



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2018 – 03:53 PM EST

PDB ID : 5XDX  
Title : Bovine heart cytochrome c oxidase in the reduced state with pH 7.3 at 1.99 angstrom resolution  
Authors : Luo, F.J.; Shimada, A.; Hagimoto, N.; Shimada, S.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.  
Deposited on : 2017-03-30  
Resolution : 1.99 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

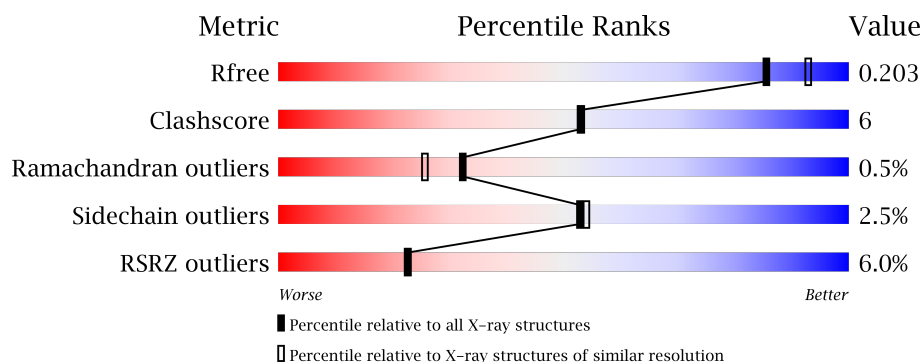
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>0.0%</div> <div> <div></div> <div>88%</div> <div>12%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>15%</div> <div>.</div> </div> </div>
2	O	227	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
3	C	260	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	P	260	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	94	
6	S	94	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
14	HEA	N	602	X	-	-	-
16	MG	A	604	-	-	-	X
16	MG	N	604	-	-	-	X
18	TGL	A	606	-	-	-	X
18	TGL	D	201	-	-	-	X
18	TGL	L	101	-	-	-	X
18	TGL	O	302	-	-	-	X
18	TGL	Q	201	-	-	-	X
18	TGL	Y	101	-	-	-	X
19	PGV	C	305	-	-	-	X
19	PGV	C	306	-	-	-	X
19	PGV	M	101	-	-	-	X
19	PGV	N	606	-	-	-	X
19	PGV	P	303	-	-	-	X
19	PGV	P	304	-	-	-	X
20	EDO	A	610	-	-	-	X
20	EDO	A	611	-	-	-	X
20	EDO	A	612	-	-	-	X
20	EDO	A	614	-	-	-	X
20	EDO	A	615	-	-	-	X
20	EDO	C	309	-	-	-	X
20	EDO	D	203	-	-	-	X
20	EDO	F	104	-	-	-	X
20	EDO	N	609	-	-	-	X
20	EDO	N	612	-	-	-	X
20	EDO	N	613	-	-	X	X
20	EDO	N	614	-	-	-	X
20	EDO	N	615	-	-	-	X
20	EDO	N	617	-	-	-	X
20	EDO	R	201	-	-	-	X
20	EDO	S	103	-	-	-	X
21	CUA	B	301	-	-	-	X
22	CHD	C	308	-	-	-	X
22	CHD	J	101	-	-	-	X
22	CHD	W	101	-	-	-	X
23	PEK	C	303	-	-	-	X
23	PEK	T	102	-	-	-	X
24	CDL	C	307	-	-	-	X
24	CDL	G	101	-	-	-	X
24	CDL	P	305	-	-	-	X
24	CDL	T	104	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	DMU	C	313	-	-	-	X
25	DMU	P	309	-	-	-	X
25	DMU	Z	101	-	-	-	X
26	PSC	E	201	-	-	-	X
26	PSC	O	304	-	-	-	X
27	ZN	F	101	-	-	-	X

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33247 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	20	0
			4128	2774	626	685	43			
1	N	514	Total	C	N	O	S	0	21	0
			4132	2773	627	687	45			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	7	0
			1854	1209	281	343	21			
2	O	227	Total	C	N	O	S	0	6	0
			1849	1205	281	343	20			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	13	0
			2173	1461	338	358	16			
3	P	259	Total	C	N	O	S	0	12	0
			2168	1457	337	357	17			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			857	548	144	162	3			
5	R	105	Total	C	N	O	S	0	1	0
			857	548	144	162	3			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	1	0
			721	448	127	140	6			
6	S	94	Total	C	N	O	S	0	1	0
			721	448	127	140	6			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit VIIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	2	0
			471	305	78	84	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	2	0
			471	305	78	84	4			

- Molecule 11 is a protein called Cytochrome c oxidase subunit VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase subunit VIIc.

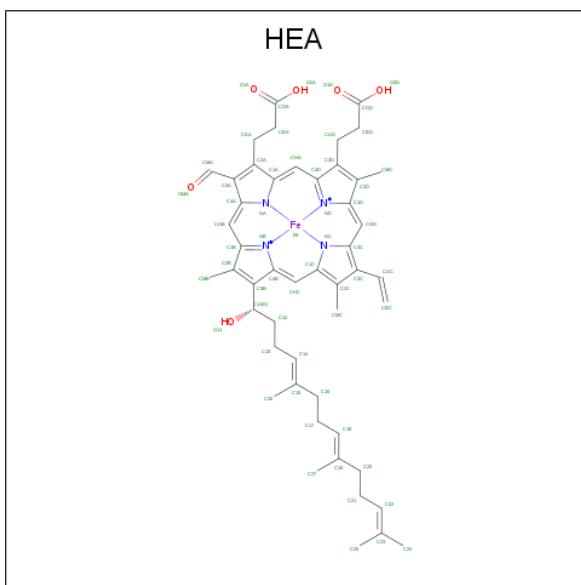
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			385	258	64	60	3			

- Molecule 13 is a protein called Cytochrome c oxidase subunit VIII-heart.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	1	0
			340	228	53	59			
13	Z	43	Total	C	N	O	0	1	0
			340	228	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

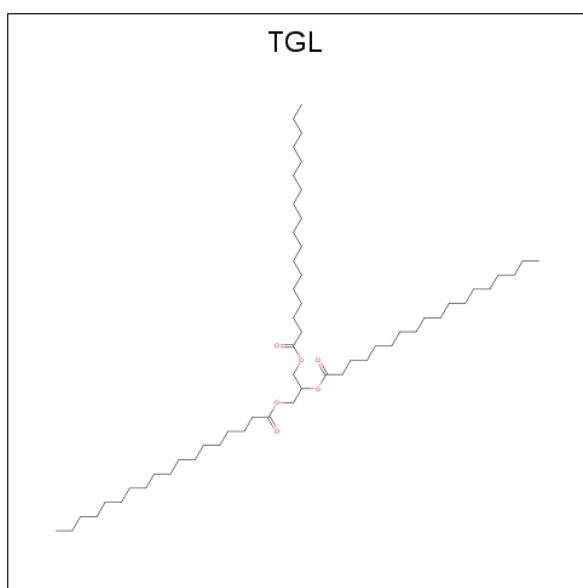
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

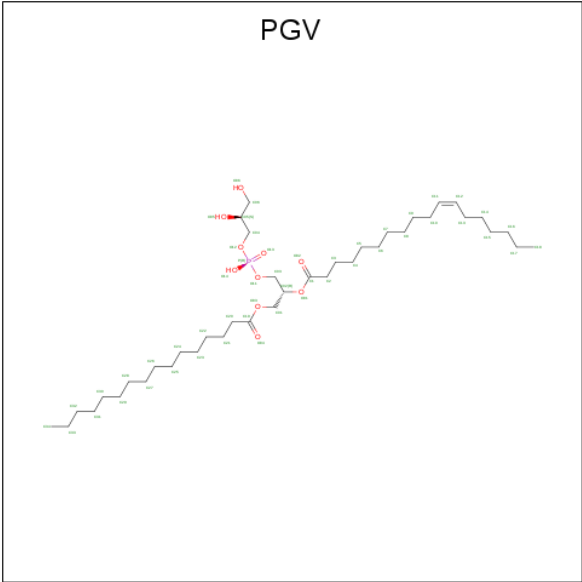
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	1	Total Na 1 1	0	0
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



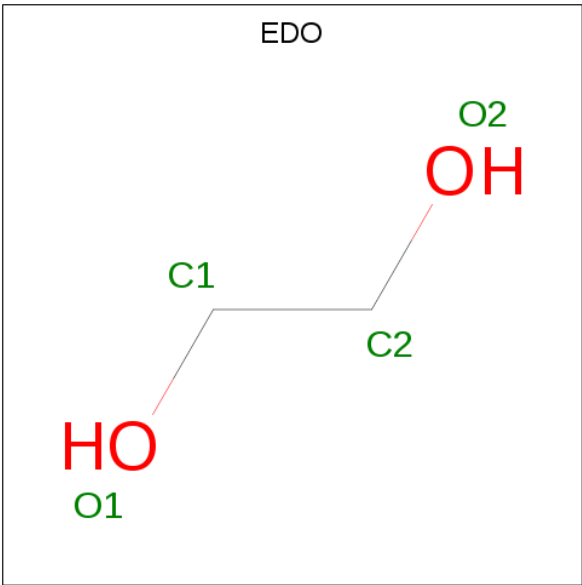
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	D	1	Total C O 63 57 6	0	0
18	L	1	Total C O 63 57 6	0	0
18	O	1	Total C O 63 57 6	0	0
18	Q	1	Total C O 63 57 6	0	0
18	Y	1	Total C O 63 57 6	0	0

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	M	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



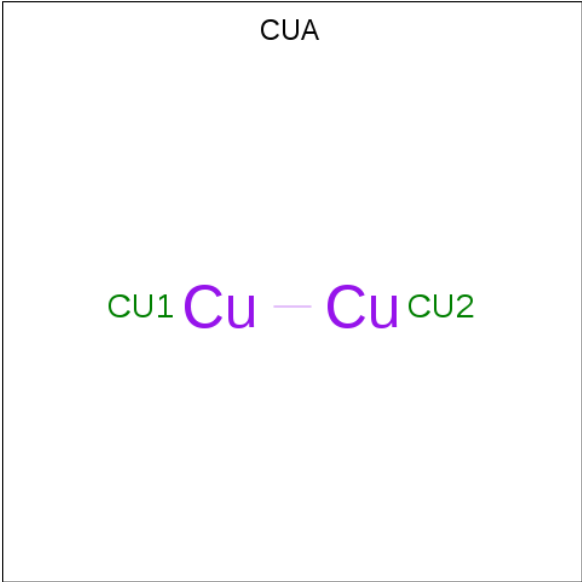
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	B	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	D	1	Total	C	O	0	0
			4	2	2		

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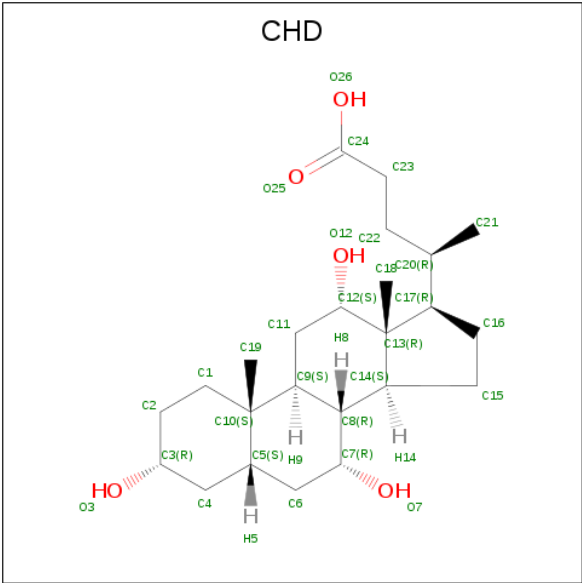
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	D	1	Total	C	O	0	0
			4	2	2		
20	E	1	Total	C	O	0	0
			4	2	2		
20	F	1	Total	C	O	0	0
			4	2	2		
20	F	1	Total	C	O	0	0
			4	2	2		
20	F	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



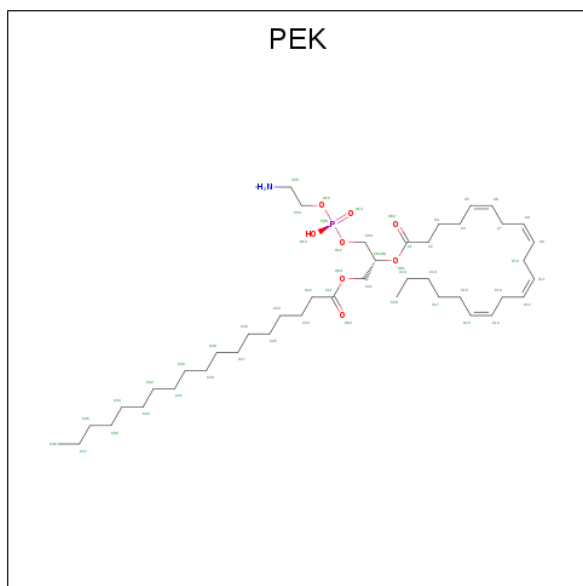
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



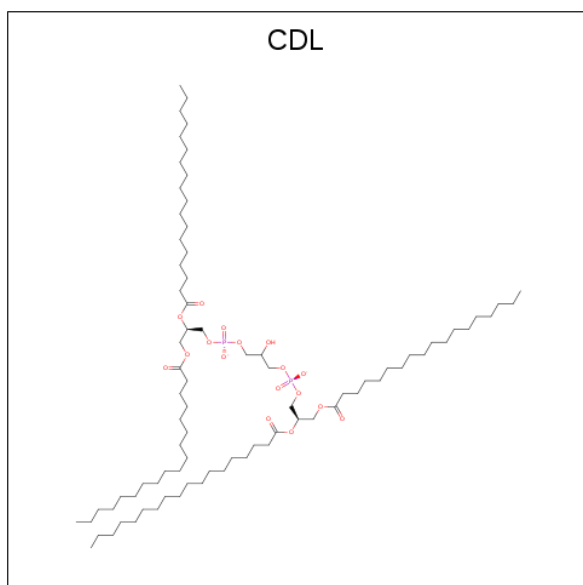
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

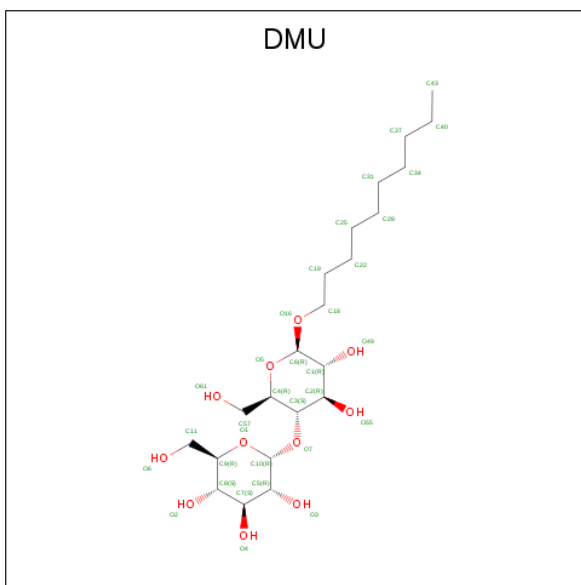
- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	O	P		0	0
			100	81	17	2			
24	G	1	Total	C	O	P		0	0
			100	81	17	2			
24	P	1	Total	C	O	P		0	0
			100	81	17	2			
24	T	1	Total	C	O	P		0	0
			100	81	17	2			

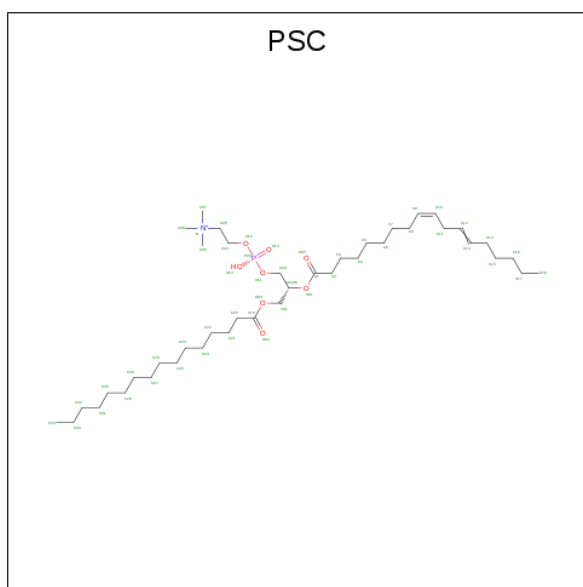
- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total 33	C 22	O 11	0	0
25	C	1	Total 33	C 22	O 11	0	0
25	M	1	Total 33	C 22	O 11	0	0
25	P	1	Total 33	C 22	O 11	0	0
25	P	1	Total 33	C 22	O 11	0	0
25	Z	1	Total 33	C 22	O 11	0	0

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula:  $C_{42}H_{81}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	S	1	Total	Zn	0	0
			1	1		
27	F	1	Total	Zn	0	0
			1	1		

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	245	Total	O	0	0
			245	245		
28	B	177	Total	O	0	1
			178	178		
28	C	103	Total	O	0	0
			103	103		
28	D	130	Total	O	0	0
			130	130		
28	E	92	Total	O	0	0
			92	92		

