



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AG3  
Title : Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-bound Fully Reduced State at 100 K  
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2010-03-19  
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

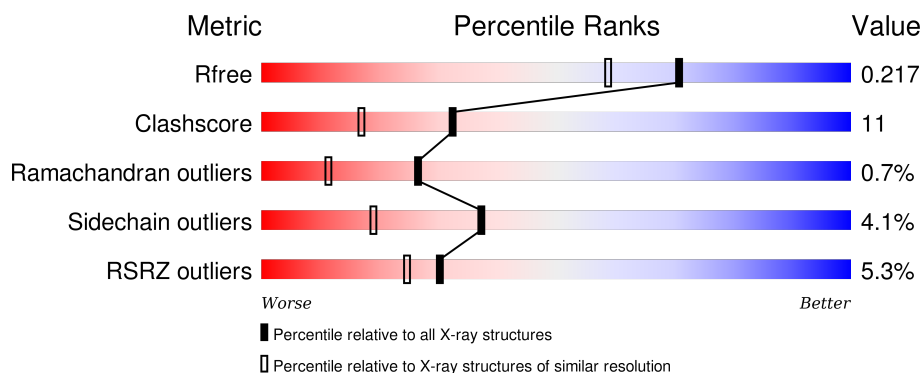
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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></div> <div>76%21%..</div> </div>
1	N	514	<div> <div>%</div> <div>76%20%..</div> </div>
2	B	227	<div> <div></div> <div>70%25%..</div> </div>
2	O	227	<div> <div>3%</div> <div>73%22%..</div> </div>
3	C	261	<div> <div>%</div> <div>78%20%..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
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	515	X	-	-	-
14	HEA	A	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	515	X	-	-	-
14	HEA	N	516	X	-	-	-
17	MG	N	518	-	-	-	X
19	TGL	A	521	-	-	-	X
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	O	1521	-	-	-	X
19	TGL	Q	1523	-	-	-	X
20	PGV	C	268	-	-	-	X
20	PGV	M	524	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	PSC	B	229	-	-	X	X
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	W	1059	X	-	-	X
25	PEK	G	1263	-	-	X	X
25	PEK	T	263	-	-	X	-
26	CDL	C	270	-	-	X	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	X	X
26	CDL	T	1269	-	-	X	X
28	DMU	G	272	X	-	-	X
28	DMU	M	526	X	-	-	X
28	DMU	P	1272	X	-	-	X
28	DMU	Z	1526	X	-	-	X

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32545 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	5	0
			4060	2712	628	684	36			
1	N	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- 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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

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

- 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 subunit 6C.

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 polypeptide 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

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			

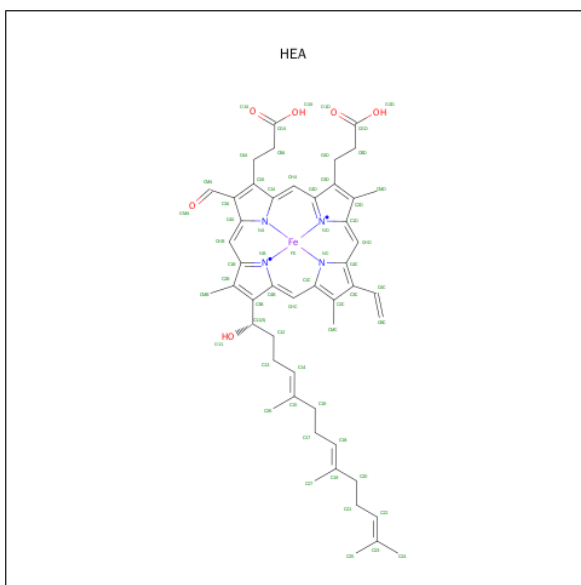
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

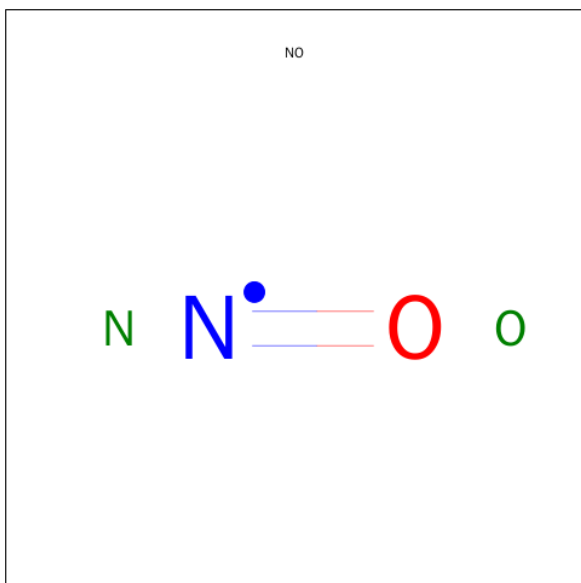
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- 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	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is NITRIC OXIDE (three-letter code: NO) (formula: NO).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total N O 2 1 1	0	0
15	N	1	Total N O 2 1 1	0	0

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

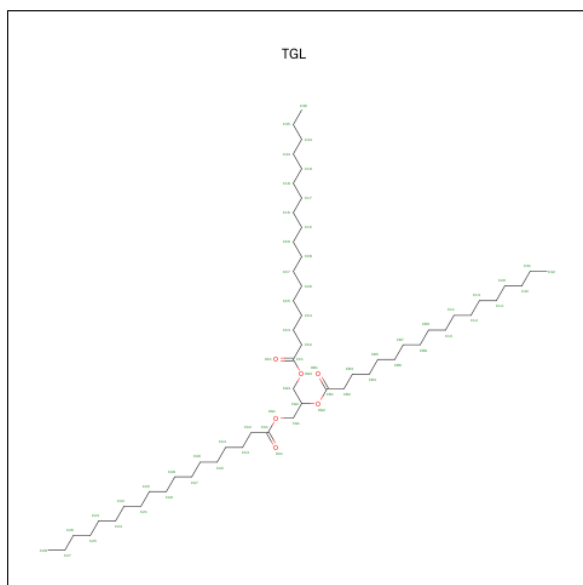
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

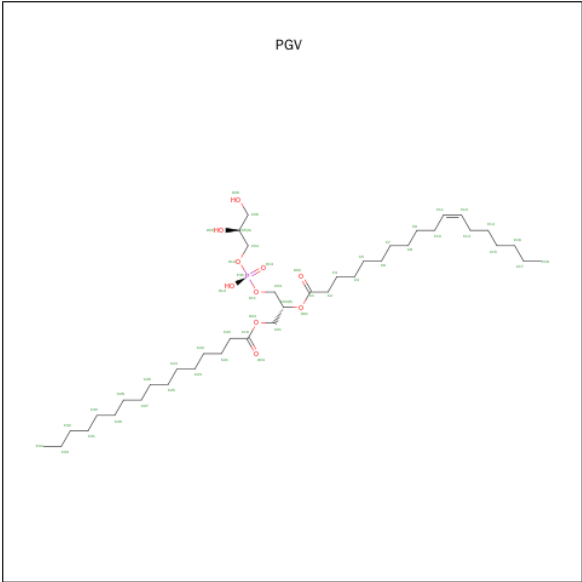
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



