67,75	0
25	CLA	c	506	65/65	0.89	0.23	0.75	36,49,70,74	0
27	BCR	H	102	40/40	0.80	0.32	0.75	34,51,59,65	0
25	CLA	C	511	65/65	0.85	0.26	0.69	45,57,66,70	0
25	CLA	b	617	65/65	0.89	0.22	0.69	34,45,63,73	0
26	PHO	A	608	64/64	0.93	0.21	0.68	23,32,37,43	0
31	LHG	a	614	35/49	0.90	0.23	0.68	36,47,56,58	0
25	CLA	C	501	65/65	0.92	0.21	0.68	34,42,49,54	0
25	CLA	c	508	65/65	0.87	0.25	0.65	34,49,72,78	0
25	CLA	B	605	65/65	0.92	0.19	0.64	24,34,40,42	0
27	BCR	A	610	40/40	0.92	0.20	0.62	22,34,44,47	0
25	CLA	b	605	65/65	0.90	0.22	0.58	31,43,56,58	0
31	LHG	l	101	49/49	0.90	0.21	0.57	30,45,54,56	0
25	CLA	C	505	65/65	0.91	0.21	0.57	33,41,55,62	0
25	CLA	B	607	65/65	0.92	0.20	0.55	26,36,44,54	0
25	CLA	b	619	65/65	0.90	0.24	0.55	30,44,72,80	0
25	CLA	b	606	65/65	0.93	0.20	0.53	24,36,50,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	B	602	65/65	0.94	0.22	0.47	29,39,47,52	0
33	DGD	C	517	62/66	0.92	0.22	0.45	39,51,74,83	0
25	CLA	A	607	57/65	0.93	0.20	0.44	29,37,49,67	0
25	CLA	C	513	65/65	0.88	0.29	0.44	41,62,74,83	0
25	CLA	B	616	65/65	0.89	0.24	0.43	32,44,70,76	0
31	LHG	a	613	49/49	0.93	0.20	0.43	26,43,56,60	0
25	CLA	b	610	65/65	0.93	0.19	0.42	23,37,51,54	0
25	CLA	c	503	65/65	0.93	0.21	0.41	27,40,46,52	0
25	CLA	B	614	65/65	0.88	0.22	0.40	32,42,63,82	0
25	CLA	c	512	65/65	0.91	0.23	0.40	31,47,56,64	0
23	SQD	f	101	43/54	0.87	0.25	0.38	51,70,77,84	0
27	BCR	b	621	40/40	0.90	0.22	0.37	31,42,57,59	0
25	CLA	B	613	65/65	0.92	0.23	0.34	19,33,48,69	0
25	CLA	c	507	65/65	0.90	0.21	0.33	32,44,61,64	0
25	CLA	b	611	65/65	0.89	0.24	0.30	27,41,54,57	0
27	BCR	c	517	40/40	0.92	0.20	0.28	19,39,50,52	0
33	DGD	c	518	62/66	0.90	0.21	0.26	28,46,63,79	0
26	PHO	a	608	64/64	0.93	0.20	0.25	19,28,38,42	0
25	CLA	C	510	65/65	0.89	0.24	0.23	41,51,58,60	0
25	CLA	C	508	65/65	0.90	0.22	0.22	38,49,82,90	0
27	BCR	h	101	40/40	0.84	0.27	0.19	31,45,55,62	0
25	CLA	b	613	65/65	0.92	0.20	0.18	24,35,43,45	0
25	CLA	b	618	65/65	0.90	0.20	0.17	28,40,47,56	0
25	CLA	C	507	65/65	0.89	0.22	0.16	32,42,52,67	0
25	CLA	B	604	65/65	0.90	0.23	0.15	28,37,57,65	0
26	PHO	D	401	64/64	0.92	0.21	0.14	27,37,47,54	0
25	CLA	d	403	65/65	0.92	0.19	0.13	24,36,45,50	0
25	CLA	B	610	65/65	0.92	0.21	0.12	25,33,39,45	0
25	CLA	B	611	65/65	0.93	0.22	0.11	21,31,38,44	0
27	BCR	a	610	40/40	0.93	0.19	0.06	19,32,45,47	0
31	LHG	A	616	49/49	0.92	0.20	0.05	24,41,54,58	0
25	CLA	a	606	65/65	0.93	0.18	-0.01	23,31,38,39	0
25	CLA	b	607	65/65	0.91	0.20	-0.01	24,34,48,53	0
25	CLA	c	509	65/65	0.91	0.20	-0.02	30,39,51,55	0
25	CLA	B	612	65/65	0.93	0.20	-0.08	26,35,42,46	0
25	CLA	B	615	65/65	0.92	0.19	-0.09	27,41,51,57	0
25	CLA	b	612	65/65	0.91	0.19	-0.15	28,41,55,61	0
25	CLA	B	609	65/65	0.89	0.20	-0.18	24,44,52,58	0
25	CLA	b	616	65/65	0.92	0.20	-0.20	25,33,51,62	0
25	CLA	a	612	65/65	0.94	0.17	-0.22	17,29,37,39	0
25	CLA	c	513	65/65	0.89	0.22	-0.23	42,52,58,60	0
25	CLA	C	506	65/65	0.90	0.20	-0.23	32,47,64,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	UNL	M	102	17/-	0.88	0.22	-0.29	31,37,49,51	0
25	CLA	a	607	59/65	0.94	0.17	-0.34	27,37,55,72	0
34	HEM	v	201	43/43	0.94	0.17	-0.40	32,41,48,52	0
25	CLA	b	615	65/65	0.94	0.18	-0.41	22,32,41,50	0
34	HEM	E	101	43/43	0.92	0.20	-0.46	42,54,67,69	0
34	HEM	V	201	43/43	0.93	0.17	-0.49	31,44,52,56	0
25	CLA	b	614	65/65	0.93	0.18	-0.57	25,35,41,50	0
34	HEM	e	101	43/43	0.89	0.21	-0.57	50,62,69,70	0
30	UNL	B	624	11/-	0.88	0.18	-0.71	26,31,38,41	0
32	BCT	A	620	4/4	0.95	0.15	-1.37	26,36,37,44	0
24	CL	a	604	1/1	0.93	0.14	-1.70	42,42,42,42	0
32	BCT	a	605	4/4	0.96	0.10	-1.99	44,47,49,50	0
24	CL	A	604	1/1	0.93	0.10	-2.11	43,43,43,43	0
24	CL	A	605	1/1	0.96	0.13	-2.23	44,44,44,44	0
21	OEX	A	601	10/10	0.98	0.10	-2.52	33,40,45,46	0
22	FE2	a	602	1/1	0.91	0.08	-3.25	62,62,62,62	0
21	OEX	a	601	10/10	0.98	0.08	-4.14	40,44,48,51	0
22	FE2	A	602	1/1	0.96	0.05	-6.60	46,46,46,46	0
30	UNL	B	623	11/-	0.81	0.23	-	35,40,47,48	0
29	LMG	b	625	9/55	0.65	0.42	-	40,46,52,55	0
30	UNL	H	101	8/-	0.84	0.20	-	29,35,43,47	0
30	UNL	j	101	9/-	0.80	0.28	-	40,49,60,63	0
30	UNL	B	622	6/-	0.86	0.24	-	26,42,50,56	0
30	UNL	M	101	6/-	0.83	0.31	-	41,46,52,65	0
30	UNL	m	101	5/-	0.80	0.28	-	26,32,37,41	0
30	UNL	i	101	12/-	0.84	0.29	-	24,39,51,51	0
30	UNL	A	614	7/-	0.89	0.19	-	32,38,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.