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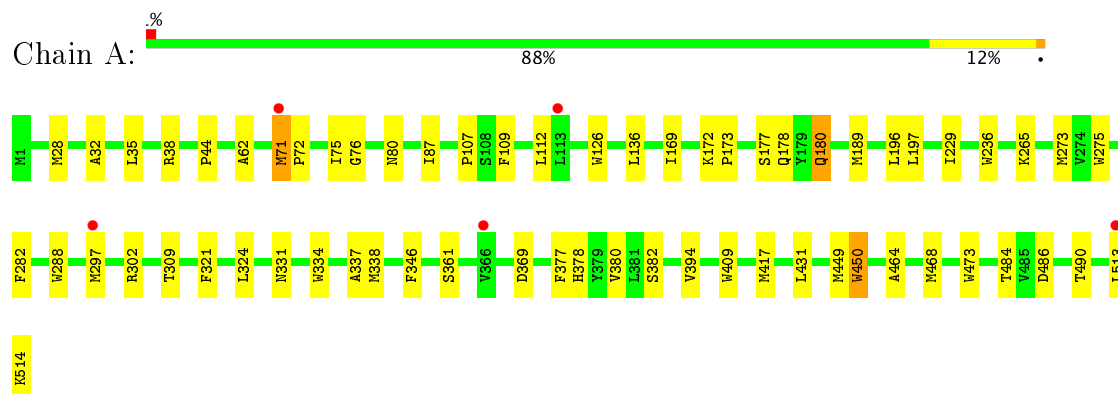
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	92	Total 92	O 92	0	0
28	G	58	Total 58	O 58	0	0
28	H	56	Total 56	O 56	0	0
28	I	48	Total 48	O 48	0	0
28	J	28	Total 28	O 28	0	0
28	K	42	Total 42	O 42	0	0
28	L	26	Total 26	O 26	0	0
28	M	27	Total 27	O 27	0	0
28	N	214	Total 214	O 214	0	0
28	O	128	Total 128	O 128	0	0
28	P	99	Total 99	O 99	0	0
28	Q	58	Total 58	O 58	0	0
28	R	62	Total 62	O 62	0	0
28	S	64	Total 64	O 64	0	0
28	T	51	Total 51	O 51	0	0
28	U	45	Total 45	O 45	0	0
28	V	31	Total 31	O 31	0	0
28	W	19	Total 19	O 19	0	0
28	X	11	Total 11	O 11	0	0
28	Y	21	Total 21	O 21	0	0
28	Z	14	Total 14	O 14	0	0

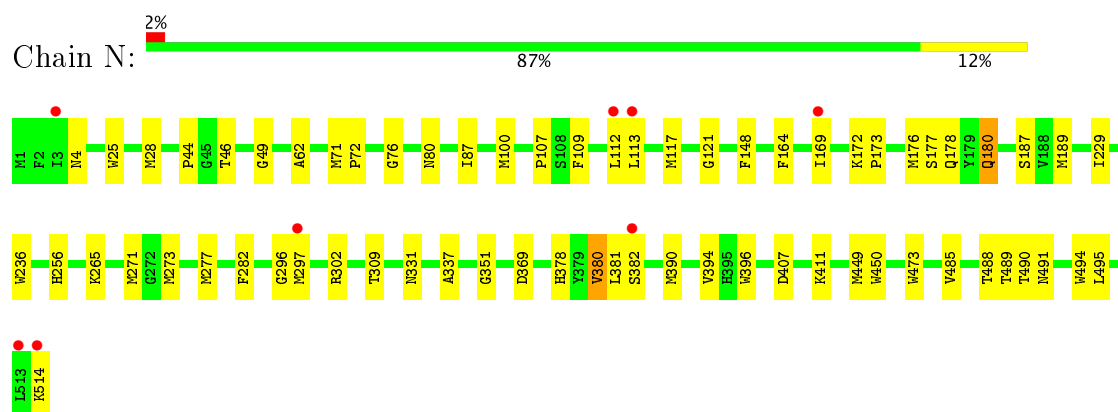
### 3 Residue-property plots [i](#)

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

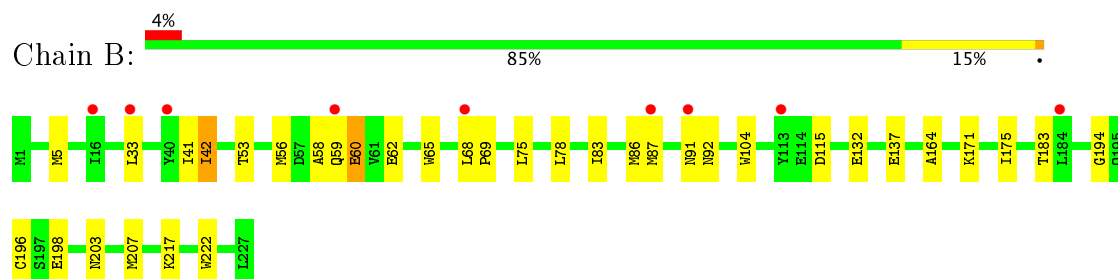
#### • Molecule 1: Cytochrome c oxidase subunit 1



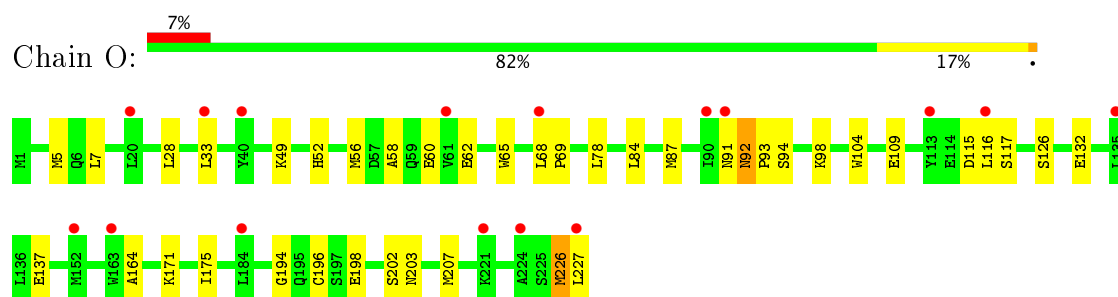
#### • Molecule 1: Cytochrome c oxidase subunit 1



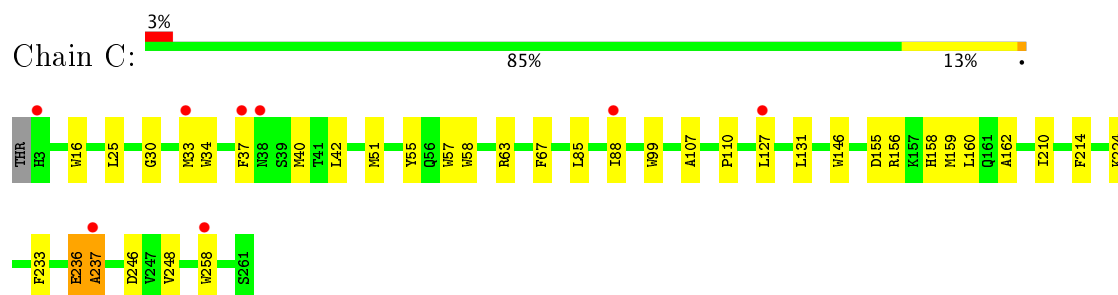
#### • Molecule 2: Cytochrome c oxidase subunit 2



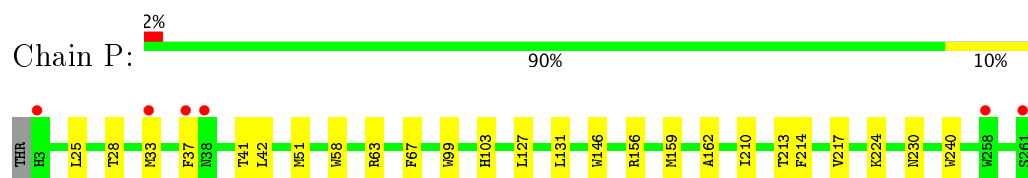
#### • Molecule 2: Cytochrome c oxidase subunit 2



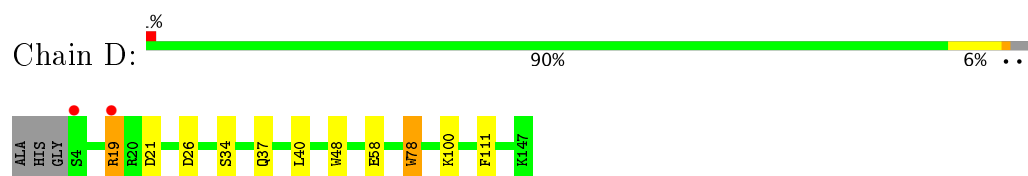
- Molecule 3: Cytochrome c oxidase subunit 3



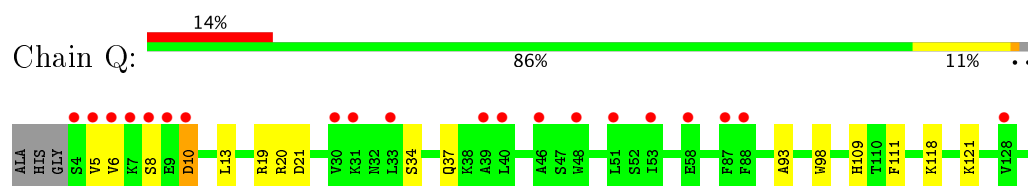
- Molecule 3: Cytochrome c oxidase subunit 3



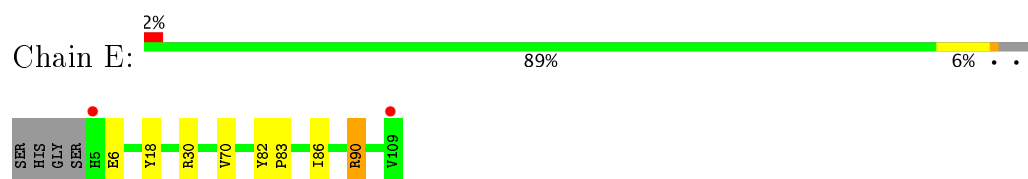
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



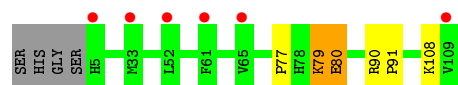
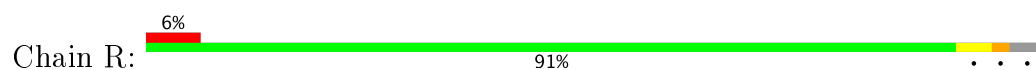
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



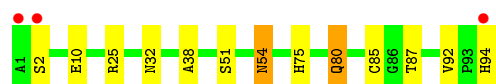
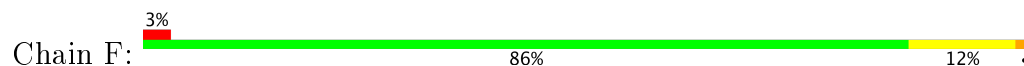
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



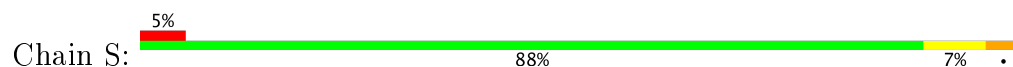
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



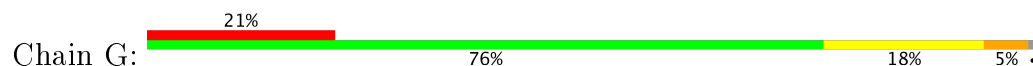
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



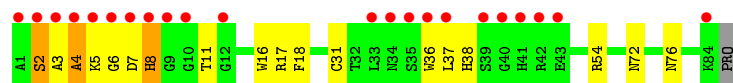
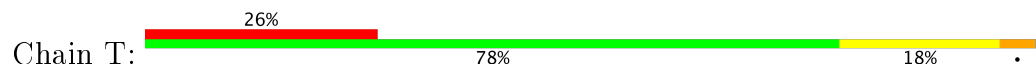
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



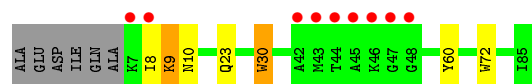
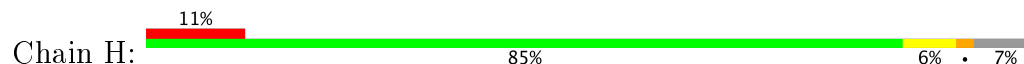
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



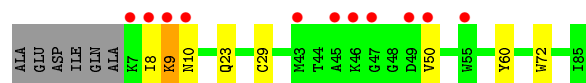
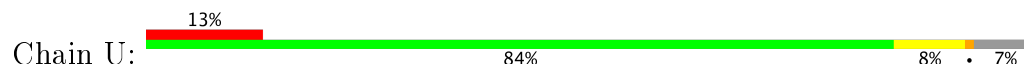
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



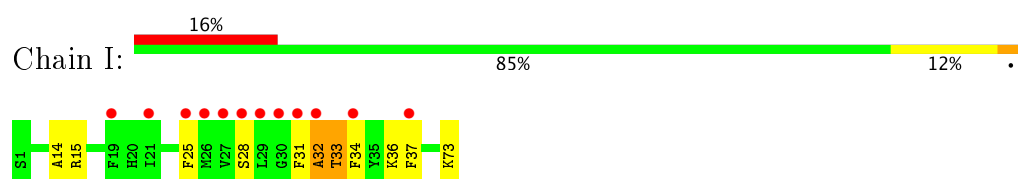
- Molecule 8: Cytochrome c oxidase subunit 6B1



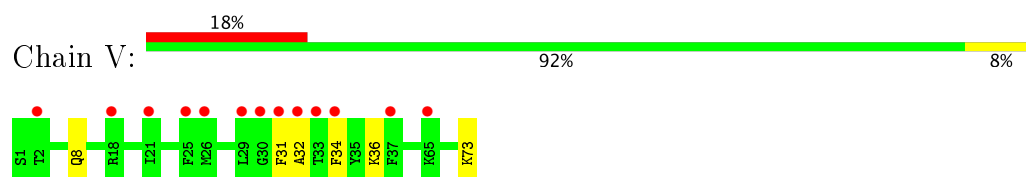
- Molecule 8: Cytochrome c oxidase subunit 6B1



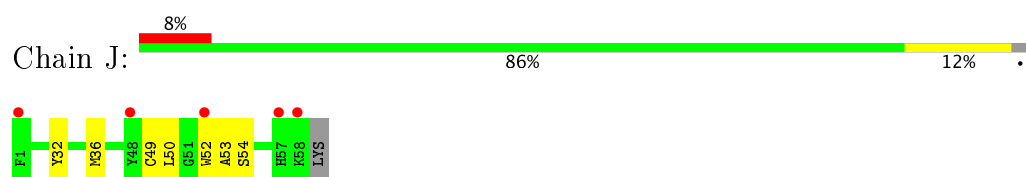
- Molecule 9: Cytochrome c oxidase polypeptide VIc



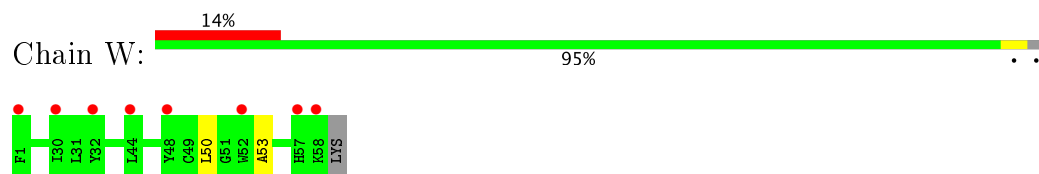
- Molecule 9: Cytochrome c oxidase polypeptide VIc



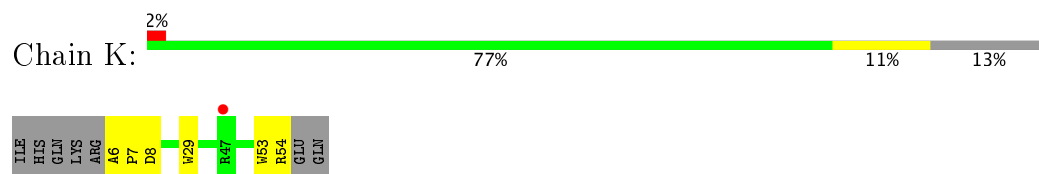
- Molecule 10: Cytochrome c oxidase subunit VIIa-heart



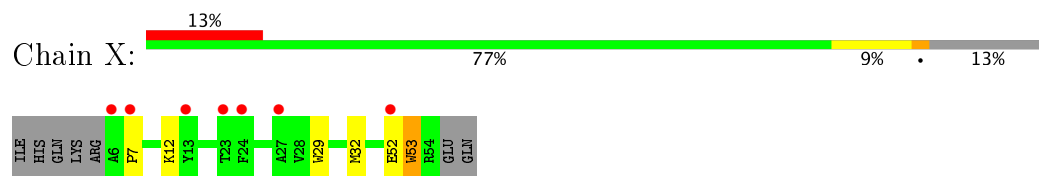
- Molecule 10: Cytochrome c oxidase subunit VIIa-heart