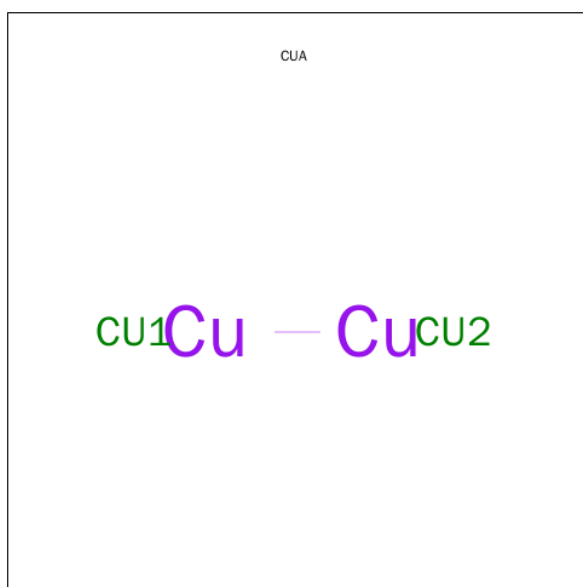
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 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).



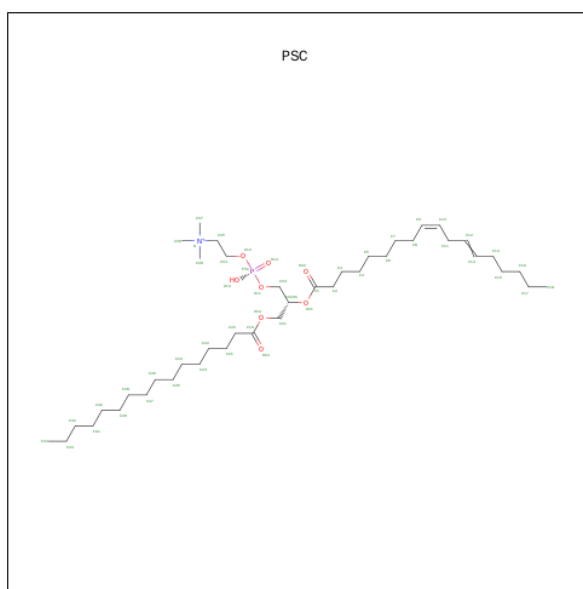
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	M	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- 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 (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<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



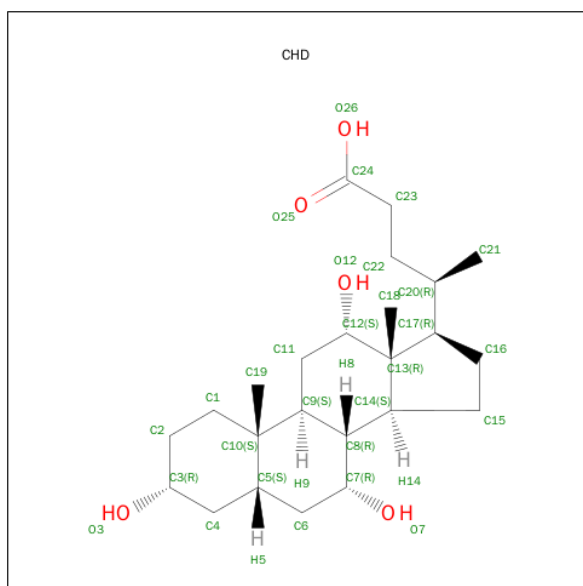
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).

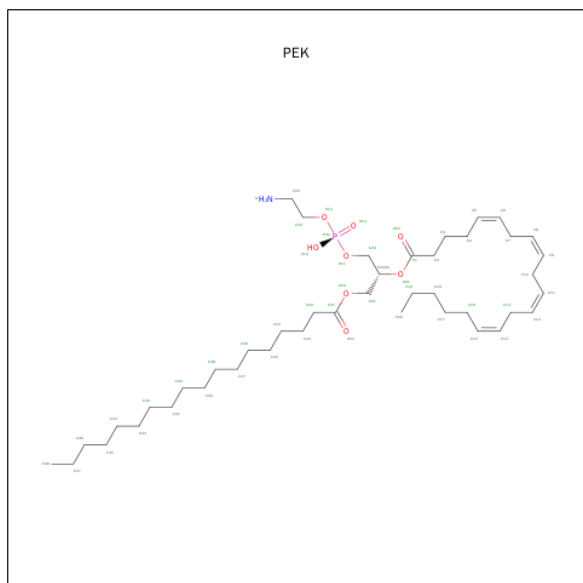


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

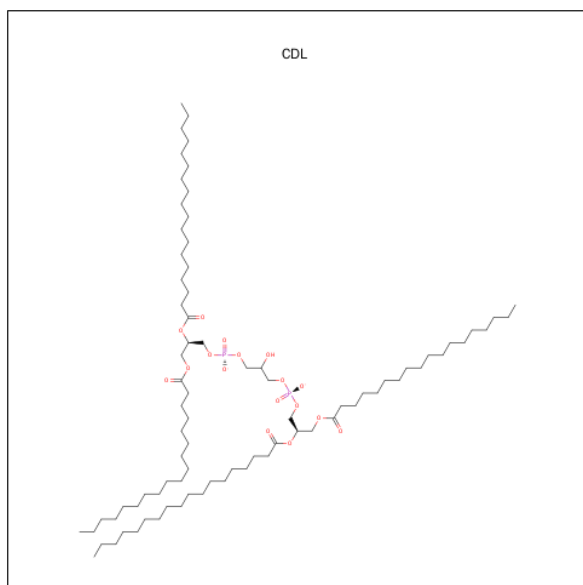
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 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
25	C	1	Total C N O P 53 43 1 8 1	0	0
25	G	1	Total C N O P 53 43 1 8 1	0	0
25	G	1	Total C N O P 53 43 1 8 1	0	0
25	P	1	Total C N O P 53 43 1 8 1	0	0
25	P	1	Total C N O P 53 43 1 8 1	0	0
25	T	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).