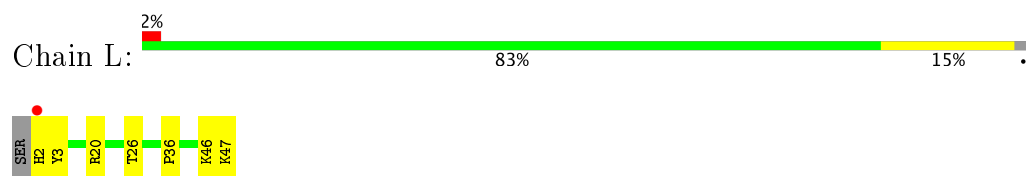
- Molecule 11: Cytochrome c oxidase subunit VIIb



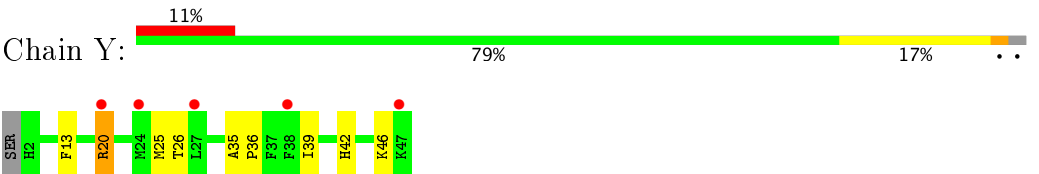
- Molecule 11: Cytochrome c oxidase subunit VIIb



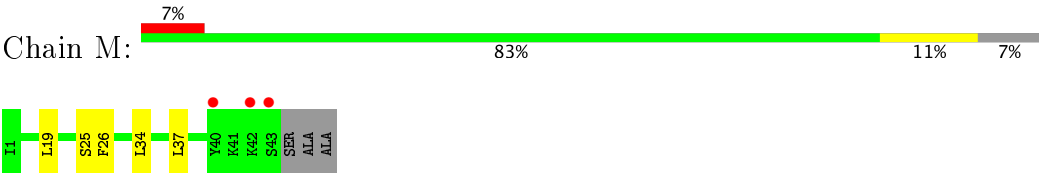
- Molecule 12: Cytochrome c oxidase subunit VIIc



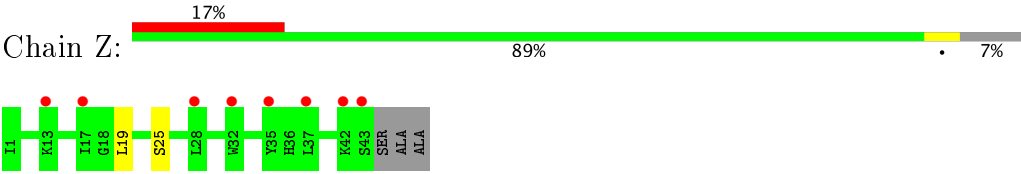
- Molecule 12: Cytochrome c oxidase subunit VIIc



● Molecule 13: Cytochrome c oxidase subunit VIII-heart



● Molecule 13: Cytochrome c oxidase subunit VIII-heart





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.04Å 205.69Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.99 108.39 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.99) 99.7 (108.39-1.99)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.182 , 0.203 0.182 , 0.203	Depositor DCC
$R_{free}$ test set	23022 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33247	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, EDO, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

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	0.66	6/4315 (0.1%)	0.61	2/5889 (0.0%)
1	N	0.63	4/4322 (0.1%)	0.59	0/5896
2	B	0.61	3/1911 (0.2%)	0.66	0/2602
2	O	0.53	2/1903 (0.1%)	0.61	0/2592
3	C	0.71	5/2299 (0.2%)	0.58	1/3140 (0.0%)
3	P	0.69	3/2291 (0.1%)	0.53	0/3128
4	D	0.63	2/1229 (0.2%)	0.54	0/1658
4	Q	0.58	2/1229 (0.2%)	0.53	0/1658
5	E	0.52	0/879	0.55	0/1192
5	R	0.49	0/879	0.54	0/1192
6	F	0.54	0/740	0.57	0/1003
6	S	0.54	0/740	0.55	0/1003
7	G	0.68	1/690 (0.1%)	0.60	0/937
7	T	0.69	2/690 (0.3%)	0.61	0/937
8	H	0.63	2/682 (0.3%)	0.55	0/921
8	U	0.62	1/682 (0.1%)	0.57	0/921
9	I	0.45	0/605	0.56	0/802
9	V	0.38	0/605	0.50	0/802
10	J	0.52	0/488	0.52	0/658
10	W	0.52	0/488	0.50	0/658
11	K	0.70	2/398 (0.5%)	0.53	0/546
11	X	0.67	2/398 (0.5%)	0.50	0/546
12	L	0.60	0/393	0.55	0/526
12	Y	0.54	0/401	0.49	0/536
13	M	0.58	0/353	0.53	0/481
13	Z	0.54	0/353	0.50	0/481
All	All	0.62	37/29963 (0.1%)	0.57	3/40705 (0.0%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	6.34	1.35	1.23
1	A	126	TRP	CD2-CE2	5.79	1.48	1.41
2	B	65	TRP	CD2-CE2	5.54	1.48	1.41
8	H	72	TRP	CD2-CE2	5.51	1.48	1.41
11	K	29	TRP	CD2-CE2	5.46	1.47	1.41
3	C	58	TRP	CD2-CE2	5.45	1.47	1.41
2	O	65	TRP	CD2-CE2	5.43	1.47	1.41
4	D	48	TRP	CD2-CE2	5.39	1.47	1.41
2	B	222	TRP	CD2-CE2	5.39	1.47	1.41
1	N	396	TRP	CD2-CE2	5.37	1.47	1.41
7	T	36	TRP	CD2-CE2	5.34	1.47	1.41
3	P	240	TRP	CD2-CE2	5.30	1.47	1.41
8	U	72	TRP	CD2-CE2	5.29	1.47	1.41
1	A	409	TRP	CD2-CE2	5.28	1.47	1.41
1	A	288	TRP	CD2-CE2	5.27	1.47	1.41
7	G	36	TRP	CD2-CE2	5.21	1.47	1.41
3	C	57	TRP	CD2-CE2	5.20	1.47	1.41
11	K	53	TRP	CD2-CE2	5.19	1.47	1.41
1	N	25	TRP	CD2-CE2	5.16	1.47	1.41
1	N	473	TRP	CD2-CE2	5.16	1.47	1.41
3	P	58	TRP	CD2-CE2	5.15	1.47	1.41
1	A	473	TRP	CD2-CE2	5.15	1.47	1.41
7	T	16	TRP	CD2-CE2	5.14	1.47	1.41
4	D	78	TRP	CD2-CE2	5.13	1.47	1.41
3	P	99	TRP	CD2-CE2	5.13	1.47	1.41
1	A	450	TRP	CD2-CE2	5.12	1.47	1.41
8	H	30	TRP	CD2-CE2	5.11	1.47	1.41
2	O	198	GLU	C-O	5.09	1.33	1.23
3	C	99	TRP	CD2-CE2	5.08	1.47	1.41
3	C	16	TRP	CD2-CE2	5.07	1.47	1.41
11	X	29	TRP	CD2-CE2	5.07	1.47	1.41
4	Q	138	TRP	CD2-CE2	5.06	1.47	1.41
1	A	275	TRP	CD2-CE2	5.04	1.47	1.41
1	N	450	TRP	CD2-CE2	5.04	1.47	1.41
3	C	258	TRP	CD2-CE2	5.02	1.47	1.41
4	Q	98	TRP	CD2-CE2	5.01	1.47	1.41
11	X	53	TRP	CD2-CE2	5.01	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71[A]	MET	CG-SD-CE	-5.71	91.06	100.20
1	A	71[B]	MET	CG-SD-CE	-5.71	91.06	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	236	GLU	C-N-CA	-5.35	108.33	121.70

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	4128	0	4171	59	0
1	N	4132	0	4169	75	0
2	B	1854	0	1888	23	0
2	O	1849	0	1879	21	0
3	C	2173	0	2130	34	0
3	P	2168	0	2122	23	0
4	D	1195	0	1183	14	0
4	Q	1195	0	1183	11	0
5	E	857	0	854	4	0
5	R	857	0	854	5	0
6	F	721	0	706	13	0
6	S	721	0	706	11	0
7	G	675	0	644	16	0
7	T	675	0	643	15	0
8	H	662	0	623	6	0
8	U	662	0	623	2	0
9	I	601	0	613	9	0
9	V	601	0	613	3	0
10	J	471	0	474	9	0
10	W	471	0	474	3	0
11	K	384	0	366	2	0
11	X	384	0	366	5	0
12	L	380	0	380	9	0
12	Y	385	0	389	10	0
13	M	340	0	363	5	0
13	Z	340	0	363	2	0
14	A	120	0	108	6	0
14	N	120	0	108	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	63	0	110	3	0
18	D	63	0	110	4	0
18	L	63	0	110	4	0
18	O	63	0	110	2	0
18	Q	63	0	110	0	0
18	Y	63	0	110	5	0
19	A	51	0	76	2	0
19	C	102	0	152	4	0
19	M	51	0	76	2	0
19	N	102	0	152	4	0
19	P	102	0	152	4	0
20	A	36	0	54	5	0
20	B	4	0	6	0	0
20	C	12	0	18	0	0
20	D	8	0	12	2	0
20	E	4	0	6	1	0
20	F	12	0	18	0	0
20	N	40	0	60	9	0
20	P	4	0	6	0	0
20	R	4	0	6	0	0
20	S	8	0	12	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	3	0
22	J	29	0	38	0	0
22	O	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	39	1	0
23	C	106	0	154	5	0
23	G	53	0	77	0	0
23	T	159	0	231	7	0
24	C	100	0	156	10	0
24	G	100	0	156	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	P	100	0	156	8	0
24	T	100	0	156	13	0
25	C	66	0	84	12	0
25	M	33	0	42	0	0
25	P	66	0	84	9	0
25	Z	33	0	42	0	0
26	E	52	0	80	10	0
26	O	52	0	80	6	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	245	0	0	12	0
28	B	178	0	0	5	0
28	C	103	0	0	2	0
28	D	130	0	0	2	0
28	E	92	0	0	0	0
28	F	92	0	0	1	0
28	G	58	0	0	0	0
28	H	56	0	0	2	0
28	I	48	0	0	0	0
28	J	28	0	0	1	0
28	K	42	0	0	1	0
28	L	26	0	0	0	0
28	M	27	0	0	0	0
28	N	214	0	0	6	0
28	O	128	0	0	1	0
28	P	99	0	0	1	0
28	Q	58	0	0	1	0
28	R	62	0	0	0	0
28	S	64	0	0	0	0
28	T	51	0	0	0	0
28	U	45	0	0	0	0
28	V	31	0	0	1	0
28	W	19	0	0	0	0
28	X	11	0	0	3	0
28	Y	21	0	0	0	0
28	Z	14	0	0	0	0
All	All	33247	0	32270	397	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 6.