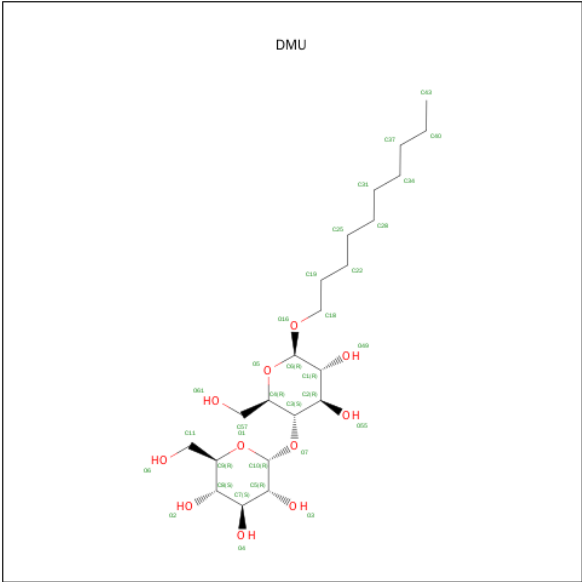


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- 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 SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	218	Total	O	0	0
			218	218		
29	B	143	Total	O	0	0
			143	143		
29	C	116	Total	O	0	0
			116	116		
29	D	80	Total	O	0	0
			80	80		
29	E	49	Total	O	0	0
			49	49		
29	F	61	Total	O	0	0
			61	61		
29	G	45	Total	O	0	0
			45	45		
29	H	51	Total	O	0	0
			51	51		

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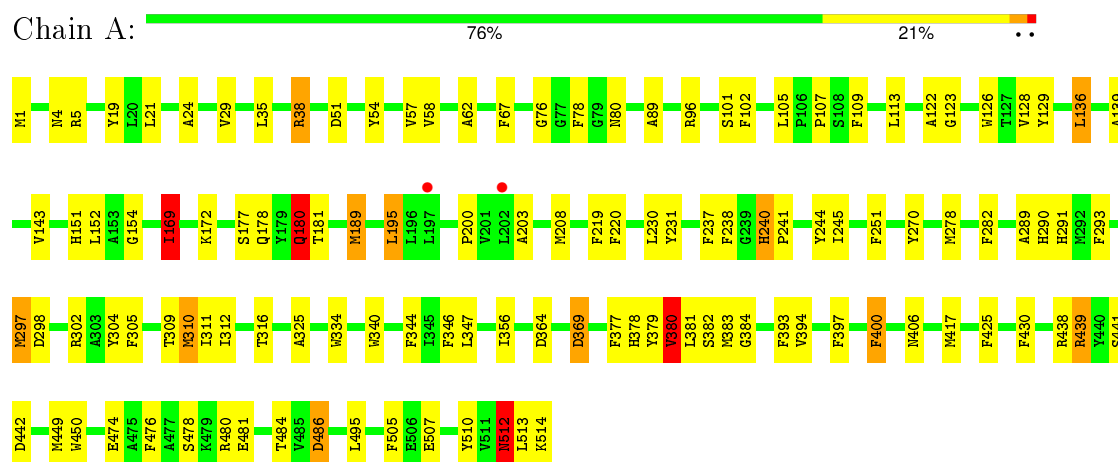
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	37	Total 37	O 37	0	0
29	J	24	Total 24	O 24	0	0
29	K	29	Total 29	O 29	0	0
29	L	23	Total 23	O 23	0	0
29	M	31	Total 31	O 31	0	0
29	N	222	Total 222	O 222	0	0
29	O	137	Total 137	O 137	0	0
29	P	102	Total 102	O 102	0	0
29	Q	65	Total 65	O 65	0	0
29	R	47	Total 47	O 47	0	0
29	S	64	Total 64	O 64	0	0
29	T	47	Total 47	O 47	0	0
29	U	49	Total 49	O 49	0	0
29	V	27	Total 27	O 27	0	0
29	W	19	Total 19	O 19	0	0
29	X	22	Total 22	O 22	0	0
29	Y	21	Total 21	O 21	0	0
29	Z	14	Total 14	O 14	0	0

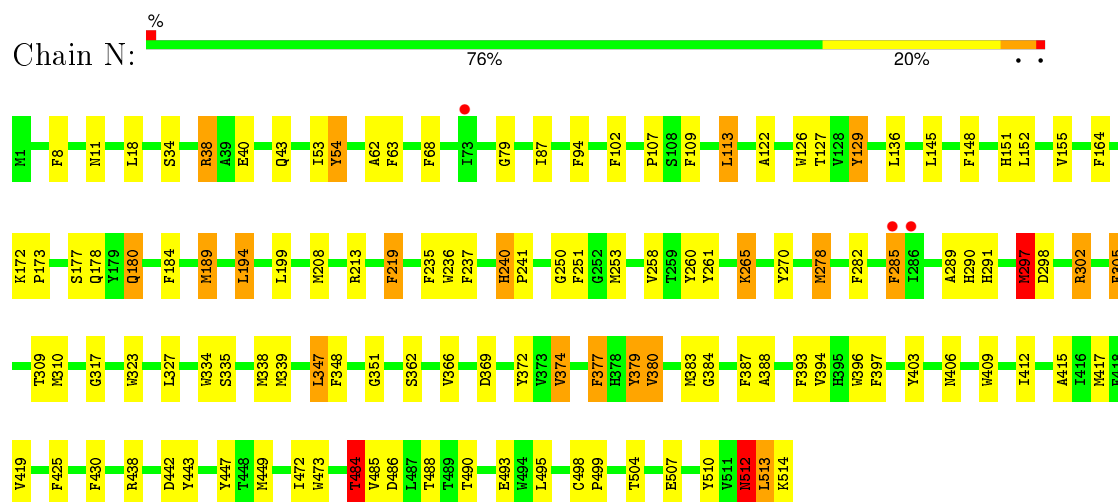
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

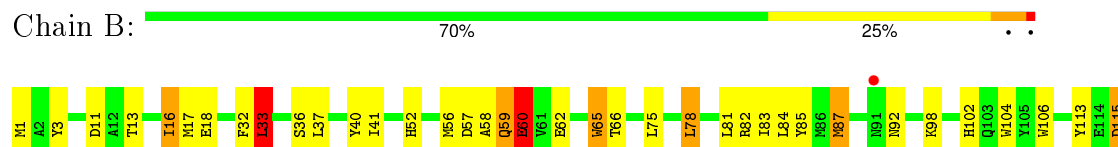
#### • Molecule 1: Cytochrome c oxidase subunit 1



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

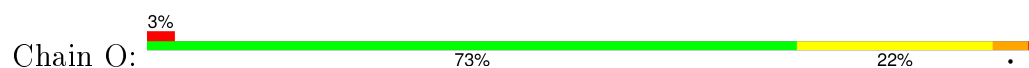


#### • Molecule 2: Cytochrome c oxidase subunit 2





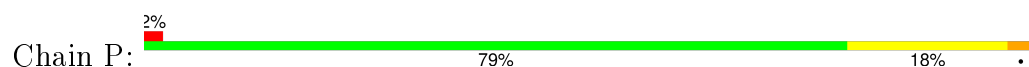
• Molecule 2: Cytochrome c oxidase subunit 2



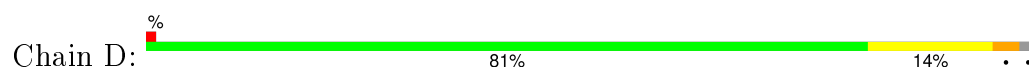
• Molecule 3: Cytochrome c oxidase subunit 3



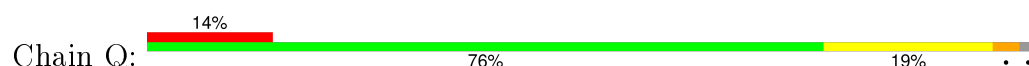
• Molecule 3: Cytochrome c oxidase subunit 3

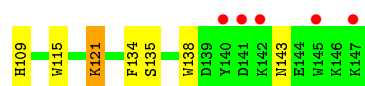


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

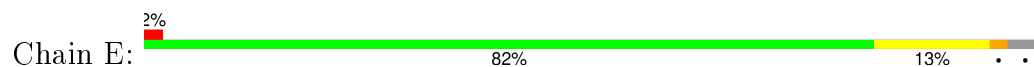


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

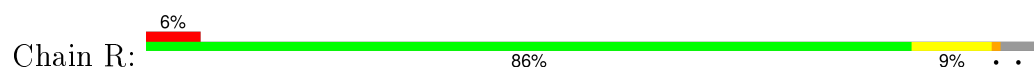




- Molecule 5: Cytochrome c oxidase subunit 5A



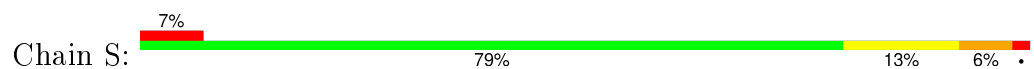
- Molecule 5: Cytochrome c oxidase subunit 5A



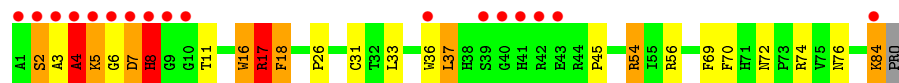
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 7: Cytochrome c oxidase subunit 6A2

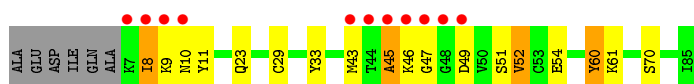


- Molecule 7: Cytochrome c oxidase subunit 6A2

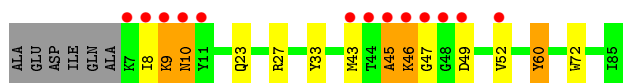
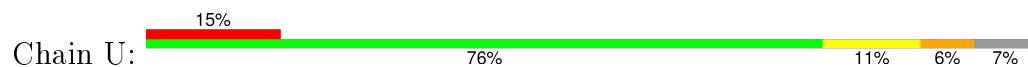


- Molecule 8: Cytochrome c oxidase subunit 6B1

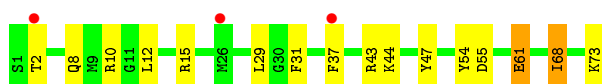
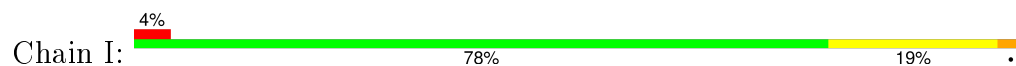




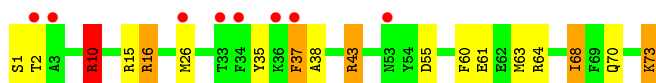
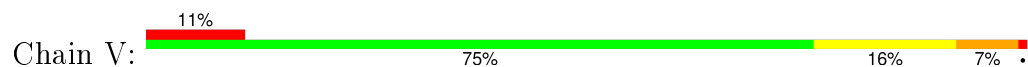
- Molecule 8: Cytochrome c oxidase subunit 6B1



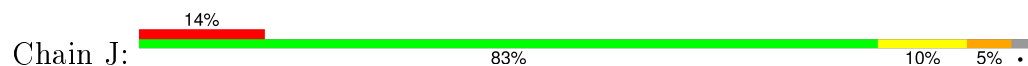
- Molecule 9: Cytochrome c oxidase subunit 6C



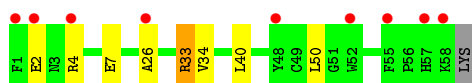
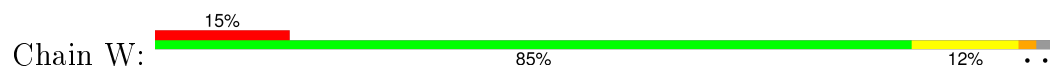
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



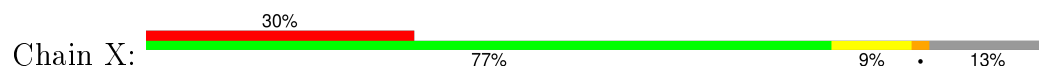
- Molecule 10: Cytochrome c oxidase polypeptide 7A1

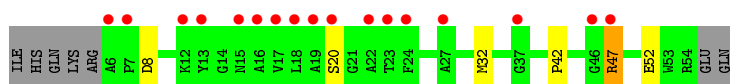


- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B





• Molecule 12: Cytochrome c oxidase subunit 7C



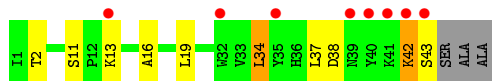
• Molecule 12: Cytochrome c oxidase subunit 7C



• Molecule 13: Cytochrome c oxidase subunit 8B



• Molecule 13: Cytochrome c oxidase subunit 8B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 83.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 99.6 (83.50-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, $R_{free}$	0.175 , 0.203 0.190 , 0.217	Depositor DCC
$R_{free}$ test set	30650 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.7	EDS
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 617373 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	32545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PEK, ZN, CHD, HEA, SAC, CDL, PSC, NO, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CU, DMU