All (397) 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)
3:C:236:GLU:O	3:C:237:ALA:CB	1.79	1.26
1:N:113[B]:LEU:HG	1:N:117[B]:MET:CE	1.69	1.22
20:A:615:EDO:H22	28:A:920:HOH:O	1.42	1.19
3:C:33[B]:MET:SD	25:C:313:DMU:H11	1.83	1.18
1:A:28[B]:MET:HA	1:A:28[B]:MET:CE	1.83	1.09
1:N:113[B]:LEU:HG	1:N:117[B]:MET:HE2	1.15	1.08
26:O:304:PSC:H02	26:O:304:PSC:H212	1.37	1.07
3:C:236:GLU:O	3:C:237:ALA:HB3	1.45	1.05
1:N:113[B]:LEU:CG	1:N:117[B]:MET:HE2	1.85	1.05
1:A:28[B]:MET:HA	1:A:28[B]:MET:HE3	1.07	1.03
6:S:85:CYS:SG	6:S:87:THR:HG23	1.99	1.02
25:C:313:DMU:H8	10:J:53:ALA:HB2	1.43	1.00
3:C:67:PHE:HE2	24:C:307:CDL:H1	1.24	0.99
7:G:84:LYS:HD2	7:G:84:LYS:H	1.27	0.99
20:N:615:EDO:H22	28:N:884:HOH:O	1.64	0.96
1:N:113[B]:LEU:CG	1:N:117[B]:MET:CE	2.43	0.96
3:P:33[B]:MET:SD	25:P:309:DMU:H11	2.06	0.95
25:C:313:DMU:C19	10:J:53:ALA:HB2	1.97	0.94
1:A:28[B]:MET:CA	1:A:28[B]:MET:HE3	2.00	0.91
11:X:32:MET:HB2	28:X:101:HOH:O	1.71	0.90
3:C:236:GLU:O	3:C:237:ALA:HB2	1.72	0.90
3:C:63:ARG:HE	24:C:307:CDL:HA21	1.37	0.88
1:N:491:ASN:HA	20:N:613:EDO:H12	1.56	0.87
3:P:67:PHE:HE2	24:P:305:CDL:H1	1.39	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.85
6:F:85:CYS:SG	6:F:87:THR:HG23	2.17	0.84
1:N:28[B]:MET:HA	1:N:28[B]:MET:CE	2.08	0.83
6:F:75:HIS:H	6:F:80:GLN:HE22	1.27	0.82
3:C:33[B]:MET:SD	25:C:313:DMU:H6	2.20	0.82
4:Q:93:ALA:HB1	28:X:101:HOH:O	1.80	0.81
9:I:31:PHE:O	9:I:34:PHE:N	2.14	0.81
26:O:304:PSC:H02	26:O:304:PSC:C21	2.11	0.80
6:S:43:LYS:H	6:S:43:LYS:HD2	1.47	0.80
25:P:309:DMU:C19	10:W:53:ALA:HB2	2.12	0.79
1:N:117[A]:MET:HE3	12:Y:39:ILE:HG23	1.65	0.79
8:H:23:GLN:NE2	28:H:101:HOH:O	2.16	0.79
23:C:303:PEK:HN2	7:G:76:ASN:HD21	1.32	0.78
1:N:113[B]:LEU:CD1	1:N:117[B]:MET:HE2	2.13	0.78
1:N:297[B]:MET:HG3	1:N:302:ARG:HG3	1.64	0.78
5:R:80:GLU:CD	5:R:80:GLU:H	1.88	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.31	0.76
3:P:63:ARG:HE	24:P:305:CDL:HA22	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:72:ASN:H	7:T:76:ASN:HD22	1.33	0.76
1:N:28[B]:MET:HE2	1:N:28[B]:MET:HA	1.67	0.75
12:L:20:ARG:HH22	18:L:101:TGL:HC32	1.52	0.74
6:S:75:HIS:H	6:S:80:GLN:HE22	1.34	0.73
1:N:113[B]:LEU:HG	1:N:117[B]:MET:HE1	1.69	0.72
1:A:417[B]:MET:HE2	1:A:464:ALA:HB3	1.70	0.72
1:A:297[B]:MET:HG2	28:A:780:HOH:O	1.89	0.72
1:N:297[B]:MET:HG2	28:N:788:HOH:O	1.89	0.71
8:U:9:LYS:HD3	8:U:10:ASN:H	1.55	0.71
20:N:612:EDO:H11	20:N:613:EDO:H11	1.72	0.70
6:S:43:LYS:CD	6:S:43:LYS:H	2.04	0.70
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.73	0.70
4:D:78:TRP:CA	18:D:201:TGL:HB22	2.21	0.69
4:D:78:TRP:HA	18:D:201:TGL:HB22	1.74	0.69
7:T:2:SER:OG	23:T:101:PEK:H311	1.94	0.68
24:T:104:CDL:H542	24:T:104:CDL:H251	1.75	0.68
1:N:113[B]:LEU:CG	1:N:117[B]:MET:HE1	2.22	0.68
3:C:67:PHE:CE2	24:C:307:CDL:H1	2.17	0.67
7:T:76:ASN:HD21	23:T:102:PEK:HN2	1.40	0.67
1:N:46:THR:HG22	1:N:49:GLY:H	1.58	0.67
6:S:85:CYS:SG	6:S:87:THR:CG2	2.81	0.67
4:D:19:ARG:HH21	4:D:19:ARG:HG2	1.59	0.67
25:P:309:DMU:H9	10:W:53:ALA:HB2	1.76	0.67
9:I:33:THR:HA	9:I:36:LYS:HB3	1.77	0.67
6:F:54:ASN:HD22	6:F:54:ASN:H	1.42	0.66
2:B:53:THR:HG21	28:D:305:HOH:O	1.94	0.66
1:A:28[B]:MET:CA	1:A:28[B]:MET:CE	2.59	0.66
19:N:606:PGV:H311	13:Z:19:LEU:HD23	1.76	0.66
23:T:103:PEK:H382	24:T:104:CDL:H273	1.77	0.65
7:G:84:LYS:H	7:G:84:LYS:CD	2.04	0.65
1:A:361[A]:SER:OG	28:A:701:HOH:O	2.15	0.64
1:N:113[B]:LEU:CD2	1:N:117[B]:MET:HE1	2.27	0.64
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.79	0.64
25:C:313:DMU:H20	10:J:50:LEU:HB2	1.78	0.64
25:P:309:DMU:H8	10:W:53:ALA:HB2	1.79	0.64
1:A:394[A]:VAL:HG12	20:A:611:EDO:H22	1.80	0.63
6:S:43:LYS:N	6:S:43:LYS:HD2	2.13	0.63
4:D:26:ASP:HB3	20:D:202:EDO:H21	1.81	0.63
1:N:117[A]:MET:HA	1:N:117[A]:MET:HE2	1.80	0.63
3:P:210:ILE:HD13	19:P:303:PGV:H301	1.80	0.63
7:T:31:CYS:SG	24:T:104:CDL:H552	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.79	0.62
25:C:313:DMU:H9	10:J:49:CYS:O	1.99	0.62
1:A:417[B]:MET:HE2	1:A:464:ALA:CB	2.29	0.62
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.30	0.62
25:C:313:DMU:H9	10:J:53:ALA:HB2	1.78	0.61
1:N:28[B]:MET:CE	1:N:28[B]:MET:CA	2.79	0.61
3:C:233:PHE:O	3:C:236:GLU:O	2.19	0.61
1:N:46:THR:CG2	1:N:49:GLY:H	2.13	0.61
1:A:112:LEU:C	1:A:112:LEU:HD23	2.21	0.60
1:A:71[B]:MET:HB3	1:A:72:PRO:HD3	1.83	0.60
2:O:28:LEU:HD21	18:O:302:TGL:HG12	1.83	0.60
9:V:8:GLN:CD	28:V:103:HOH:O	2.40	0.60
3:P:63:ARG:HE	24:P:305:CDL:CA2	2.14	0.60
7:T:31:CYS:SG	24:T:104:CDL:H532	2.42	0.60
24:C:307:CDL:OB6	24:C:307:CDL:HB21	2.02	0.60
2:B:56:MET:HA	26:E:201:PSC:H201	1.84	0.60
24:C:307:CDL:HA22	28:J:201:HOH:O	2.02	0.59
4:D:34:SER:H	4:D:37:GLN:NE2	1.99	0.59
18:L:101:TGL:HC41	18:L:101:TGL:OC1	2.02	0.59
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.84	0.59
1:N:256:HIS:HE1	20:N:613:EDO:H22	1.67	0.59
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.38	0.58
14:N:601:HEA:HMC1	14:N:601:HEA:HBC1	1.85	0.58
12:L:20:ARG:NH2	18:L:101:TGL:HC32	2.17	0.58
3:P:37:PHE:CE2	25:P:309:DMU:H13	2.38	0.58
1:A:297[B]:MET:HG3	1:A:302:ARG:HG3	1.84	0.58
4:Q:10:ASP:HB3	4:Q:13:LEU:HD12	1.86	0.58
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.34	0.57
1:N:113[B]:LEU:CD1	1:N:117[B]:MET:CE	2.78	0.57
1:N:113[B]:LEU:HD21	1:N:117[B]:MET:HE1	1.86	0.57
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.87	0.57
2:O:56:MET:HA	26:O:304:PSC:H201	1.85	0.57
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.44	0.57
3:P:33[B]:MET:SD	25:P:309:DMU:H6	2.45	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.05	0.56
1:N:87:ILE:O	1:N:173:PRO:HD3	2.06	0.56
1:A:112:LEU:HG	28:A:932:HOH:O	2.05	0.56
3:C:30:GLY:HA2	3:C:42[B]:LEU:HB3	1.88	0.56
24:T:104:CDL:OA7	24:T:104:CDL:H331	2.05	0.56
1:A:282:PHE:HA	7:T:4:ALA:CB	2.35	0.56
9:I:31:PHE:O	9:I:32:ALA:C	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:33[B]:MET:SD	25:P:309:DMU:C22	2.90	0.55
12:Y:13:PHE:HB3	18:Y:101:TGL:HA21	1.89	0.55
2:B:183:THR:HG23	28:B:556:HOH:O	2.06	0.55
13:M:19:LEU:HD23	19:M:101:PGV:H311	1.87	0.55
3:C:156:ARG:HE	22:C:308:CHD:C24	2.20	0.55
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.89	0.55
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.54
26:E:201:PSC:H21	26:E:201:PSC:H231	1.88	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.54
9:I:33:THR:O	9:I:37:PHE:N	2.33	0.54
9:I:28:SER:O	9:I:32:ALA:N	2.31	0.54
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.89	0.54
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.89	0.54
14:A:602:HEA:HMD1	14:A:602:HEA:HBD2	1.90	0.54
2:B:87:MET:HE2	28:B:413:HOH:O	2.08	0.54
2:O:58:ALA:O	2:O:62:GLU:HG3	2.08	0.54
1:A:484:THR:HG22	28:A:933:HOH:O	2.07	0.54
19:P:303:PGV:H171	24:P:305:CDL:H651	1.89	0.54
3:C:85:LEU:HD23	3:C:88[B]:ILE:HD11	1.90	0.53
4:D:78:TRP:N	18:D:201:TGL:HB22	2.23	0.53
25:C:313:DMU:H10	10:J:49:CYS:HB3	1.90	0.53
6:S:43:LYS:HE2	6:S:88:HIS:CE1	2.43	0.53
1:A:331[B]:ASN:ND2	4:D:21:ASP:HB3	2.24	0.53
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.91	0.53
1:A:334:TRP:CZ3	18:D:201:TGL:HA52	2.44	0.53
1:A:71[B]:MET:HG3	1:A:75:ILE:HD12	1.91	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.09	0.53
1:N:273:MET:HE2	28:N:827:HOH:O	2.09	0.53
1:A:321:PHE:CD1	26:E:201:PSC:H341	2.44	0.53
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.38	0.52
2:B:58:ALA:O	2:B:62:GLU:HG3	2.09	0.52
1:N:117[A]:MET:HE2	12:Y:42:HIS:CD2	2.45	0.52
19:N:607:PGV:H322	23:T:102:PEK:H371	1.90	0.52
3:C:210:ILE:HG12	19:C:305:PGV:H132	1.90	0.52
3:C:33[B]:MET:SD	25:C:313:DMU:C22	2.76	0.52
6:F:54:ASN:HD22	6:F:54:ASN:N	2.04	0.52
6:S:67:SER:OG	20:S:103:EDO:H21	2.10	0.52
1:N:28[B]:MET:HE3	1:N:28[B]:MET:CA	2.40	0.52
1:A:297[A]:MET:HB2	28:A:780:HOH:O	2.09	0.51
1:N:76:GLY:O	1:N:80:ASN:HB2	2.09	0.51
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.93	0.51
11:X:7:PRO:HB2	11:X:12:LYS:HE3	1.91	0.51
12:Y:25:MET:HG2	18:Y:101:TGL:HA62	1.92	0.51
26:E:201:PSC:H252	26:E:201:PSC:H41	1.93	0.51
1:N:256:HIS:CE1	20:N:613:EDO:H22	2.43	0.51
1:A:28[B]:MET:HE1	13:M:26:PHE:HE2	1.76	0.51
12:L:2:HIS:CG	12:L:3:TYR:H	2.28	0.51
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.93	0.51
20:A:616:EDO:H22	28:A:715:HOH:O	2.10	0.51
7:G:3:ALA:O	7:G:4:ALA:CB	2.59	0.50
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.50
3:C:33[B]:MET:SD	25:C:313:DMU:C18	2.95	0.50
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.47	0.50
23:C:304:PEK:H132	7:G:25:LEU:HD22	1.92	0.50
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.50
3:C:210:ILE:HG21	19:C:305:PGV:H282	1.92	0.50
1:A:449[A]:MET:SD	2:B:5[A]:MET:HG2	2.52	0.50
2:B:68[B]:LEU:HD23	26:E:201:PSC:H171	1.93	0.50
7:G:1:ALA:HB2	19:P:304:PGV:H321	1.92	0.50
7:T:38:HIS:NE2	24:T:104:CDL:H111	2.26	0.50
6:F:51:SER:O	6:F:94:HIS:N	2.35	0.49
1:N:4[B]:ASN:ND2	28:N:702:HOH:O	2.44	0.49
25:P:308:DMU:H35	28:P:426:HOH:O	2.11	0.49
1:A:417[B]:MET:HE3	28:A:841:HOH:O	2.12	0.49
19:M:101:PGV:H012	19:M:101:PGV:H32	1.94	0.49
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.95	0.49
1:N:236:TRP:HH2	14:N:602:HEA:HBD1	1.77	0.49
25:P:309:DMU:H29	25:P:309:DMU:H32	1.94	0.49
1:A:76:GLY:O	1:A:80:ASN:HB2	2.13	0.49
12:L:46:LYS:O	12:L:47:LYS:HB2	2.12	0.49
3:C:51[A]:MET:SD	24:C:307:CDL:H612	2.53	0.49
1:N:177:SER:H	1:N:180:GLN:NE2	2.11	0.49
5:R:80:GLU:N	5:R:80:GLU:CD	2.64	0.49
7:T:72:ASN:H	7:T:76:ASN:ND2	2.08	0.49
3:C:155:ASP:OD2	6:F:2:SER:HA	2.13	0.49
4:D:19:ARG:NH2	28:D:302:HOH:O	2.45	0.49
1:N:309:THR:HG22	14:N:602:HEA:HMB2	1.95	0.49
24:T:104:CDL:H581	24:T:104:CDL:H762	1.95	0.49
7:T:37:LEU:HD23	24:T:104:CDL:H381	1.95	0.48
24:T:104:CDL:H542	24:T:104:CDL:C25	2.42	0.48
3:C:37:PHE:CE2	25:C:313:DMU:H13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.13	0.48
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.95	0.48
5:E:86:ILE:O	5:E:90:ARG:HG2	2.13	0.48
8:H:23:GLN:HG3	28:H:141:HOH:O	2.13	0.48
9:I:31:PHE:O	9:I:33:THR:N	2.46	0.48
3:C:248:VAL:HG22	23:T:101:PEK:H161	1.95	0.48
7:T:3:ALA:O	7:T:4:ALA:CB	2.61	0.48
1:A:177:SER:H	1:A:180:GLN:HE21	1.61	0.48
5:R:77:PRO:HA	5:R:79:LYS:HE3	1.94	0.48
3:C:160:LEU:HD13	22:C:308:CHD:H181	1.95	0.48
1:N:100[B]:MET:CE	19:N:607:PGV:H82	2.44	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
1:N:112:LEU:HD23	1:N:112:LEU:C	2.34	0.48
10:J:54:SER:O	12:L:46:LYS:HE2	2.14	0.47
12:Y:20:ARG:HD3	12:Y:20:ARG:C	2.34	0.47
25:C:313:DMU:H7	10:J:52:TRP:CE3	2.49	0.47
1:N:71[A]:MET:HB2	1:N:72:PRO:HD3	1.94	0.47
6:F:54:ASN:H	6:F:54:ASN:ND2	2.09	0.47
7:T:17:ARG:HH22	23:T:103:PEK:H041	1.79	0.47
12:Y:13:PHE:HB3	18:Y:101:TGL:CA2	2.45	0.47
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.62	0.47
4:D:19:ARG:HH21	4:D:19:ARG:CG	2.25	0.47
3:P:33[A]:MET:HE1	3:P:41:THR:HB	1.96	0.47
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.96	0.47
3:P:127:LEU:HB3	24:T:104:CDL:OB3	2.15	0.47
1:N:488:THR:HB	1:N:495:LEU:HD13	1.97	0.47
1:N:46:THR:HG21	1:N:49:GLY:HA2	1.96	0.47
2:O:126:SER:OG	28:O:401:HOH:O	2.20	0.47
1:A:136[B]:LEU:HD11	28:A:937:HOH:O	2.13	0.47
18:A:606:TGL:HA41	18:A:606:TGL:HA92	1.97	0.46
2:B:41:ILE:HG21	26:E:201:PSC:H342	1.96	0.46
7:G:37:LEU:HD22	24:G:101:CDL:H381	1.96	0.46
1:N:351:GLY:C	1:N:380:VAL:HG13	2.35	0.46
2:B:41:ILE:HD13	26:E:201:PSC:H342	1.97	0.46
7:G:72:ASN:N	7:G:76:ASN:HD22	2.02	0.46
9:I:31:PHE:CD1	9:I:31:PHE:C	2.88	0.46
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.46
22:C:308:CHD:H42	28:C:499:HOH:O	2.14	0.46
1:N:297[B]:MET:SD	1:N:302:ARG:CG	3.03	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.46
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:84:LEU:HA	2:O:87:MET:HE2	1.96	0.46
24:C:307:CDL:H191	24:C:307:CDL:H752	1.98	0.46
8:H:9:LYS:O	8:H:10:ASN:HB2	2.14	0.46
3:P:224:LYS:HE3	24:P:305:CDL:HB32	1.97	0.46
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.46	0.46
2:B:217:LYS:HG2	28:B:506:HOH:O	2.16	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.98	0.46
22:O:301:CHD:H212	22:O:301:CHD:H12	1.96	0.46
19:N:606:PGV:H011	19:N:606:PGV:H221	1.98	0.46
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.98	0.46
3:P:213:THR:HG23	24:P:305:CDL:H771	1.98	0.46
1:A:377:PHE:HA	1:A:380:VAL:HG12	1.97	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.97	0.45
3:C:107:ALA:HB2	19:C:306:PGV:H031	1.96	0.45
28:N:728:HOH:O	2:O:87:MET:SD	2.61	0.45
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.51	0.45
4:Q:109:HIS:HD2	28:Q:338:HOH:O	1.99	0.45
1:A:87:ILE:O	1:A:173:PRO:HD3	2.15	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.46	0.45
2:B:68[B]:LEU:HB3	2:B:69:PRO:HD3	1.99	0.45
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.14	0.45
26:E:201:PSC:H31	9:I:14:ALA:HB1	1.99	0.44
1:N:271:MET:HB2	20:N:617:EDO:H12	1.98	0.44
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.99	0.44
12:Y:20:ARG:NH2	18:Y:101:TGL:HC32	2.32	0.44
19:A:607:PGV:H262	19:C:305:PGV:H292	1.99	0.44
6:F:92:VAL:O	6:F:92:VAL:HG23	2.17	0.44
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.63	0.44
3:P:210:ILE:HG21	19:P:303:PGV:H282	1.98	0.44
7:T:11:TPO:HA	7:T:11:TPO:O2P	2.16	0.44
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.16	0.44
23:T:102:PEK:H32	23:T:102:PEK:H71	1.98	0.44
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.00	0.44
1:N:297[B]:MET:HG3	1:N:302:ARG:CG	2.43	0.44
1:A:486:ASP:OD2	4:D:19:ARG:HD2	2.18	0.44
1:N:169:ILE:HG13	1:N:189[A]:MET:CE	2.48	0.44
2:O:52:HIS:HE1	26:O:304:PSC:H211	1.82	0.44
9:V:31:PHE:O	9:V:34:PHE:N	2.46	0.44
2:B:83:ILE:HA	2:B:86[B]:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:LYS:O	12:L:47:LYS:CB	2.66	0.43
26:O:304:PSC:H251	26:O:304:PSC:H222	1.56	0.43
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.52	0.43
1:A:273:MET:HE2	28:A:725:HOH:O	2.18	0.43
2:B:56:MET:HB3	26:E:201:PSC:H222	2.00	0.43
7:G:84:LYS:HD2	7:G:84:LYS:N	2.10	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.92	0.43
1:A:196:LEU:HD21	3:C:88[B]:ILE:HG13	2.00	0.43
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.01	0.43
24:C:307:CDL:OA5	24:C:307:CDL:HB22	2.18	0.43
1:A:169:ILE:HD11	1:A:189[A]:MET:HE3	2.01	0.43
2:B:60:GLU:CD	2:B:60:GLU:H	2.21	0.43
23:C:303:PEK:H11	23:C:303:PEK:H172	2.00	0.43
3:P:217:VAL:HG22	24:P:305:CDL:H732	2.00	0.43
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.47	0.43
10:J:32:TYR:CZ	10:J:36[B]:MET:HG3	2.54	0.43
1:N:378:HIS:O	1:N:382:SER:HB2	2.19	0.43
1:N:331[B]:ASN:ND2	4:Q:21:ASP:HB3	2.33	0.43
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.81	0.43
3:C:131:LEU:HD21	24:G:101:CDL:H521	2.00	0.43
1:N:164:PHE:HE2	20:N:615:EDO:H21	1.84	0.43
2:O:68[B]:LEU:HB3	2:O:69:PRO:HD3	2.00	0.43
2:O:116:LEU:HD12	2:O:117:SER:N	2.33	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
18:A:606:TGL:HA82	18:A:606:TGL:H142	2.00	0.43
1:A:71[B]:MET:HB2	1:A:71[B]:MET:HE3	1.96	0.43
2:B:183:THR:HG22	28:B:428:HOH:O	2.19	0.43
8:H:9:LYS:O	8:H:10:ASN:CB	2.67	0.43
3:C:224:LYS:CD	24:C:307:CDL:HB31	2.49	0.42
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.42	0.42
2:O:7:LEU:HD11	18:O:302:TGL:H191	2.01	0.42
6:S:54:ASN:HD22	6:S:54:ASN:C	2.22	0.42
19:A:607:PGV:H183	23:C:303:PEK:H322	2.01	0.42
3:C:158:HIS:CE1	6:F:2:SER:H	2.36	0.42
1:N:173:PRO:HD2	1:N:176[B]:MET:HE2	2.01	0.42
3:C:158:HIS:HE1	6:F:2:SER:H	1.67	0.42
5:E:18:TYR:CE2	20:E:202:EDO:H22	2.54	0.42
24:G:101:CDL:H212	24:G:101:CDL:H511	2.01	0.42
1:N:187:SER:HB3	1:N:277[B]:MET:CE	2.50	0.42
24:G:101:CDL:H361	2:O:78:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42
1:N:489:THR:HA	6:S:71:TRP:O	2.19	0.42
12:L:26:THR:HG23	13:M:25:SER:CB	2.49	0.42
22:W:101:CHD:H183	22:W:101:CHD:H222	2.02	0.42
13:M:34:LEU:HA	13:M:37[A]:LEU:HG	2.02	0.42
3:C:55:TYR:HA	24:C:307:CDL:H551	2.02	0.42
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.02	0.42
3:P:103:HIS:ND1	22:P:301:CHD:O25	2.53	0.42
3:C:246:ASP:HB2	28:C:481:HOH:O	2.19	0.42
23:C:304:PEK:H041	7:G:17:ARG:HH22	1.84	0.42
1:N:187:SER:HB3	1:N:277[B]:MET:HE1	2.01	0.42
26:E:201:PSC:H042	26:E:201:PSC:H062	1.80	0.42
1:A:197:LEU:HD21	7:T:2:SER:HB2	2.02	0.42
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.55	0.42
18:L:101:TGL:H231	18:L:101:TGL:H202	1.84	0.42
1:N:180:GLN:HB2	1:N:180:GLN:HE21	1.69	0.42
1:N:169:ILE:HG13	1:N:189[A]:MET:HE1	2.02	0.42
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.20	0.42
1:N:309:THR:CG2	14:N:602:HEA:HMB2	2.50	0.42
1:A:169:ILE:CD1	1:A:189[A]:MET:HE3	2.50	0.42
1:A:309:THR:CG2	14:A:602:HEA:HMB2	2.50	0.42
28:B:455:HOH:O	24:T:104:CDL:H332	2.20	0.42
1:A:346[A]:PHE:HZ	18:A:606:TGL:H122	1.85	0.41
1:A:236:TRP:HH2	14:A:602:HEA:HBD1	1.85	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.02	0.41
1:A:417[B]:MET:CE	28:A:841:HOH:O	2.68	0.41
1:A:514:LYS:HE2	28:F:220:HOH:O	2.19	0.41
20:A:608:EDO:H22	6:F:32:ASN:HD21	1.84	0.41
1:N:494:TRP:CH2	20:N:608:EDO:H12	2.55	0.41
20:D:202:EDO:C2	5:E:30:ARG:HH21	2.33	0.41
3:P:67:PHE:CE2	24:P:305:CDL:H1	2.32	0.41
3:C:85:LEU:HA	3:C:88[B]:ILE:HG12	2.01	0.41
5:R:108:LYS:HA	5:R:108:LYS:HD3	1.78	0.41
1:A:468:MET:HG3	20:A:611:EDO:O1	2.19	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.56	0.41
24:T:104:CDL:H541	24:T:104:CDL:H712	2.02	0.41
11:K:6:ALA:HA	11:K:7:PRO:HD3	1.96	0.41
11:X:52:GLU:HG2	28:X:103:HOH:O	2.20	0.41
28:A:814:HOH:O	4:D:100:LYS:HD3	2.19	0.41
1:N:407:ASP:O	1:N:411:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:449:MET:SD	2:O:5:MET:HG2	2.60	0.41
26:O:304:PSC:H063	26:O:304:PSC:H042	1.85	0.41
3:P:156:ARG:HH21	22:P:306:CHD:C24	2.34	0.41
1:A:378:HIS:HA	1:A:382:SER:HB2	2.03	0.41
1:A:44:PRO:HG3	4:D:111:PHE:CZ	2.56	0.41
3:P:51[B]:MET:HE2	3:P:51[B]:MET:HB2	1.83	0.41
20:N:614:EDO:H11	28:N:884:HOH:O	2.21	0.41
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.90	0.41
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.03	0.41
3:P:33[B]:MET:HG3	3:P:42:LEU:HD12	2.02	0.41
12:Y:26:THR:HG23	13:Z:25:SER:HB2	2.03	0.41
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.03	0.40
11:K:8:ASP:HB2	28:K:117:HOH:O	2.20	0.40
1:N:148:PHE:HB3	3:P:28:THR:HB	2.02	0.40
1:N:390:MET:O	1:N:394[A]:VAL:HG22	2.21	0.40
9:I:73:LYS:HD3	9:I:73:LYS:HA	1.90	0.40
9:V:32:ALA:O	9:V:36:LYS:HB2	2.20	0.40
1:N:117[A]:MET:CE	12:Y:42:HIS:CD2	3.04	0.40
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.19	0.40
18:Y:101:TGL:H202	18:Y:101:TGL:H231	1.95	0.40
24:G:101:CDL:H751	24:G:101:CDL:H561	2.03	0.40
12:L:26:THR:HG23	13:M:25:SER:HB3	2.04	0.40
1:N:113[B]:LEU:HD11	1:N:117[B]:MET:CE	2.50	0.40
3:P:131:LEU:HD11	24:T:104:CDL:H561	2.04	0.40
22:P:301:CHD:H212	22:P:301:CHD:H12	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	532/514 (104%)	520 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	533/514 (104%)	520 (98%)	13 (2%)	0	100	100
2	B	232/227 (102%)	227 (98%)	4 (2%)	1 (0%)	38	33
2	O	231/227 (102%)	225 (97%)	5 (2%)	1 (0%)	38	33
3	C	270/260 (104%)	263 (97%)	6 (2%)	1 (0%)	38	33
3	P	269/260 (104%)	262 (97%)	7 (3%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	25	18
5	E	104/109 (95%)	103 (99%)	0	1 (1%)	18	10
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
6	S	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
7	G	81/85 (95%)	71 (88%)	6 (7%)	4 (5%)	2	0
7	T	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	2	0
8	H	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	14	7
8	U	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
9	I	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	13	6
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
10	W	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	8	3
13	M	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
13	Z	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
All	All	3586/3604 (100%)	3478 (97%)	91 (2%)	17 (0%)	32	26