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	1.80	66/4189 (1.6%)	1.47	43/5722 (0.8%)
1	N	1.81	63/4189 (1.5%)	1.38	35/5722 (0.6%)
2	B	1.84	41/1860 (2.2%)	1.48	19/2534 (0.7%)
2	O	1.61	21/1860 (1.1%)	1.31	14/2534 (0.6%)
3	C	1.66	26/2197 (1.2%)	1.33	18/3005 (0.6%)
3	P	1.68	21/2197 (1.0%)	1.33	18/3005 (0.6%)
4	D	1.65	12/1229 (1.0%)	1.46	16/1658 (1.0%)
4	Q	1.53	10/1229 (0.8%)	1.30	10/1658 (0.6%)
5	E	1.56	4/871 (0.5%)	1.35	8/1182 (0.7%)
5	R	1.39	3/871 (0.3%)	1.13	2/1182 (0.2%)
6	F	1.66	8/765 (1.0%)	1.32	5/1038 (0.5%)
6	S	1.62	4/765 (0.5%)	1.42	4/1038 (0.4%)
7	G	1.69	10/690 (1.4%)	1.68	8/937 (0.9%)
7	T	1.59	4/690 (0.6%)	1.64	8/937 (0.9%)
8	H	1.59	5/682 (0.7%)	1.21	2/921 (0.2%)
8	U	1.33	2/682 (0.3%)	1.11	0/921
9	I	1.56	4/605 (0.7%)	1.20	4/802 (0.5%)
9	V	1.44	0/605	1.25	6/802 (0.7%)
10	J	1.40	1/471 (0.2%)	1.19	4/636 (0.6%)
10	W	1.55	5/471 (1.1%)	1.20	2/636 (0.3%)
11	K	1.63	5/398 (1.3%)	1.26	3/546 (0.5%)
11	X	1.27	1/398 (0.3%)	1.05	1/546 (0.2%)
12	L	1.68	6/393 (1.5%)	1.27	2/526 (0.4%)
12	Y	1.75	9/393 (2.3%)	1.24	0/526
13	M	1.64	5/345 (1.4%)	1.32	4/470 (0.9%)
13	Z	1.40	2/345 (0.6%)	1.16	3/470 (0.6%)
All	All	1.67	338/29390 (1.2%)	1.36	239/39954 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is



detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	1	0
6	F	0	1
6	S	0	1
All	All	1	3

The worst 5 of 338 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	167	SER	CB-OG	-12.15	1.26	1.42
7	T	36	TRP	CB-CG	11.41	1.70	1.50
7	G	36	TRP	CB-CG	11.12	1.70	1.50
6	S	54	ASN	CB-CG	-10.52	1.26	1.51
4	Q	121	LYS	CE-NZ	10.12	1.74	1.49

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	17	ARG	NE-CZ-NH1	23.02	131.81	120.30
7	G	17	ARG	NE-CZ-NH2	-22.34	109.13	120.30
7	G	17	ARG	NE-CZ-NH1	22.31	131.46	120.30
7	T	17	ARG	NE-CZ-NH2	-21.59	109.50	120.30
4	D	20	ARG	NE-CZ-NH2	-21.22	109.69	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	66	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	TYR	Sidechain
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide

## 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	4060	0	4037	59	0
1	N	4060	0	4037	67	0
2	B	1824	0	1833	29	0
2	O	1824	0	1833	34	1
3	C	2110	0	2027	30	0
3	P	2110	0	2027	31	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	10	0
5	E	852	0	845	8	0
5	R	852	0	845	8	1
6	F	748	0	728	17	0
6	S	748	0	728	19	1
7	G	675	0	643	43	0
7	T	675	0	643	51	0
8	H	662	0	623	13	0
8	U	662	0	623	11	0
9	I	601	0	613	6	1
9	V	601	0	613	14	0
10	J	460	0	459	5	0
10	W	460	0	459	6	0
11	K	384	0	366	1	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	8	0
13	M	335	0	352	10	0
13	Z	335	0	352	2	0
14	A	120	0	107	9	0
14	N	120	0	108	8	0
15	A	2	0	0	0	0
15	N	2	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	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	8	0
19	L	63	0	110	15	0
19	N	63	0	110	15	0
19	O	63	0	110	10	0
19	Q	63	0	110	12	0
20	A	51	0	76	0	0
20	C	102	0	152	8	0
20	M	51	0	76	15	0
20	N	102	0	152	9	0
20	P	102	0	152	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	26	0
22	R	52	0	80	15	0
23	B	29	0	36	2	0
23	C	58	0	73	4	0
23	J	29	0	36	1	0
23	O	29	0	39	3	0
23	P	58	0	73	6	0
23	W	29	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	53	0	77	8	0
25	G	106	0	154	43	0
25	P	106	0	154	24	0
25	T	53	0	77	21	0
26	C	100	0	156	26	0
26	G	100	0	156	30	0
26	P	100	0	156	25	0
26	T	100	0	156	27	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	37	4	0
28	M	33	0	37	0	0
28	P	33	0	39	6	0
28	Z	33	0	38	2	0
29	A	218	0	0	5	0
29	B	143	0	0	7	0
29	C	116	0	0	3	0
29	D	80	0	0	3	0
29	E	49	0	0	0	0
29	F	61	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	G	45	0	0	2	0
29	H	51	0	0	1	0
29	I	37	0	0	2	0
29	J	24	0	0	0	0
29	K	29	0	0	0	0
29	L	23	0	0	1	0
29	M	31	0	0	2	0
29	N	222	0	0	7	0
29	O	137	0	0	5	0
29	P	102	0	0	0	0
29	Q	65	0	0	3	0
29	R	47	0	0	0	0
29	S	64	0	0	0	0
29	T	47	0	0	2	0
29	U	49	0	0	2	0
29	V	27	0	0	2	0
29	W	19	0	0	0	0
29	X	22	0	0	2	0
29	Y	21	0	0	1	0
29	Z	14	0	0	1	0
All	All	32545	0	31351	653	2

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 11.

The worst 5 of 653 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)
25:P:1265:PEK:H383	26:T:1269:CDL:C27	1.21	1.67
1:N:484:THR:CG2	1:N:484:THR:CB	1.77	1.60
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.70	1.55
1:N:189:MET:CB	1:N:189:MET:CG	1.82	1.52
4:Q:121:LYS:CE	4:Q:121:LYS:NZ	1.74	1.50

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:OG1	5:R:80:GLU:OE1[3_647]	1.64	0.56
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	2.11	0.09

## 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	517/514 (101%)	504 (98%)	13 (2%)	0	100	100
1	N	517/514 (101%)	501 (97%)	16 (3%)	0	100	100
2	B	225/227 (99%)	220 (98%)	4 (2%)	1 (0%)	39	23
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	39	23
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	26	11
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5	0
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5	0
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2	0
7	T	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	3	0
8	H	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2	0
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3514/3614 (97%)	3380 (96%)	108 (3%)	26 (1%)	26	11

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

### 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	430/426 (101%)	419 (97%)	11 (3%)	54	37
1	N	430/426 (101%)	418 (97%)	12 (3%)	51	35
2	B	210/210 (100%)	201 (96%)	9 (4%)	35	17
2	O	210/210 (100%)	198 (94%)	12 (6%)	25	10
3	C	224/226 (99%)	222 (99%)	2 (1%)	84	80
3	P	224/226 (99%)	218 (97%)	6 (3%)	52	36
4	D	128/129 (99%)	125 (98%)	3 (2%)	58	42
4	Q	128/129 (99%)	122 (95%)	6 (5%)	32	14
5	E	92/95 (97%)	91 (99%)	1 (1%)	80	74
5	R	92/95 (97%)	91 (99%)	1 (1%)	80	74
6	F	81/81 (100%)	78 (96%)	3 (4%)	41	23
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	5
7	G	67/68 (98%)	60 (90%)	7 (10%)	9	2
7	T	67/68 (98%)	59 (88%)	8 (12%)	6	1
8	H	71/75 (95%)	68 (96%)	3 (4%)	36	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	69 (97%)	2 (3%)	51	35
9	I	57/57 (100%)	50 (88%)	7 (12%)	6	1
9	V	57/57 (100%)	50 (88%)	7 (12%)	6	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	49
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	49
11	K	39/46 (85%)	37 (95%)	2 (5%)	29	12
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	12
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	37
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16	5
13	M	37/38 (97%)	32 (86%)	5 (14%)	5	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	5	1
All	All	3048/3082 (99%)	2922 (96%)	126 (4%)	37	19

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	109	PHE
2	O	65	TRP
11	X	20	SER
1	N	241	PRO
1	N	443	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	8	GLN
1	N	180	GLN
7	T	76	ASN
10	J	29	ASN
1	N	99	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	8,9,10	2.32	2 (25%)	6,9,11	10.18	3 (50%)
2	FME	B	1	2	8,9,10	3.80	5 (62%)	6,9,11	11.14	4 (66%)
7	TPO	G	11	7	8,10,11	2.40	5 (62%)	7,14,16	1.66	2 (28%)
9	SAC	I	1	9	7,8,9	2.85	3 (42%)	7,9,11	1.46	2 (28%)
1	FME	N	1	1	8,9,10	1.24	1 (12%)	6,9,11	9.52	3 (50%)
2	FME	O	1	2	8,9,10	2.04	3 (37%)	6,9,11	7.10	4 (66%)
7	TPO	T	11	7	8,10,11	2.48	4 (50%)	7,14,16	1.68	2 (28%)
9	SAC	V	1	9	7,8,9	3.12	2 (28%)	7,9,11	1.52	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	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

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-6.01	1.03	1.22
2	O	1	FME	O1-CN	-4.53	1.08	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	FME	O1-CN	-3.08	1.13	1.22
2	B	1	FME	CG-SD	-2.95	1.64	1.81
2	O	1	FME	CG-SD	-2.23	1.68	1.81

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O1-CN-N	-23.08	91.52	124.76
1	A	1	FME	CA-N-CN	-22.50	88.22	122.82
1	N	1	FME	CA-N-CN	-19.41	92.96	122.82
2	O	1	FME	CA-N-CN	-16.83	96.94	122.82
2	B	1	FME	CA-N-CN	-13.91	101.44	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
1	N	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
2	B	1	FME	3	0
7	G	11	TPO	3	0
7	T	11	TPO	2	0
9	V	1	SAC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 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	515	1	40,67,67	1.31	5 (12%)	41,103,103	2.79	20 (48%)
14	HEA	A	516	1,15	40,67,67	1.49	7 (17%)	41,103,103	2.50	13 (31%)
15	NO	A	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.32	6 (9%)	65,65,65	1.83	13 (20%)
20	PGV	A	522	-	50,50,50	1.18	5 (10%)	51,56,56	1.50	10 (19%)
23	CHD	B	1085	-	29,32,32	2.15	9 (31%)	48,51,51	5.30	33 (68%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	229	-	51,51,51	1.23	3 (5%)	55,59,59	1.30	7 (12%)
25	PEK	C	264	-	51,52,52	1.13	4 (7%)	52,57,57	2.35	11 (21%)
20	PGV	C	267	-	50,50,50	0.89	1 (2%)	51,56,56	1.39	12 (23%)
20	PGV	C	268	-	50,50,50	1.30	4 (8%)	51,56,56	1.67	5 (9%)
26	CDL	C	270	-	99,99,99	1.44	15 (15%)	101,111,111	1.82	18 (17%)
23	CHD	C	271	-	29,32,32	0.99	1 (3%)	48,51,51	5.12	32 (66%)
23	CHD	C	525	-	29,32,32	1.56	5 (17%)	48,51,51	5.20	33 (68%)
19	TGL	D	523	-	62,62,62	1.55	7 (11%)	65,65,65	1.74	15 (23%)
25	PEK	G	1263	-	51,52,52	1.43	4 (7%)	52,57,57	1.52	7 (13%)
25	PEK	G	265	-	51,52,52	1.45	4 (7%)	52,57,57	1.66	8 (15%)
26	CDL	G	269	-	99,99,99	1.43	14 (14%)	101,111,111	1.64	22 (21%)
28	DMU	G	272	-	34,34,34	1.42	6 (17%)	45,45,45	3.68	24 (53%)
23	CHD	J	60	-	29,32,32	1.05	2 (6%)	48,51,51	5.16	34 (70%)
19	TGL	L	522	-	62,62,62	1.64	7 (11%)	65,65,65	2.13	16 (24%)
20	PGV	M	524	-	50,50,50	1.17	2 (4%)	51,56,56	1.58	10 (19%)
28	DMU	M	526	-	34,34,34	1.21	4 (11%)	45,45,45	3.67	27 (60%)
20	PGV	N	1266	-	50,50,50	1.20	4 (8%)	51,56,56	1.56	8 (15%)
19	TGL	N	1522	-	62,62,62	1.62	10 (16%)	65,65,65	1.96	17 (26%)
20	PGV	N	1524	-	50,50,50	1.28	4 (8%)	51,56,56	1.43	8 (15%)
14	HEA	N	515	1	40,67,67	1.16	2 (5%)	41,103,103	2.59	16 (39%)
14	HEA	N	516	1,15	40,67,67	1.31	7 (17%)	41,103,103	2.33	18 (43%)
15	NO	N	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	TGL	O	1521	-	62,62,62	1.38	6 (9%)	65,65,65	1.81	12 (18%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.98	10 (34%)	48,51,51	5.54	33 (68%)
25	PEK	P	1264	-	51,52,52	0.93	2 (3%)	52,57,57	2.42	12 (23%)
25	PEK	P	1265	-	51,52,52	1.43	6 (11%)	52,57,57	1.54	9 (17%)
20	PGV	P	1267	-	50,50,50	1.04	2 (4%)	51,56,56	1.65	12 (23%)
20	PGV	P	1268	-	50,50,50	1.41	3 (6%)	51,56,56	1.75	9 (17%)
26	CDL	P	1270	-	99,99,99	1.45	14 (14%)	101,111,111	1.88	23 (22%)
23	CHD	P	1271	-	29,32,32	0.88	1 (3%)	48,51,51	5.33	34 (70%)
28	DMU	P	1272	-	34,34,34	1.65	6 (17%)	45,45,45	3.53	28 (62%)
23	CHD	P	1525	-	29,32,32	1.95	12 (41%)	48,51,51	5.64	35 (72%)
19	TGL	Q	1523	-	62,62,62	1.49	7 (11%)	65,65,65	1.51	10 (15%)
22	PSC	R	1229	-	51,51,51	1.38	3 (5%)	55,59,59	1.33	6 (10%)
26	CDL	T	1269	-	99,99,99	1.34	12 (12%)	101,111,111	1.70	19 (18%)
25	PEK	T	263	-	51,52,52	1.26	4 (7%)	52,57,57	1.45	8 (15%)
23	CHD	W	1059	-	29,32,32	0.90	1 (3%)	48,51,51	5.17	34 (70%)
28	DMU	Z	1526	-	34,34,34	1.13	4 (11%)	45,45,45	3.50	25 (55%)