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	237	ALA
7	G	4	ALA
7	G	8	HIS

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Mol	Chain	Res	Type
4	Q	8	SER
7	T	4	ALA
7	G	5	LYS
7	T	8	HIS
5	E	6	GLU
7	T	5	LYS
7	T	7	ASP
9	I	32	ALA
12	Y	46	LYS
8	H	8	ILE
2	O	92	ASN
2	B	92	ASN
7	G	9	GLY
7	T	6	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/426 (105%)	439 (98%)	7 (2%)	68	72
1	N	447/426 (105%)	441 (99%)	6 (1%)	73	78
2	B	217/210 (103%)	208 (96%)	9 (4%)	35	31
2	O	216/210 (103%)	207 (96%)	9 (4%)	34	30
3	C	237/225 (105%)	234 (99%)	3 (1%)	73	78
3	P	236/225 (105%)	233 (99%)	3 (1%)	73	78
4	D	128/129 (99%)	127 (99%)	1 (1%)	85	88
4	Q	128/129 (99%)	125 (98%)	3 (2%)	56	58
5	E	93/95 (98%)	91 (98%)	2 (2%)	57	60
5	R	93/95 (98%)	91 (98%)	2 (2%)	57	60
6	F	79/78 (101%)	77 (98%)	2 (2%)	53	54
6	S	79/78 (101%)	74 (94%)	5 (6%)	21	15
7	G	67/68 (98%)	60 (90%)	7 (10%)	8	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	63 (94%)	4 (6%)	22	17
8	H	71/75 (95%)	69 (97%)	2 (3%)	49	49
8	U	71/75 (95%)	66 (93%)	5 (7%)	18	12
9	I	57/57 (100%)	54 (95%)	3 (5%)	26	21
9	V	57/57 (100%)	56 (98%)	1 (2%)	64	68
10	J	51/50 (102%)	51 (100%)	0	100	100
10	W	51/50 (102%)	50 (98%)	1 (2%)	60	64
11	K	39/46 (85%)	38 (97%)	1 (3%)	51	52
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	40/40 (100%)	39 (98%)	1 (2%)	53	54
13	M	38/38 (100%)	38 (100%)	0	100	100
13	Z	38/38 (100%)	38 (100%)	0	100	100
All	All	3124/3074 (102%)	3047 (98%)	77 (2%)	53	54

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35[A]	LEU
1	A	35[B]	LEU
1	A	38	ARG
1	A	109	PHE
1	A	180	GLN
1	A	338	MET
1	A	369	ASP
2	B	33	LEU
2	B	42	ILE
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE

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Mol	Chain	Res	Type
4	D	19	ARG
5	E	70	VAL
5	E	90	ARG
6	F	54	ASN
6	F	80	GLN
7	G	2	SER
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	60	TYR
9	I	15	ARG
9	I	25	PHE
9	I	33	THR
11	K	54	ARG
1	N	109	PHE
1	N	180	GLN
1	N	369	ASP
1	N	380	VAL
1	N	381	LEU
1	N	485	VAL
2	O	33	LEU
2	O	60	GLU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	171	LYS
2	O	202	SER
2	O	226	MET
2	O	227	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	5	VAL
4	Q	6	VAL
4	Q	10	ASP
5	R	79	LYS
5	R	80	GLU
6	S	43	LYS

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Mol	Chain	Res	Type
6	S	54	ASN
6	S	80	GLN
6	S	87	THR
6	S	94	HIS
7	T	2	SER
7	T	8	HIS
7	T	18	PHE
7	T	54	ARG
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	50	VAL
8	U	60	TYR
9	V	73	LYS
10	W	50	LEU
12	Y	20	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	52	HIS
2	B	59	GLN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
3	C	149	HIS
4	D	37	GLN
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
1	N	180	GLN
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN

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Mol	Chain	Res	Type
2	O	203	ASN
3	P	3	HIS
3	P	68	GLN
3	P	149	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN
10	W	29	ASN
11	X	35	GLN
12	Y	42	HIS
13	Z	39	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z  > 2$
1	FME	A	1	1	9,9,10	0.56	0	7,9,11	1.40	1 (14%)
2	FME	B	1	2	9,9,10	0.72	0	7,9,11	1.67	2 (28%)
7	TPO	G	11	7	9,10,11	1.27	1 (11%)	10,14,16	0.87	0
9	SAC	I	1	9	8,8,9	1.86	2 (25%)	6,9,11	0.97	0
1	FME	N	1	1	9,9,10	0.50	0	7,9,11	1.20	1 (14%)
2	FME	O	1	2	9,9,10	0.61	0	7,9,11	1.24	1 (14%)
7	TPO	T	11	7	9,10,11	1.33	1 (11%)	10,14,16	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SAC	V	1	9	8,8,9	1.95	2 (25%)	6,9,11	1.28	1 (16%)

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
1	FME	A	1	1	-	0/6/9/11	0/0/0/0
2	FME	B	1	2	-	0/6/9/11	0/0/0/0
7	TPO	G	11	7	-	1/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	0/6/9/11	0/0/0/0
2	FME	O	1	2	-	0/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	2.23	1.49	1.46
7	T	11	TPO	P-O1P	2.55	1.59	1.50
7	G	11	TPO	P-O1P	2.59	1.59	1.50
9	V	1	SAC	CA-N	2.82	1.50	1.46
9	V	1	SAC	OAC-C1A	4.41	1.33	1.23
9	I	1	SAC	OAC-C1A	4.45	1.33	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CB-CA-C	-2.61	107.35	111.65
1	N	1	FME	O-C-CA	-2.50	119.32	125.15
2	B	1	FME	O-C-CA	-2.48	119.36	125.15
1	A	1	FME	O-C-CA	-2.44	119.45	125.15
2	O	1	FME	O-C-CA	-2.27	119.85	125.15
9	V	1	SAC	O-C-CA	-2.01	120.46	125.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	OG1-CB-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 10 are monoatomic - leaving 79 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	$\# Z  > 2$
14	HEA	A	601	1	44,67,67	1.06	4 (9%)	37,103,103	1.86	14 (37%)
14	HEA	A	602	1	44,67,67	0.99	3 (6%)	37,103,103	1.27	7 (18%)
18	TGL	A	606	-	62,62,62	1.24	6 (9%)	65,65,65	1.47	8 (12%)
19	PGV	A	607	-	50,50,50	0.87	2 (4%)	51,56,56	0.95	3 (5%)
20	EDO	A	608	-	3,3,3	0.42	0	2,2,2	0.42	0
20	EDO	A	609	-	3,3,3	0.55	0	2,2,2	0.54	0
20	EDO	A	610	-	3,3,3	0.46	0	2,2,2	0.52	0
20	EDO	A	611	-	3,3,3	0.42	0	2,2,2	0.32	0
20	EDO	A	612	-	3,3,3	0.52	0	2,2,2	0.44	0
20	EDO	A	613	-	3,3,3	0.50	0	2,2,2	0.49	0
20	EDO	A	614	-	3,3,3	0.36	0	2,2,2	0.43	0
20	EDO	A	615	-	3,3,3	0.41	0	2,2,2	0.46	0
20	EDO	A	616	-	3,3,3	0.42	0	2,2,2	0.20	0
21	CUA	B	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	B	302	-	29,32,32	0.62	0	47,51,51	1.06	2 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	B	303	-	3,3,3	0.40	0	2,2,2	0.42	0
22	CHD	C	301	-	29,32,32	0.59	0	47,51,51	0.92	1 (2%)
23	PEK	C	303	-	52,52,52	0.82	2 (3%)	54,57,57	0.93	3 (5%)
23	PEK	C	304	-	52,52,52	0.95	2 (3%)	54,57,57	1.00	2 (3%)
19	PGV	C	305	-	50,50,50	0.84	2 (4%)	51,56,56	0.84	2 (3%)
19	PGV	C	306	-	50,50,50	0.94	2 (4%)	51,56,56	1.01	2 (3%)
24	CDL	C	307	-	99,99,99	1.31	12 (12%)	101,111,111	1.14	4 (3%)
22	CHD	C	308	-	29,32,32	0.52	0	47,51,51	1.56	10 (21%)
20	EDO	C	309	-	3,3,3	0.46	0	2,2,2	0.34	0
20	EDO	C	310	-	3,3,3	0.48	0	2,2,2	0.38	0
20	EDO	C	311	-	3,3,3	0.57	0	2,2,2	0.26	0
25	DMU	C	312	-	34,34,34	0.56	1 (2%)	45,45,45	1.31	5 (11%)
25	DMU	C	313	-	34,34,34	0.59	1 (2%)	45,45,45	1.09	3 (6%)
18	TGL	D	201	-	62,62,62	1.24	6 (9%)	65,65,65	1.01	4 (6%)
20	EDO	D	202	-	3,3,3	0.50	0	2,2,2	0.27	0
20	EDO	D	203	-	3,3,3	0.49	0	2,2,2	0.42	0
26	PSC	E	201	-	51,51,51	1.10	3 (5%)	56,59,59	1.08	3 (5%)
20	EDO	E	202	-	3,3,3	0.42	0	2,2,2	0.35	0
20	EDO	F	102	-	3,3,3	0.41	0	2,2,2	0.46	0
20	EDO	F	103	-	3,3,3	0.60	0	2,2,2	0.44	0
20	EDO	F	104	-	3,3,3	0.47	0	2,2,2	0.50	0
24	CDL	G	101	-	99,99,99	1.30	12 (12%)	101,111,111	1.11	6 (5%)
23	PEK	G	102	-	52,52,52	0.93	2 (3%)	54,57,57	1.02	2 (3%)
22	CHD	J	101	-	29,32,32	0.48	0	47,51,51	1.61	8 (17%)
18	TGL	L	101	-	62,62,62	1.25	6 (9%)	65,65,65	1.09	4 (6%)
19	PGV	M	101	-	50,50,50	0.96	2 (4%)	51,56,56	1.05	3 (5%)
25	DMU	M	102	-	34,34,34	0.47	0	45,45,45	0.72	0
14	HEA	N	601	1	44,67,67	1.04	3 (6%)	37,103,103	1.65	10 (27%)
14	HEA	N	602	1	44,67,67	1.00	3 (6%)	37,103,103	1.48	7 (18%)
19	PGV	N	606	-	50,50,50	0.96	2 (4%)	51,56,56	1.02	2 (3%)
19	PGV	N	607	-	50,50,50	0.88	2 (4%)	51,56,56	0.89	2 (3%)
20	EDO	N	608	-	3,3,3	0.51	0	2,2,2	0.26	0
20	EDO	N	609	-	3,3,3	0.40	0	2,2,2	0.45	0
20	EDO	N	610	-	3,3,3	0.47	0	2,2,2	0.40	0
20	EDO	N	611	-	3,3,3	0.42	0	2,2,2	0.28	0
20	EDO	N	612	-	3,3,3	0.57	0	2,2,2	0.20	0
20	EDO	N	613	-	3,3,3	0.35	0	2,2,2	0.63	0
20	EDO	N	614	-	3,3,3	0.47	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	N	615	-	3,3,3	0.38	0	2,2,2	0.43	0
20	EDO	N	616	-	3,3,3	0.46	0	2,2,2	0.35	0
20	EDO	N	617	-	3,3,3	0.41	0	2,2,2	0.44	0
22	CHD	O	301	-	29,32,32	0.57	0	47,51,51	1.16	4 (8%)
18	TGL	O	302	-	62,62,62	1.24	6 (9%)	65,65,65	1.14	3 (4%)
21	CUA	O	303	2	0,1,1	0.00	-	0,0,0	0.00	-
26	PSC	O	304	-	51,51,51	1.11	3 (5%)	56,59,59	1.08	3 (5%)
22	CHD	P	301	-	29,32,32	0.56	0	47,51,51	0.95	2 (4%)
19	PGV	P	303	-	50,50,50	0.89	2 (4%)	51,56,56	0.86	3 (5%)
19	PGV	P	304	-	50,50,50	0.96	2 (4%)	51,56,56	0.97	2 (3%)
24	CDL	P	305	-	99,99,99	1.30	12 (12%)	101,111,111	1.15	7 (6%)
22	CHD	P	306	-	29,32,32	0.48	0	47,51,51	1.68	12 (25%)
20	EDO	P	307	-	3,3,3	0.46	0	2,2,2	0.35	0
25	DMU	P	308	-	34,34,34	0.59	1 (2%)	45,45,45	1.04	2 (4%)
25	DMU	P	309	-	34,34,34	0.59	1 (2%)	45,45,45	0.88	1 (2%)
18	TGL	Q	201	-	62,62,62	1.24	6 (9%)	65,65,65	1.14	6 (9%)
20	EDO	R	201	-	3,3,3	0.52	0	2,2,2	0.44	0
20	EDO	S	102	-	3,3,3	0.46	0	2,2,2	0.42	0
20	EDO	S	103	-	3,3,3	0.48	0	2,2,2	0.15	0
23	PEK	T	101	-	52,52,52	0.93	2 (3%)	54,57,57	0.99	2 (3%)
23	PEK	T	102	-	52,52,52	0.88	2 (3%)	54,57,57	0.91	3 (5%)
23	PEK	T	103	-	52,52,52	0.95	2 (3%)	54,57,57	0.94	3 (5%)
24	CDL	T	104	-	99,99,99	1.30	12 (12%)	101,111,111	1.14	5 (4%)
22	CHD	W	101	-	29,32,32	0.47	0	47,51,51	1.51	7 (14%)
18	TGL	Y	101	-	62,62,62	1.24	6 (9%)	65,65,65	1.05	3 (4%)
25	DMU	Z	101	-	34,34,34	0.46	0	45,45,45	0.75	2 (4%)