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	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	NO	A	520	14,16	-	0/0/0/0	0/0/0/0
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
20	PGV	A	522	-	-	0/55/55/55	0/0/0/0
23	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	229	-	-	0/55/55/55	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
23	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
25	PEK	G	265	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
28	DMU	G	272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
20	PGV	M	524	-	-	2/55/55/55	0/0/0/0
28	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	NO	N	520	14,16	-	0/0/0/0	0/0/0/0
19	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	-	0/7/74/74	0/4/4/4
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
23	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
22	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1059	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 235 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1085	CHD	C10-C5	-5.01	1.46	1.55
23	P	1525	CHD	C6-C5	-4.23	1.46	1.53
23	C	525	CHD	C11-C12	-3.77	1.46	1.53
23	B	1085	CHD	C8-C7	-3.67	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	522	TGL	C20-CA9	-3.66	1.30	1.51

The worst 5 of 746 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C18-C13-C12	-11.11	98.26	109.09
23	P	1271	CHD	C23-C22-C20	-10.75	102.07	114.75
23	P	1525	CHD	C23-C22-C20	-10.58	102.27	114.75
23	P	1271	CHD	C18-C13-C12	-10.33	99.01	109.09
23	O	229	CHD	C19-C10-C9	-10.09	96.05	111.18

5 of 38 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C5
28	P	1272	DMU	C6
28	P	1272	DMU	C9
28	P	1272	DMU	C4
28	P	1272	DMU	C2

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C02-O01-C1-O02
20	N	1524	PGV	C02-O01-C1-C2
20	M	524	PGV	C02-O01-C1-O02
20	M	524	PGV	C02-O01-C1-C2

There are no ring outliers.

39 monomers are involved in 370 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	4	0
14	A	516	HEA	5	0
19	A	521	TGL	8	0
23	B	1085	CHD	2	0
22	B	229	PSC	26	0
25	C	264	PEK	8	0
20	C	267	PGV	5	0
20	C	268	PGV	3	0
26	C	270	CDL	26	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	271	CHD	4	0
19	D	523	TGL	8	0
25	G	1263	PEK	24	0
25	G	265	PEK	19	0
26	G	269	CDL	30	0
28	G	272	DMU	4	0
23	J	60	CHD	1	0
19	L	522	TGL	15	0
20	M	524	PGV	15	0
20	N	1266	PGV	1	0
19	N	1522	TGL	15	0
20	N	1524	PGV	8	0
14	N	515	HEA	4	0
14	N	516	HEA	4	0
19	O	1521	TGL	10	0
23	O	229	CHD	3	0
25	P	1264	PEK	7	0
25	P	1265	PEK	17	0
20	P	1267	PGV	5	0
20	P	1268	PGV	1	0
26	P	1270	CDL	25	0
23	P	1271	CHD	5	0
28	P	1272	DMU	6	0
23	P	1525	CHD	1	0
19	Q	1523	TGL	12	0
22	R	1229	PSC	15	0
26	T	1269	CDL	27	0
25	T	263	PEK	21	0
23	W	1059	CHD	1	0
28	Z	1526	DMU	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.06	2 (0%) 93 91	21, 25, 33, 64	0
1	N	513/514 (99%)	0.04	3 (0%) 90 88	24, 28, 36, 63	0
2	B	226/227 (99%)	-0.32	1 (0%) 93 91	20, 30, 48, 68	0
2	O	226/227 (99%)	-0.25	7 (3%) 52 47	25, 34, 58, 80	0
3	C	259/261 (99%)	-0.34	2 (0%) 87 85	23, 27, 39, 61	0
3	P	259/261 (99%)	-0.16	6 (2%) 64 59	25, 30, 41, 58	0
4	D	144/147 (97%)	-0.39	1 (0%) 89 87	27, 34, 48, 64	0
4	Q	144/147 (97%)	0.87	21 (14%) 3 2	31, 40, 65, 115	0
5	E	105/109 (96%)	-0.08	2 (1%) 70 66	28, 33, 58, 98	0
5	R	105/109 (96%)	0.48	7 (6%) 21 17	29, 37, 58, 101	0
6	F	98/98 (100%)	0.38	8 (8%) 14 11	26, 35, 79, 127	0
6	S	98/98 (100%)	0.27	7 (7%) 19 15	27, 37, 85, 121	0
7	G	83/85 (97%)	0.82	17 (20%) 1 1	25, 33, 90, 108	0
7	T	83/85 (97%)	0.89	17 (20%) 1 1	26, 34, 91, 107	0
8	H	79/85 (92%)	0.26	11 (13%) 4 3	27, 37, 83, 109	0
8	U	79/85 (92%)	0.47	13 (16%) 2 2	30, 41, 88, 109	0
9	I	72/73 (98%)	0.20	3 (4%) 40 34	28, 40, 57, 67	0
9	V	72/73 (98%)	0.66	8 (11%) 7 5	30, 44, 61, 77	0
10	J	58/59 (98%)	0.41	8 (13%) 4 3	27, 35, 56, 97	0
10	W	58/59 (98%)	0.56	9 (15%) 3 2	29, 37, 57, 102	0
11	K	49/56 (87%)	0.31	4 (8%) 14 11	30, 37, 52, 66	0
11	X	49/56 (87%)	1.69	17 (34%) 0 0	34, 42, 56, 72	0
12	L	46/47 (97%)	-0.37	2 (4%) 39 32	25, 31, 48, 73	0
12	Y	46/47 (97%)	-0.26	1 (2%) 65 60	29, 34, 51, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.11	4 (9%) 11 8	27, 31, 69, 98	0
13	Z	43/46 (93%)	0.66	8 (18%) 2 1	32, 37, 79, 106	0
All	All	3550/3614 (98%)	0.11	189 (5%) 30 25	20, 31, 58, 127	0