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
14	HEA	A	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1	2/2/7/16	0/24/76/76	0/0/8/8
18	TGL	A	606	-	-	0/65/65/65	0/0/0/0
19	PGV	A	607	-	-	0/55/55/55	0/0/0/0
20	EDO	A	608	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	609	-	-	0/1/1/1	0/0/0/0
20	EDO	A	610	-	-	0/1/1/1	0/0/0/0
20	EDO	A	611	-	-	0/1/1/1	0/0/0/0
20	EDO	A	612	-	-	0/1/1/1	0/0/0/0
20	EDO	A	613	-	-	0/1/1/1	0/0/0/0
20	EDO	A	614	-	-	0/1/1/1	0/0/0/0
20	EDO	A	615	-	-	0/1/1/1	0/0/0/0
20	EDO	A	616	-	-	0/1/1/1	0/0/0/0
21	CUA	B	301	2	-	0/0/0/0	0/0/0/0
22	CHD	B	302	-	-	0/7/74/74	0/4/4/4
20	EDO	B	303	-	-	0/1/1/1	0/0/0/0
22	CHD	C	301	-	-	0/7/74/74	0/4/4/4
23	PEK	C	303	-	-	0/56/56/56	0/0/0/0
23	PEK	C	304	-	-	0/56/56/56	0/0/0/0
19	PGV	C	305	-	-	0/55/55/55	0/0/0/0
19	PGV	C	306	-	-	0/55/55/55	0/0/0/0
24	CDL	C	307	-	-	0/110/110/110	0/0/0/0
22	CHD	C	308	-	-	0/7/74/74	0/4/4/4
20	EDO	C	309	-	-	0/1/1/1	0/0/0/0
20	EDO	C	310	-	-	0/1/1/1	0/0/0/0
20	EDO	C	311	-	-	0/1/1/1	0/0/0/0
25	DMU	C	312	-	-	0/19/59/59	0/2/2/2
25	DMU	C	313	-	-	0/19/59/59	0/2/2/2
18	TGL	D	201	-	-	0/65/65/65	0/0/0/0
20	EDO	D	202	-	-	0/1/1/1	0/0/0/0
20	EDO	D	203	-	-	0/1/1/1	0/0/0/0
26	PSC	E	201	-	-	0/55/55/55	0/0/0/0
20	EDO	E	202	-	-	0/1/1/1	0/0/0/0
20	EDO	F	102	-	-	0/1/1/1	0/0/0/0
20	EDO	F	103	-	-	0/1/1/1	0/0/0/0
20	EDO	F	104	-	-	0/1/1/1	0/0/0/0
24	CDL	G	101	-	-	0/110/110/110	0/0/0/0
23	PEK	G	102	-	-	0/56/56/56	0/0/0/0
22	CHD	J	101	-	-	0/7/74/74	0/4/4/4
18	TGL	L	101	-	-	0/65/65/65	0/0/0/0
19	PGV	M	101	-	-	0/55/55/55	0/0/0/0
25	DMU	M	102	-	-	0/19/59/59	0/2/2/2
14	HEA	N	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1	2/2/7/16	0/24/76/76	0/0/8/8
19	PGV	N	606	-	-	0/55/55/55	0/0/0/0
19	PGV	N	607	-	-	0/55/55/55	0/0/0/0
20	EDO	N	608	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	609	-	-	0/1/1/1	0/0/0/0
20	EDO	N	610	-	-	0/1/1/1	0/0/0/0
20	EDO	N	611	-	-	0/1/1/1	0/0/0/0
20	EDO	N	612	-	-	0/1/1/1	0/0/0/0
20	EDO	N	613	-	-	0/1/1/1	0/0/0/0
20	EDO	N	614	-	-	0/1/1/1	0/0/0/0
20	EDO	N	615	-	-	0/1/1/1	0/0/0/0
20	EDO	N	616	-	-	0/1/1/1	0/0/0/0
20	EDO	N	617	-	-	0/1/1/1	0/0/0/0
22	CHD	O	301	-	-	0/7/74/74	0/4/4/4
18	TGL	O	302	-	-	0/65/65/65	0/0/0/0
21	CUA	O	303	2	-	0/0/0/0	0/0/0/0
26	PSC	O	304	-	-	0/55/55/55	0/0/0/0
22	CHD	P	301	-	-	0/7/74/74	0/4/4/4
19	PGV	P	303	-	-	0/55/55/55	0/0/0/0
19	PGV	P	304	-	-	0/55/55/55	0/0/0/0
24	CDL	P	305	-	-	0/110/110/110	0/0/0/0
22	CHD	P	306	-	-	0/7/74/74	0/4/4/4
20	EDO	P	307	-	-	0/1/1/1	0/0/0/0
25	DMU	P	308	-	-	0/19/59/59	0/2/2/2
25	DMU	P	309	-	-	0/19/59/59	0/2/2/2
18	TGL	Q	201	-	-	0/65/65/65	0/0/0/0
20	EDO	R	201	-	-	0/1/1/1	0/0/0/0
20	EDO	S	102	-	-	0/1/1/1	0/0/0/0
20	EDO	S	103	-	-	0/1/1/1	0/0/0/0
23	PEK	T	101	-	-	0/56/56/56	0/0/0/0
23	PEK	T	102	-	-	0/56/56/56	0/0/0/0
23	PEK	T	103	-	-	0/56/56/56	0/0/0/0
24	CDL	T	104	-	-	0/110/110/110	0/0/0/0
22	CHD	W	101	-	-	0/7/74/74	0/4/4/4
18	TGL	Y	101	-	-	0/65/65/65	0/0/0/0
25	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	101	TGL	C20-CA9	-3.25	1.33	1.51
18	L	101	TGL	C20-CA9	-3.22	1.33	1.51
24	T	104	CDL	C62-C61	-3.18	1.33	1.51
24	C	307	CDL	C59-C58	-3.18	1.33	1.51
18	L	101	TGL	C10-CB9	-3.17	1.33	1.51
24	G	101	CDL	C22-C21	-3.17	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	101	CDL	C19-C18	-3.17	1.33	1.51
24	P	305	CDL	C22-C21	-3.16	1.33	1.51
24	T	104	CDL	C19-C18	-3.16	1.33	1.51
18	O	302	TGL	C20-CA9	-3.15	1.33	1.51
24	P	305	CDL	C59-C58	-3.15	1.33	1.51
24	T	104	CDL	C22-C21	-3.15	1.33	1.51
24	C	307	CDL	C62-C61	-3.15	1.33	1.51
24	T	104	CDL	C59-C58	-3.15	1.33	1.51
24	C	307	CDL	C82-C81	-3.14	1.33	1.51
24	P	305	CDL	C19-C18	-3.14	1.33	1.51
18	O	302	TGL	C15-CC9	-3.14	1.33	1.51
18	Y	101	TGL	C15-CC9	-3.14	1.33	1.51
24	C	307	CDL	C79-C78	-3.14	1.33	1.51
24	P	305	CDL	C42-C41	-3.13	1.33	1.51
24	G	101	CDL	C39-C38	-3.13	1.33	1.51
18	Y	101	TGL	C10-CB9	-3.13	1.33	1.51
24	T	104	CDL	C42-C41	-3.13	1.33	1.51
24	T	104	CDL	C39-C38	-3.13	1.33	1.51
24	C	307	CDL	C22-C21	-3.12	1.33	1.51
18	A	606	TGL	C20-CA9	-3.12	1.33	1.51
24	T	104	CDL	C79-C78	-3.11	1.33	1.51
18	Q	201	TGL	C10-CB9	-3.11	1.33	1.51
24	C	307	CDL	C19-C18	-3.11	1.33	1.51
24	P	305	CDL	C62-C61	-3.11	1.33	1.51
24	G	101	CDL	C62-C61	-3.10	1.33	1.51
18	A	606	TGL	C10-CB9	-3.10	1.33	1.51
24	G	101	CDL	C59-C58	-3.10	1.33	1.51
24	G	101	CDL	C42-C41	-3.10	1.33	1.51
24	P	305	CDL	C79-C78	-3.10	1.33	1.51
18	O	302	TGL	C10-CB9	-3.10	1.33	1.51
24	C	307	CDL	C42-C41	-3.10	1.33	1.51
18	A	606	TGL	C15-CC9	-3.09	1.33	1.51
18	D	201	TGL	C10-CB9	-3.09	1.34	1.51
18	D	201	TGL	C15-CC9	-3.09	1.34	1.51
18	L	101	TGL	C15-CC9	-3.09	1.34	1.51
24	P	305	CDL	C82-C81	-3.08	1.34	1.51
24	P	305	CDL	C39-C38	-3.08	1.34	1.51
24	G	101	CDL	C79-C78	-3.06	1.34	1.51
18	Q	201	TGL	C20-CA9	-3.06	1.34	1.51
24	G	101	CDL	C82-C81	-3.06	1.34	1.51
24	T	104	CDL	C82-C81	-3.05	1.34	1.51
18	D	201	TGL	C20-CA9	-3.05	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	201	TGL	C15-CC9	-3.05	1.34	1.51
24	C	307	CDL	C39-C38	-3.02	1.34	1.51
14	A	602	HEA	C4A-NA	-2.62	1.33	1.36
14	N	601	HEA	C1A-NA	-2.35	1.34	1.36
14	A	601	HEA	C1D-ND	-2.35	1.34	1.36
14	A	601	HEA	C4A-NA	-2.24	1.34	1.36
14	A	601	HEA	C1A-NA	-2.08	1.34	1.36
14	N	602	HEA	C4B-NB	-2.05	1.34	1.36
14	N	601	HEA	C4A-NA	-2.03	1.34	1.36
14	N	602	HEA	C4A-NA	-2.01	1.34	1.36
14	N	601	HEA	O11-C11	2.00	1.47	1.42
14	A	602	HEA	C4C-CHD	2.04	1.45	1.40
14	A	602	HEA	O11-C11	2.05	1.47	1.42
14	N	602	HEA	C4C-CHD	2.18	1.45	1.40
14	A	601	HEA	O11-C11	2.20	1.48	1.42
25	P	309	DMU	O16-C6	2.20	1.44	1.40
25	C	312	DMU	O16-C6	2.27	1.44	1.40
25	P	308	DMU	O16-C6	2.36	1.44	1.40
25	C	313	DMU	O16-C6	2.46	1.44	1.40
19	A	607	PGV	O01-C1	3.29	1.43	1.34
19	N	607	PGV	O01-C1	3.30	1.43	1.34
19	C	305	PGV	O01-C1	3.44	1.44	1.34
23	C	303	PEK	O03-C21	3.60	1.43	1.33
23	T	102	PEK	O01-C1	3.63	1.44	1.34
23	C	303	PEK	O01-C1	3.67	1.44	1.34
19	P	303	PGV	O01-C1	3.68	1.45	1.34
26	E	201	PSC	C13-C12	3.78	1.52	1.31
19	C	305	PGV	O03-C19	3.79	1.44	1.33
26	O	304	PSC	C13-C12	3.81	1.53	1.31
19	P	303	PGV	O03-C19	3.85	1.44	1.33
18	D	201	TGL	OG2-CB1	3.94	1.45	1.34
23	T	102	PEK	O03-C21	4.03	1.45	1.33
18	Y	101	TGL	OG1-CA1	4.10	1.45	1.33
24	P	305	CDL	OB6-CB5	4.11	1.46	1.34
24	P	305	CDL	OA6-CA5	4.14	1.46	1.34
24	G	101	CDL	OA6-CA5	4.15	1.46	1.34
24	T	104	CDL	OA6-CA5	4.17	1.46	1.34
24	C	307	CDL	OA6-CA5	4.19	1.46	1.34
19	M	101	PGV	O01-C1	4.20	1.46	1.34
26	O	304	PSC	O01-C1	4.22	1.46	1.34
23	G	102	PEK	O01-C1	4.22	1.46	1.34
24	C	307	CDL	OB6-CB5	4.23	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	607	PGV	O03-C19	4.23	1.45	1.33
19	N	606	PGV	O01-C1	4.23	1.46	1.34
19	C	306	PGV	O03-C19	4.24	1.45	1.33
23	T	101	PEK	O01-C1	4.25	1.46	1.34
19	P	304	PGV	O01-C1	4.26	1.46	1.34
18	L	101	TGL	OG3-CC1	4.27	1.45	1.33
19	N	607	PGV	O03-C19	4.28	1.45	1.33
24	T	104	CDL	OA8-CA7	4.29	1.46	1.33
19	C	306	PGV	O01-C1	4.30	1.46	1.34
26	E	201	PSC	O01-C1	4.33	1.46	1.34
26	E	201	PSC	O03-C19	4.33	1.46	1.33
23	T	103	PEK	O01-C1	4.33	1.46	1.34
23	G	102	PEK	O03-C21	4.34	1.46	1.33
18	O	302	TGL	OG3-CC1	4.35	1.46	1.33
24	T	104	CDL	OB6-CB5	4.36	1.46	1.34
24	G	101	CDL	OA8-CA7	4.36	1.46	1.33
18	Q	201	TGL	OG1-CA1	4.36	1.46	1.33
23	C	304	PEK	O01-C1	4.37	1.47	1.34
24	G	101	CDL	OB6-CB5	4.37	1.47	1.34
18	A	606	TGL	OG3-CC1	4.38	1.46	1.33
23	T	101	PEK	O03-C21	4.39	1.46	1.33
18	A	606	TGL	OG1-CA1	4.41	1.46	1.33
23	T	103	PEK	O03-C21	4.42	1.46	1.33
18	Y	101	TGL	OG2-CB1	4.43	1.47	1.34
18	O	302	TGL	OG2-CB1	4.43	1.47	1.34
26	O	304	PSC	O03-C19	4.43	1.46	1.33
18	Q	201	TGL	OG3-CC1	4.44	1.46	1.33
19	P	304	PGV	O03-C19	4.44	1.46	1.33
18	O	302	TGL	OG1-CA1	4.44	1.46	1.33
18	Q	201	TGL	OG2-CB1	4.44	1.47	1.34
18	D	201	TGL	OG3-CC1	4.45	1.46	1.33
23	C	304	PEK	O03-C21	4.45	1.46	1.33
24	P	305	CDL	OB8-CB7	4.47	1.46	1.33
18	Y	101	TGL	OG3-CC1	4.47	1.46	1.33
19	M	101	PGV	O03-C19	4.47	1.46	1.33
18	L	101	TGL	OG2-CB1	4.47	1.47	1.34
24	G	101	CDL	OB8-CB7	4.49	1.46	1.33
24	T	104	CDL	OB8-CB7	4.50	1.46	1.33
19	N	606	PGV	O03-C19	4.50	1.46	1.33
18	L	101	TGL	OG1-CA1	4.51	1.46	1.33
18	A	606	TGL	OG2-CB1	4.53	1.47	1.34
24	P	305	CDL	OA8-CA7	4.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	307	CDL	OB8-CB7	4.57	1.46	1.33
24	C	307	CDL	OA8-CA7	4.59	1.46	1.33
18	D	201	TGL	OG1-CA1	4.70	1.47	1.33

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C17-C13-C14	-4.92	95.08	100.08
22	W	101	CHD	C17-C13-C14	-3.95	96.06	100.08
22	C	308	CHD	C23-C22-C20	-3.78	109.63	114.72
14	N	601	HEA	CAA-CBA-CGA	-3.65	106.43	112.66
14	N	602	HEA	CAD-CBD-CGD	-3.59	106.52	112.66
14	A	601	HEA	C13-C12-C11	-3.35	109.39	114.46
14	N	602	HEA	OMA-CMA-C3A	-3.31	117.46	125.08
25	C	312	DMU	C6-O5-C4	-3.17	107.75	113.72
18	A	606	TGL	OG3-CC1-OC1	-3.13	115.77	123.55
14	A	601	HEA	C1B-C2B-C3B	-2.97	104.93	107.00
22	O	301	CHD	C6-C5-C4	-2.96	107.77	111.13
14	A	601	HEA	CAA-CBA-CGA	-2.93	107.66	112.66
14	N	601	HEA	C13-C12-C11	-2.87	110.12	114.46
14	A	601	HEA	CMB-C2B-C1B	-2.82	124.12	128.46
14	A	602	HEA	C20-C19-C18	-2.82	115.33	121.10
24	P	305	CDL	CB4-OB6-CB5	-2.77	111.34	117.88
22	C	308	CHD	C14-C8-C9	-2.76	105.88	109.64
19	A	607	PGV	O03-C19-O04	-2.73	116.77	123.55
22	C	308	CHD	C17-C13-C12	-2.71	115.18	117.67
14	A	601	HEA	CMC-C2C-C1C	-2.68	124.35	128.46
22	J	101	CHD	C23-C22-C20	-2.66	111.14	114.72
22	P	306	CHD	C14-C8-C9	-2.66	106.02	109.64
18	A	606	TGL	CG3-CG2-CG1	-2.65	105.88	111.86
22	P	306	CHD	C1-C10-C9	-2.56	107.31	111.39
14	A	602	HEA	C13-C12-C11	-2.54	110.62	114.46
14	A	601	HEA	OMA-CMA-C3A	-2.53	119.25	125.08
14	A	602	HEA	C4B-C3B-C2B	-2.53	105.10	106.87
24	P	305	CDL	OB8-CB7-OB9	-2.52	117.31	123.55
22	P	306	CHD	C23-C22-C20	-2.46	111.40	114.72
18	Q	201	TGL	OG3-CC1-OC1	-2.45	117.46	123.55
22	J	101	CHD	C6-C5-C4	-2.45	108.35	111.13
26	E	201	PSC	C11-C12-C13	-2.43	110.53	124.90
14	N	602	HEA	C4B-C3B-C2B	-2.43	105.17	106.87
22	C	308	CHD	C13-C17-C20	-2.41	116.57	119.49
22	O	301	CHD	C13-C17-C20	-2.35	116.64	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C1B-C2B-C3B	-2.34	105.37	107.00
14	A	601	HEA	C13-C14-C15	-2.32	121.86	127.68
19	N	607	PGV	O03-C19-O04	-2.25	117.97	123.55
22	P	306	CHD	C5-C4-C3	-2.24	109.58	112.87
14	A	601	HEA	C17-C18-C19	-2.24	122.05	127.68
14	A	601	HEA	C26-C15-C14	-2.23	117.75	123.69
23	T	103	PEK	O03-C21-O04	-2.22	118.04	123.55
14	N	601	HEA	CMC-C2C-C1C	-2.20	125.08	128.46
23	C	303	PEK	O03-C01-C02	-2.20	103.13	108.66
14	N	602	HEA	CAA-CBA-CGA	-2.20	108.91	112.66
18	D	201	TGL	OG3-CC1-OC1	-2.19	118.11	123.55
18	Q	201	TGL	OG1-CA1-OA1	-2.17	118.16	123.55
22	W	101	CHD	C23-C22-C20	-2.14	111.84	114.72
18	L	101	TGL	OG3-CC1-OC1	-2.13	118.26	123.55
22	J	101	CHD	C21-C20-C17	-2.12	109.63	112.95
25	Z	101	DMU	C10-O7-C3	-2.10	112.88	118.00
26	O	304	PSC	C11-C12-C13	-2.09	112.53	124.90
24	G	101	CDL	OA6-CA5-OA7	-2.07	118.50	123.68
22	P	301	CHD	C19-C10-C1	-2.07	104.84	108.24
24	T	104	CDL	OA8-CA7-OA9	-2.04	118.48	123.55
19	P	303	PGV	O03-C19-O04	-2.01	118.56	123.55
23	T	102	PEK	O03-C21-O04	-2.00	118.58	123.55
19	M	101	PGV	O03-C19-O04	-2.00	118.58	123.55
14	N	602	HEA	CMC-C2C-C3C	2.00	128.61	124.89
22	J	101	CHD	C15-C14-C13	2.01	105.57	103.57
25	P	308	DMU	O7-C3-C2	2.02	112.06	107.19
19	C	305	PGV	O03-C19-C20	2.03	117.81	111.90
19	P	303	PGV	O03-C19-C20	2.06	117.89	111.90
24	G	101	CDL	CB6-OB8-CB7	2.06	123.34	117.13
19	A	607	PGV	O01-C1-C2	2.11	115.92	111.55
22	P	306	CHD	C2-C1-C10	2.11	116.47	112.80
22	W	101	CHD	C9-C10-C5	2.13	111.70	108.63
25	P	308	DMU	O16-C6-C1	2.13	111.70	108.23
19	P	303	PGV	O01-C1-C2	2.14	115.99	111.55
14	A	601	HEA	CMD-C2D-C3D	2.15	128.99	124.94
14	A	602	HEA	CMD-C2D-C3D	2.16	129.02	124.94
14	N	601	HEA	CMC-C2C-C3C	2.16	128.91	124.89
14	A	602	HEA	CMC-C2C-C3C	2.19	128.96	124.89
23	C	303	PEK	C01-O03-C21	2.21	123.79	117.13
22	B	302	CHD	C14-C8-C7	2.22	114.82	111.80
25	C	312	DMU	C18-O16-C6	2.26	117.75	113.87
18	D	201	TGL	CG1-OG1-CA1	2.27	123.95	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C12-C11-C3B	2.30	118.27	112.65
25	Z	101	DMU	C1-C2-C3	2.37	114.52	109.61
22	C	308	CHD	C16-C17-C13	2.41	105.97	103.57
14	A	602	HEA	CBD-CAD-C3D	2.42	117.11	112.48
24	P	305	CDL	CB6-OB8-CB7	2.43	124.44	117.13
22	O	301	CHD	C11-C9-C8	2.43	114.34	110.82
22	P	306	CHD	C6-C7-C8	2.45	114.10	111.50
19	C	305	PGV	O01-C1-C2	2.45	116.64	111.55
14	A	601	HEA	CMC-C2C-C3C	2.48	129.49	124.89
22	O	301	CHD	C15-C14-C13	2.49	106.05	103.57
14	A	602	HEA	C27-C19-C20	2.50	119.63	115.29
14	N	601	HEA	CMD-C2D-C3D	2.52	129.70	124.94
24	T	104	CDL	OB8-CB7-C71	2.53	119.27	111.90
18	Y	101	TGL	OG1-CA1-CA2	2.54	119.28	111.90
18	Q	201	TGL	OG1-CG1-CG2	2.55	115.06	108.66
18	Y	101	TGL	OG3-CC1-CC2	2.56	119.33	111.90
14	N	601	HEA	C3C-C4C-NC	2.56	112.52	109.21
22	P	306	CHD	C15-C14-C13	2.56	106.12	103.57
22	C	301	CHD	C15-C14-C13	2.56	106.12	103.57
24	C	307	CDL	OA8-CA7-C31	2.59	119.43	111.90
22	W	101	CHD	C6-C5-C10	2.60	115.50	112.66
25	C	313	DMU	O5-C4-C3	2.60	115.08	109.75
14	N	602	HEA	C27-C19-C20	2.61	119.82	115.29
24	G	101	CDL	OB8-CB7-C71	2.63	119.55	111.90
22	C	308	CHD	C9-C10-C5	2.64	112.44	108.63
14	N	601	HEA	C26-C15-C16	2.65	119.88	115.29
22	P	301	CHD	C6-C7-C8	2.65	114.32	111.50
23	T	102	PEK	O01-C1-C2	2.66	117.08	111.55
18	D	201	TGL	OG1-CA1-CA2	2.66	119.64	111.90
18	A	606	TGL	OG1-CA1-CA2	2.70	119.77	111.90
26	E	201	PSC	O03-C19-C20	2.73	119.86	111.90
22	W	101	CHD	C22-C20-C17	2.74	116.01	110.26
19	N	606	PGV	O03-C19-C20	2.74	119.88	111.90
18	O	302	TGL	OG1-CA1-CA2	2.76	119.93	111.90
22	P	306	CHD	C15-C14-C8	2.77	122.24	118.32
26	O	304	PSC	O03-C19-C20	2.79	120.00	111.90
14	A	601	HEA	CBA-CAA-C2A	2.80	117.81	112.47
23	G	102	PEK	O03-C21-C22	2.81	120.07	111.90
18	L	101	TGL	OG3-CC1-CC2	2.82	120.10	111.90
22	C	308	CHD	C15-C14-C8	2.82	122.31	118.32
24	P	305	CDL	OA8-CA7-C31	2.83	120.13	111.90
22	C	308	CHD	C15-C14-C13	2.83	106.39	103.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C22-C20-C17	2.86	116.26	110.26
22	C	308	CHD	C1-C2-C3	2.87	114.08	110.42
18	O	302	TGL	OG3-CC1-CC2	2.88	120.27	111.90
24	G	101	CDL	OA8-CA7-C31	2.90	120.33	111.90
18	A	606	TGL	OG2-CG2-CG1	2.93	119.09	108.44
23	C	303	PEK	O01-C1-C2	2.94	117.66	111.55
23	T	101	PEK	O03-C21-C22	2.95	120.50	111.90
25	P	309	DMU	O7-C3-C4	2.96	116.63	109.34
25	C	313	DMU	C2-C3-C4	2.96	117.17	110.88
23	C	304	PEK	O03-C21-C22	2.98	120.57	111.90
23	T	103	PEK	O03-C21-C22	3.01	120.65	111.90
22	P	306	CHD	C6-C5-C10	3.03	115.97	112.66
14	A	601	HEA	C26-C15-C16	3.06	120.59	115.29
25	C	312	DMU	C6-C1-C2	3.06	115.67	109.98
25	C	313	DMU	C1-C2-C3	3.07	115.97	109.61
24	C	307	CDL	OB8-CB7-C71	3.09	120.90	111.90
14	N	601	HEA	CBA-CAA-C2A	3.12	118.41	112.47
22	P	306	CHD	C9-C10-C5	3.12	113.14	108.63
19	C	306	PGV	O03-C19-C20	3.13	121.02	111.90
14	A	601	HEA	CMB-C2B-C3B	3.14	130.94	124.92
18	Q	201	TGL	OG2-CB1-CB2	3.14	118.07	111.55
24	T	104	CDL	OA8-CA7-C31	3.14	121.04	111.90
18	D	201	TGL	OG3-CC1-CC2	3.15	121.06	111.90
14	N	602	HEA	CBD-CAD-C3D	3.16	118.53	112.48
18	A	606	TGL	CG3-OG3-CC1	3.22	126.83	117.13
18	Q	201	TGL	OG3-CC1-CC2	3.27	121.41	111.90
18	L	101	TGL	OG1-CA1-CA2	3.30	121.49	111.90
18	Q	201	TGL	OG1-CA1-CA2	3.30	121.50	111.90
23	T	102	PEK	O03-C21-C22	3.34	121.61	111.90
24	P	305	CDL	OB8-CB7-C71	3.37	121.70	111.90
19	M	101	PGV	O03-C19-C20	3.37	121.70	111.90
22	B	302	CHD	C15-C14-C13	3.42	106.97	103.57
22	W	101	CHD	C14-C13-C12	3.42	110.63	107.39
22	W	101	CHD	C16-C17-C20	3.48	117.71	112.14
22	C	308	CHD	C10-C9-C8	3.48	115.62	111.87
19	P	304	PGV	O01-C1-C2	3.49	118.81	111.55
19	N	607	PGV	O03-C19-C20	3.52	122.14	111.90
19	P	304	PGV	O03-C19-C20	3.52	122.15	111.90
23	T	103	PEK	O01-C1-C2	3.58	118.99	111.55
25	C	312	DMU	O16-C6-C1	3.59	114.09	108.23
22	P	306	CHD	C1-C2-C3	3.60	115.01	110.42
18	L	101	TGL	OG2-CB1-CB2	3.71	119.25	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	PGV	O03-C19-C20	3.77	122.87	111.90
22	J	101	CHD	C16-C17-C20	3.83	118.28	112.14
24	P	305	CDL	OB6-CB5-C51	3.85	119.54	111.55
23	T	101	PEK	O01-C1-C2	3.85	119.55	111.55
24	P	305	CDL	OA6-CA5-C11	3.88	119.61	111.55
22	J	101	CHD	C14-C13-C12	3.97	111.15	107.39
24	T	104	CDL	OA6-CA5-C11	3.97	119.80	111.55
24	C	307	CDL	OB6-CB5-C51	3.99	119.83	111.55
25	C	312	DMU	C1-C2-C3	3.99	117.89	109.61
18	A	606	TGL	CG2-OG2-CB1	4.02	127.38	117.88
19	C	306	PGV	O01-C1-C2	4.03	119.92	111.55
23	C	304	PEK	O01-C1-C2	4.05	119.96	111.55
24	G	101	CDL	OA6-CA5-C11	4.10	120.06	111.55
19	M	101	PGV	O01-C1-C2	4.11	120.08	111.55
18	O	302	TGL	OG2-CB1-CB2	4.15	120.17	111.55
22	P	306	CHD	C10-C9-C8	4.15	116.34	111.87
23	G	102	PEK	O01-C1-C2	4.17	120.21	111.55
18	A	606	TGL	OG3-CC1-CC2	4.23	124.22	111.90
18	Y	101	TGL	OG2-CB1-CB2	4.27	120.41	111.55
26	E	201	PSC	O01-C1-C2	4.32	120.53	111.55
26	O	304	PSC	O01-C1-C2	4.33	120.55	111.55
19	N	606	PGV	O01-C1-C2	4.34	120.56	111.55
24	G	101	CDL	OB6-CB5-C51	4.38	120.64	111.55
24	C	307	CDL	OA6-CA5-C11	4.40	120.69	111.55
24	T	104	CDL	OB6-CB5-C51	4.56	121.02	111.55
18	A	606	TGL	OG2-CB1-CB2	4.75	121.41	111.55

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	601	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NB

There are no torsion outliers.

There are no ring outliers.

49 monomers are involved in 153 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	2	0
14	A	602	HEA	4	0
18	A	606	TGL	3	0
19	A	607	PGV	2	0
20	A	608	EDO	1	0
20	A	611	EDO	2	0
20	A	615	EDO	1	0
20	A	616	EDO	1	0
23	C	303	PEK	3	0
23	C	304	PEK	2	0
19	C	305	PGV	3	0
19	C	306	PGV	1	0
24	C	307	CDL	10	0
22	C	308	CHD	3	0
25	C	313	DMU	12	0
18	D	201	TGL	4	0
20	D	202	EDO	2	0
26	E	201	PSC	10	0
20	E	202	EDO	1	0
24	G	101	CDL	5	0
18	L	101	TGL	4	0
19	M	101	PGV	2	0
14	N	601	HEA	2	0
14	N	602	HEA	5	0
19	N	606	PGV	2	0
19	N	607	PGV	2	0
20	N	608	EDO	1	0
20	N	612	EDO	1	0
20	N	613	EDO	4	0
20	N	614	EDO	1	0
20	N	615	EDO	2	0
20	N	617	EDO	1	0
22	O	301	CHD	1	0
18	O	302	TGL	2	0
26	O	304	PSC	6	0
22	P	301	CHD	2	0
19	P	303	PGV	3	0
19	P	304	PGV	1	0
24	P	305	CDL	8	0
22	P	306	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	308	DMU	1	0
25	P	309	DMU	8	0
20	S	103	EDO	1	0
23	T	101	PEK	2	0
23	T	102	PEK	3	0
23	T	103	PEK	2	0
24	T	104	CDL	13	0
22	W	101	CHD	1	0
18	Y	101	TGL	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	0.56	5 (0%) 82 82	25, 31, 39, 76	0
1	N	513/514 (99%)	0.45	8 (1%) 72 71	32, 41, 53, 77	0
2	B	226/227 (99%)	0.50	9 (3%) 39 39	28, 38, 58, 75	0
2	O	226/227 (99%)	0.74	16 (7%) 17 17	40, 52, 72, 99	0
3	C	259/260 (99%)	0.68	8 (3%) 49 49	27, 36, 48, 82	0
3	P	259/260 (99%)	0.55	6 (2%) 61 60	33, 40, 51, 78	0
4	D	144/147 (97%)	0.32	2 (1%) 75 75	34, 43, 55, 75	0
4	Q	144/147 (97%)	1.26	21 (14%) 3 3	48, 63, 88, 137	0
5	E	105/109 (96%)	0.36	2 (1%) 67 66	35, 44, 63, 109	0
5	R	105/109 (96%)	0.63	6 (5%) 24 25	45, 55, 71, 115	0
6	F	94/94 (100%)	0.71	3 (3%) 48 48	32, 46, 64, 119	0
6	S	94/94 (100%)	0.66	5 (5%) 27 27	37, 51, 75, 117	0
7	G	83/85 (97%)	1.47	18 (21%) 1 1	34, 44, 114, 145	0
7	T	83/85 (97%)	1.82	22 (26%) 1 1	35, 48, 108, 150	0
8	H	79/85 (92%)	0.69	9 (11%) 6 6	36, 47, 80, 99	0
8	U	79/85 (92%)	0.99	11 (13%) 3 3	43, 54, 93, 109	0
9	I	72/73 (98%)	1.18	12 (16%) 2 2	36, 50, 82, 91	0
9	V	72/73 (98%)	1.44	13 (18%) 1 2	42, 67, 95, 103	0
10	J	58/59 (98%)	0.84	5 (8%) 11 11	38, 47, 73, 117	0
10	W	58/59 (98%)	1.04	8 (13%) 3 3	44, 55, 81, 128	0
11	K	49/56 (87%)	0.38	1 (2%) 65 65	38, 45, 58, 66	0
11	X	49/56 (87%)	0.88	7 (14%) 3 3	56, 66, 83, 90	0
12	L	46/47 (97%)	0.44	1 (2%) 62 61	31, 38, 53, 84	0
12	Y	46/47 (97%)	0.82	5 (10%) 6 6	46, 54, 70, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.56	3 (6%) 17 17	35, 38, 66, 104	0
13	Z	43/46 (93%)	0.97	8 (18%) 1 1	52, 58, 85, 118	0
All	All	3542/3604 (98%)	0.70	214 (6%) 23 23	25, 43, 75, 150	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	23.3
4	Q	5	VAL	17.0
7	T	8	HIS	12.9
7	G	3	ALA	12.7
6	F	1	ALA	12.5
7	T	3	ALA	11.9
9	I	29	LEU	11.6
6	S	1	ALA	10.9
8	U	8	ILE	10.4
7	G	2	SER	10.1
4	Q	8	SER	9.8
6	F	2	SER	9.6
9	I	30	GLY	9.2
7	T	10	GLY	8.8
9	V	29	LEU	8.5
7	T	36	TRP	8.3
9	V	30	GLY	8.1
9	V	25	PHE	8.0
8	H	45	ALA	7.7
4	Q	4	SER	7.7
5	R	109	VAL	7.5
7	T	2	SER	7.4
7	G	6	GLY	7.0
10	W	58	LYS	7.0
3	P	38[A]	ASN	6.9
4	Q	7	LYS	6.7
7	T	5	LYS	6.7
7	G	1	ALA	6.5
8	U	7	LYS	6.5
7	G	5	LYS	6.4
9	I	25	PHE	6.4
5	E	5	HIS	6.3
6	S	2	SER	6.2
10	W	57	HIS	6.1