The worst 5 of 189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	15.6
4	Q	5	VAL	14.6
6	F	1	ALA	13.9
6	S	1	ALA	13.9
6	S	97	ALA	12.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.63	0.55	-	83,86,88,88	0
7	TPO	G	11	11/12	0.50	0.31	-	66,75,101,101	0
2	FME	B	1	10/11	0.97	0.11	-	20,30,40,52	0
2	FME	O	1	10/11	0.96	0.10	-	33,34,40,48	0
1	FME	N	1	10/11	0.91	0.13	-	42,48,77,80	0
7	TPO	T	11	11/12	0.43	0.35	-	71,80,101,104	0
9	SAC	I	1	9/10	0.87	0.30	-	63,66,69,73	0
1	FME	A	1	10/11	0.94	0.12	-	38,41,68,76	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
20	PGV	M	524	51/51	0.80	0.25	11.05	40,70,127,129	0
28	DMU	G	272	33/33	0.39	0.34	9.93	72,100,115,116	0
28	DMU	P	1272	33/33	0.40	0.35	9.06	72,106,119,121	0
23	CHD	W	1059	29/29	0.68	0.39	7.88	101,108,110,112	0
23	CHD	J	60	29/29	0.60	0.41	6.21	99,104,108,108	0
26	CDL	P	1270	100/100	0.71	0.28	5.84	36,86,117,120	0
19	TGL	N	1522	63/63	0.65	0.25	5.45	49,64,84,89	0
26	CDL	C	270	100/100	0.77	0.27	4.91	42,84,109,110	0
19	TGL	D	523	63/63	0.74	0.20	4.74	53,67,97,99	0
19	TGL	L	522	63/63	0.77	0.23	4.59	36,62,78,81	0
19	TGL	A	521	63/63	0.81	0.18	4.49	53,72,88,92	0
19	TGL	O	1521	63/63	0.80	0.17	3.81	53,75,88,92	0
19	TGL	Q	1523	63/63	0.72	0.22	3.81	56,74,100,102	0
20	PGV	N	1524	51/51	0.72	0.30	3.73	41,76,121,123	0
17	MG	N	518	1/1	0.97	0.12	2.66	29,29,29,29	0
20	PGV	C	268	51/51	0.73	0.31	2.59	51,79,108,111	0
28	DMU	M	526	33/33	0.91	0.14	2.55	35,44,61,65	0
26	CDL	T	1269	100/100	0.59	0.28	2.44	59,86,115,118	0
22	PSC	B	229	52/52	0.67	0.32	2.39	45,95,136,139	0
28	DMU	Z	1526	33/33	0.82	0.25	2.38	40,50,71,75	0
25	PEK	G	1263	53/53	0.55	0.43	2.31	51,96,123,124	0
26	CDL	G	269	100/100	0.62	0.25	2.06	58,86,116,120	0
20	PGV	P	1268	51/51	0.70	0.32	2.03	57,77,111,112	0
22	PSC	R	1229	52/52	0.58	0.30	1.77	49,95,129,135	0
21	CUA	B	228	2/2	1.00	0.12	1.37	23,23,23,23	0
25	PEK	T	263	53/53	0.60	0.32	1.30	48,94,121,122	0
20	PGV	C	267	51/51	0.96	0.11	1.27	22,33,73,74	0
17	MG	A	518	1/1	0.98	0.13	1.25	24,24,24,24	0
20	PGV	P	1267	51/51	0.94	0.13	1.22	23,37,80,82	0
23	CHD	P	1271	29/29	0.90	0.20	1.15	51,63,68,69	0
25	PEK	P	1264	53/53	0.93	0.14	1.15	25,49,81,82	0
25	PEK	P	1265	53/53	0.43	0.30	0.99	46,76,107,110	0
23	CHD	C	525	29/29	0.97	0.14	0.98	21,30,35,38	0
25	PEK	G	265	53/53	0.55	0.27	0.89	47,79,103,105	0
25	PEK	C	264	53/53	0.95	0.12	0.84	24,45,77,80	0
23	CHD	C	271	29/29	0.89	0.19	0.82	54,61,65,73	0
27	ZN	F	99	1/1	0.98	0.08	0.68	31,31,31,31	0
14	HEA	N	516	60/60	0.99	0.13	0.67	22,26,31,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
20	PGV	N	1266	51/51	0.95	0.13	0.63	23,36,59,64	0
23	CHD	P	1525	29/29	0.96	0.14	0.59	27,31,35,37	0
20	PGV	A	522	51/51	0.97	0.11	0.43	20,33,67,71	0
16	CU	A	517	1/1	1.00	0.14	0.20	24,24,24,24	0
27	ZN	S	99	1/1	0.99	0.09	0.11	33,33,33,33	0
21	CUA	O	228	2/2	0.99	0.09	-0.04	27,27,27,27	0
14	HEA	A	516	60/60	0.99	0.12	-0.23	19,22,30,34	0
14	HEA	N	515	60/60	0.98	0.10	-0.27	21,26,40,44	0
14	HEA	A	515	60/60	0.99	0.11	-0.29	19,23,38,41	0
23	CHD	B	1085	29/29	0.97	0.08	-0.35	23,26,31,37	0
23	CHD	O	229	29/29	0.97	0.08	-0.43	21,25,31,33	0
18	NA	N	519	1/1	0.96	0.07	-0.59	31,31,31,31	0
18	NA	A	519	1/1	0.98	0.07	-0.63	28,28,28,28	0
15	NO	A	520	2/2	0.98	0.10	-1.90	24,24,24,25	0
15	NO	N	520	2/2	0.99	0.08	-2.21	26,26,26,31	0
24	UNX	C	262	1/1	0.40	0.47	-	81,81,81,81	0
16	CU	N	517	1/1	1.00	0.15	-	26,26,26,26	0
24	UNX	P	262	1/1	0.66	0.42	-	82,82,82,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.