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Mol	Chain	Res	Type	RSRZ
9	V	33	THR	6.0
9	V	2	THR	6.0
9	V	34	PHE	5.8
2	O	227	LEU	5.8
7	T	7	ASP	5.6
10	W	52	TRP	5.5
7	T	37	LEU	5.5
10	J	58	LYS	5.5
7	T	42	ARG	5.4
10	J	57	HIS	5.3
7	T	33	LEU	5.2
8	U	45	ALA	5.1
9	V	37	PHE	5.1
7	G	36	TRP	5.1
7	T	1	ALA	5.1
7	T	4	ALA	5.0
4	Q	33	LEU	4.9
7	G	4	ALA	4.8
9	I	37	PHE	4.8
12	Y	47	LYS	4.6
7	T	9	GLY	4.6
4	Q	87	PHE	4.6
7	G	40	GLY	4.5
11	X	13	TYR	4.5
7	T	39	SER	4.5
4	Q	10	ASP	4.4
3	C	38[A]	ASN	4.4
13	Z	32	TRP	4.3
9	V	31	PHE	4.3
5	R	5	HIS	4.3
2	O	113	TYR	4.3
3	P	37	PHE	4.2
13	Z	37[A]	LEU	4.2
10	J	52	TRP	4.2
8	H	8	ILE	4.2
7	T	40	GLY	4.1
9	I	34	PHE	4.0
6	F	94	HIS	4.0
9	I	19	PHE	3.9
7	G	8	HIS	3.9
1	N	513	LEU	3.9
9	V	32	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
7	G	42	ARG	3.7
11	X	6	ALA	3.7
7	G	37	LEU	3.6
10	J	1	PHE	3.6
7	T	41	HIS	3.6
4	Q	51	LEU	3.6
5	E	109	VAL	3.6
8	U	9	LYS	3.6
3	P	3	HIS	3.6
11	X	27	ALA	3.6
10	W	48	TYR	3.6
11	X	7	PRO	3.6
8	H	47	GLY	3.5
7	T	84	LYS	3.5
3	C	258	TRP	3.5
2	O	40	TYR	3.5
5	R	65	VAL	3.4
9	I	31	PHE	3.4
2	O	224	ALA	3.3
4	Q	48	TRP	3.3
8	U	50	VAL	3.3
3	C	37	PHE	3.3
2	B	68[A]	LEU	3.2
2	O	184	LEU	3.2
12	Y	20	ARG	3.2
4	Q	30	VAL	3.2
9	V	21	ILE	3.2
4	Q	9	GLU	3.2
7	G	7	ASP	3.2
12	Y	27	LEU	3.1
9	I	28	SER	3.1
2	B	113	TYR	3.1
2	B	87	MET	3.0
13	Z	42	LYS	3.0
13	Z	17	ILE	3.0
10	J	48	TYR	2.9
8	H	43	MET	2.9
4	Q	39	ALA	2.9
7	G	33	LEU	2.9
2	O	90	ILE	2.9
3	C	237	ALA	2.9
7	T	6	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
8	H	46	LYS	2.9
7	T	43	GLU	2.8
8	U	10	ASN	2.8
8	H	48	GLY	2.8
11	X	52	GLU	2.8
2	B	91	ASN	2.7
2	O	91	ASN	2.7
2	O	61	VAL	2.7
7	G	9	GLY	2.7
8	U	47	GLY	2.7
13	Z	43	SER	2.7
9	V	18	ARG	2.7
10	W	1	PHE	2.6
4	D	4	SER	2.6
13	M	42	LYS	2.6
8	U	55	TRP	2.6
1	N	113[A]	LEU	2.6
2	B	59	GLN	2.6
7	G	41	HIS	2.6
9	I	26	MET	2.6
12	Y	24[A]	MET	2.6
9	I	32	ALA	2.5
6	S	94	HIS	2.5
8	H	44	THR	2.5
13	M	43	SER	2.5
9	V	26	MET	2.5
4	Q	46	ALA	2.5
4	Q	31	LYS	2.5
1	A	297[A]	MET	2.4
13	Z	28	LEU	2.4
2	O	163	TRP	2.4
7	T	12	GLY	2.4
9	I	21	ILE	2.4
5	R	52	LEU	2.4
9	V	65	LYS	2.3
4	Q	128	VAL	2.3
2	O	152[A]	MET	2.3
1	A	113[A]	LEU	2.3
2	O	135	LEU	2.3
7	G	45	PRO	2.3
13	M	40	TYR	2.3
3	C	33[A]	MET	2.3

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Mol	Chain	Res	Type	RSRZ
13	Z	35	TYR	2.3
6	S	43	LYS	2.3
13	Z	13	LYS	2.2
2	O	68[A]	LEU	2.2
3	C	127	LEU	2.2
1	N	297[A]	MET	2.2
1	A	513	LEU	2.2
2	O	116	LEU	2.2
4	Q	40	LEU	2.2
3	P	33[A]	MET	2.2
4	Q	58	GLU	2.2
6	S	3	GLY	2.2
7	G	12	GLY	2.2
1	N	112	LEU	2.2
2	O	33	LEU	2.2
3	P	258	TRP	2.2
10	W	44	LEU	2.2
5	R	33[A]	MET	2.2
4	Q	88	PHE	2.2
11	X	24	PHE	2.2
11	K	47	ARG	2.2
8	U	49	ASP	2.2
3	C	3	HIS	2.2
4	D	19	ARG	2.2
12	Y	38	PHE	2.2
4	Q	147	LYS	2.2
10	W	30	ILE	2.1
2	B	184	LEU	2.1
2	O	20	LEU	2.1
2	B	16	ILE	2.1
12	L	2	HIS	2.1
2	O	221	LYS	2.1
8	H	7	LYS	2.1
1	N	382	SER	2.1
1	N	514	LYS	2.1
7	T	35	SER	2.1
7	T	34	ASN	2.1
4	Q	53	ILE	2.1
8	U	46	LYS	2.1
8	U	43	MET	2.0
10	W	32	TYR	2.0
5	R	61	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
8	H	42	ALA	2.0
7	G	10	GLY	2.0
1	N	169	ILE	2.0
3	C	88[A]	ILE	2.0
2	B	40	TYR	2.0
1	A	366[A]	VAL	2.0
9	I	27	VAL	2.0
1	N	3	ILE	2.0
2	B	33	LEU	2.0
1	A	71[A]	MET	2.0
3	P	261	SER	2.0
11	X	23	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.73	0.60	-	118,123,127,131	0
7	TPO	G	11	11/12	0.58	0.30	-	88,102,120,124	0
2	FME	O	1	10/11	0.96	0.21	-	52,53,59,60	0
7	TPO	T	11	11/12	0.48	0.35	-	93,108,122,125	0
9	SAC	I	1	9/10	0.82	0.20	-	74,75,78,79	0
1	FME	A	1	10/11	0.93	0.16	-	46,53,70,78	0
1	FME	N	1	10/11	0.94	0.21	-	58,63,83,86	0
2	FME	B	1	10/11	0.97	0.15	-	35,36,44,47	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	N	615	4/4	0.93	0.39	26.57	54,58,59,65	0
20	EDO	A	611	4/4	0.85	0.76	26.50	62,67,67,69	0
20	EDO	A	615	4/4	0.84	0.37	19.34	49,50,56,58	0
20	EDO	N	613	4/4	0.96	0.35	17.28	49,51,53,55	0
24	CDL	C	307	100/100	0.69	0.34	12.09	56,85,110,116	0
19	PGV	M	101	51/51	0.70	0.31	10.16	49,77,115,124	0
25	DMU	C	313	33/33	0.64	0.54	8.92	49,130,146,147	0
20	EDO	R	201	4/4	0.91	0.34	8.27	52,53,53,53	0
24	CDL	P	305	100/100	0.63	0.33	8.16	65,90,111,114	0
24	CDL	G	101	100/100	0.60	0.40	7.76	65,97,136,145	0
20	EDO	A	612	4/4	0.94	0.22	7.41	38,39,43,43	0
20	EDO	A	614	4/4	0.94	0.24	7.15	50,53,54,59	0
18	TGL	A	606	63/63	0.80	0.28	7.00	53,78,95,98	0
20	EDO	F	104	4/4	0.83	0.29	6.82	56,58,60,62	0
22	CHD	W	101	29/29	0.66	0.36	6.12	89,96,106,107	0
22	CHD	J	101	29/29	0.73	0.27	5.96	73,78,100,104	0
19	PGV	N	606	51/51	0.65	0.40	5.27	70,87,126,128	0
18	TGL	L	101	63/63	0.73	0.29	5.10	46,71,85,86	0
18	TGL	O	302	63/63	0.75	0.32	5.07	64,87,99,105	0
20	EDO	D	203	4/4	0.84	0.23	4.73	61,65,70,71	0
23	PEK	T	102	53/53	0.95	0.20	4.49	40,58,95,98	0
20	EDO	N	617	4/4	0.94	0.21	4.42	58,70,75,86	0
24	CDL	T	104	100/100	0.61	0.38	4.25	63,92,121,138	0
18	TGL	D	201	63/63	0.73	0.21	4.00	56,71,89,92	0
26	PSC	O	304	52/52	0.73	0.31	3.88	60,92,142,154	0
18	TGL	Q	201	63/63	0.63	0.25	3.50	67,86,96,100	0
19	PGV	P	303	51/51	0.96	0.19	3.47	38,46,76,79	0
20	EDO	S	103	4/4	0.87	0.21	3.37	57,66,69,72	0
20	EDO	N	609	4/4	0.94	0.28	3.30	63,69,69,74	0
23	PEK	C	303	53/53	0.96	0.18	3.28	35,52,84,86	0
21	CUA	B	301	2/2	0.98	0.17	3.24	30,30,30,30	0
26	PSC	E	201	52/52	0.67	0.36	3.08	56,87,141,150	0
18	TGL	Y	101	63/63	0.61	0.31	2.82	63,83,104,107	0
20	EDO	N	612	4/4	0.96	0.17	2.78	45,46,46,47	0
27	ZN	F	101	1/1	1.00	0.18	2.75	39,39,39,39	0
16	MG	A	604	1/1	0.95	0.16	2.69	30,30,30,30	0
20	EDO	N	614	4/4	0.94	0.19	2.58	46,48,49,50	0
25	DMU	Z	101	33/33	0.84	0.26	2.50	57,80,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	PGV	C	306	51/51	0.72	0.30	2.47	62,82,121,124	0
20	EDO	C	309	4/4	0.70	0.26	2.42	82,86,90,92	0
20	EDO	A	610	4/4	0.94	0.21	2.38	54,56,56,57	0
22	CHD	C	308	29/29	0.87	0.25	2.29	72,74,79,80	0
19	PGV	P	304	51/51	0.68	0.33	2.22	66,92,122,129	0
25	DMU	P	309	33/33	0.69	0.46	2.12	64,128,146,149	0
16	MG	N	604	1/1	0.85	0.17	2.10	44,44,44,44	0
19	PGV	C	305	51/51	0.97	0.18	2.07	35,41,90,101	0
20	EDO	N	611	4/4	0.81	0.17	1.96	60,62,64,66	0
20	EDO	N	610	4/4	0.89	0.20	1.89	62,64,65,66	0
20	EDO	A	616	4/4	0.94	0.23	1.84	43,45,49,49	0
20	EDO	A	613	4/4	0.92	0.15	1.38	46,49,51,52	0
27	ZN	S	101	1/1	0.99	0.15	1.14	46,46,46,46	0
22	CHD	P	306	29/29	0.87	0.19	1.05	71,76,81,81	0
19	PGV	A	607	51/51	0.97	0.17	1.04	33,40,61,66	0
19	PGV	N	607	51/51	0.97	0.15	0.68	38,46,68,70	0
23	PEK	T	103	53/53	0.54	0.26	0.67	59,85,124,134	0
23	PEK	C	304	53/53	0.47	0.27	0.67	60,91,135,141	0
14	HEA	N	602	60/60	0.97	0.14	0.56	35,37,42,44	0
20	EDO	E	202	4/4	0.95	0.13	0.54	51,52,52,53	0
23	PEK	T	101	53/53	0.59	0.33	0.50	56,94,139,144	0
20	EDO	F	102	4/4	0.96	0.16	0.49	41,44,45,47	0
14	HEA	N	601	60/60	0.97	0.14	0.46	36,42,49,51	0
21	CUA	O	303	2/2	0.99	0.14	0.46	42,42,42,43	0
23	PEK	G	102	53/53	0.66	0.29	0.46	55,101,139,150	0
25	DMU	C	312	33/33	0.70	0.25	0.34	65,100,138,139	0
25	DMU	M	102	33/33	0.90	0.15	0.21	48,58,74,77	0
20	EDO	F	103	4/4	0.98	0.14	0.16	31,33,33,33	0
22	CHD	O	301	29/29	0.97	0.14	0.12	40,42,44,47	0
25	DMU	P	308	33/33	0.43	0.29	0.08	71,126,142,143	0
20	EDO	P	307	4/4	0.86	0.29	0.06	82,88,90,97	0
20	EDO	S	102	4/4	0.98	0.13	-0.06	37,39,40,42	0
20	EDO	N	608	4/4	0.93	0.14	-0.12	37,39,40,40	0
14	HEA	A	601	60/60	0.98	0.14	-0.15	25,28,38,40	0
20	EDO	A	609	4/4	0.98	0.14	-0.25	30,32,32,33	0
22	CHD	B	302	29/29	0.96	0.14	-0.29	36,38,40,44	0
14	HEA	A	602	60/60	0.98	0.13	-0.39	26,28,34,38	0
20	EDO	A	608	4/4	0.88	0.12	-0.47	55,59,59,65	0
22	CHD	P	301	29/29	0.95	0.11	-0.76	37,40,42,45	0
22	CHD	C	301	29/29	0.96	0.11	-1.03	34,37,39,42	0
17	NA	N	605	1/1	0.99	0.09	-1.34	49,49,49,49	0
20	EDO	C	311	4/4	0.97	0.11	-1.36	40,43,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	NA	A	605	1/1	0.98	0.08	-5.60	30,30,30,30	0
20	EDO	C	310	4/4	0.37	0.22	-	71,76,80,84	0
20	EDO	B	303	4/4	0.84	0.52	-	62,72,75,79	0
17	NA	P	302	1/1	0.73	0.12	-	51,51,51,51	0
20	EDO	N	616	4/4	0.97	0.23	-	59,59,61,61	0
15	CU	A	603	1/1	1.00	0.19	-	28,28,28,28	0
20	EDO	D	202	4/4	0.87	0.32	-	54,63,65,68	0
15	CU	N	603	1/1	1.00	0.20	-	37,37,37,37	0
17	NA	C	302	1/1	0.52	0.20	-	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.