



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AG1  
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 280 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 : 2.20 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

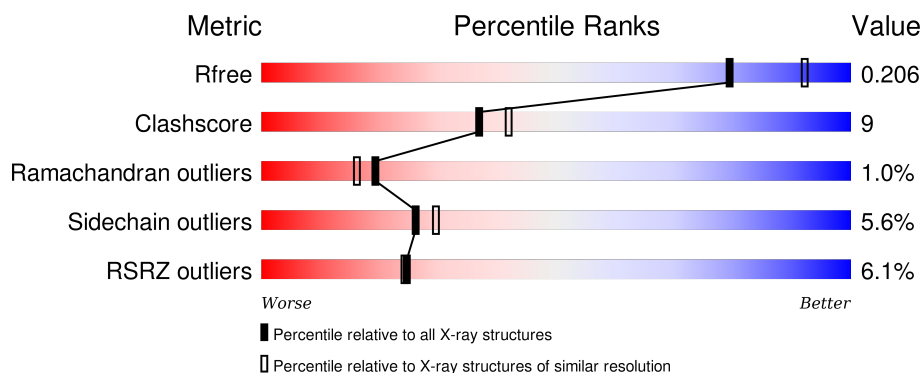
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



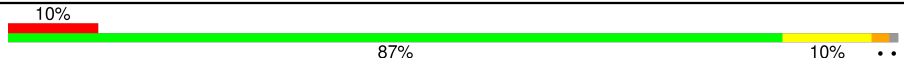

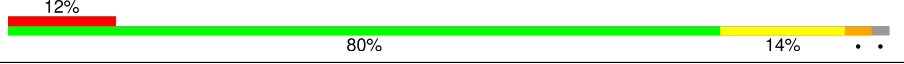
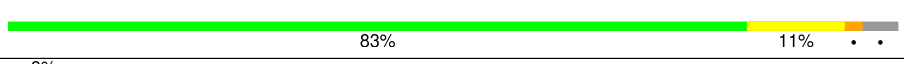

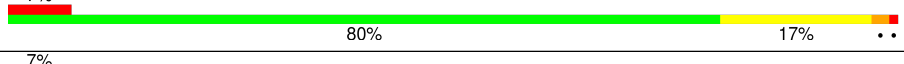


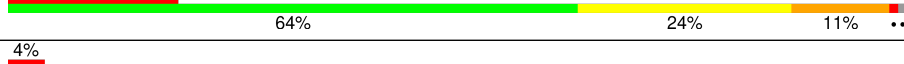


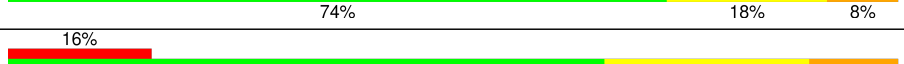

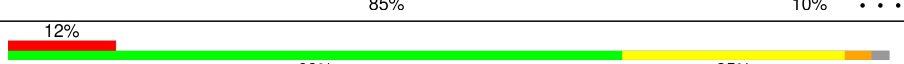
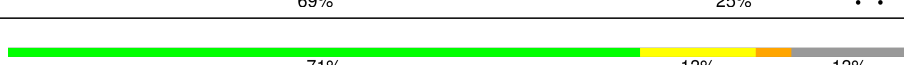
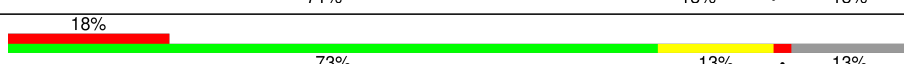
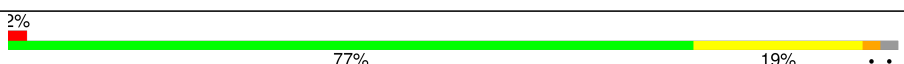
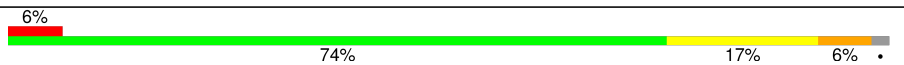
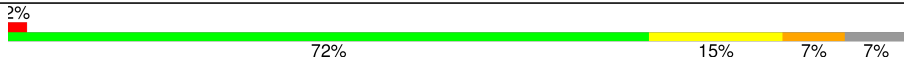

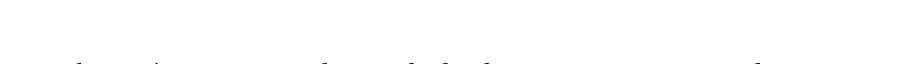
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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>3%</div> <div>85% 13% •</div> </div>
1	N	514	<div> <div>2%</div> <div>86% 12% •</div> </div>
2	B	227	<div> <div>68% 27% • •</div> </div>
2	O	227	<div> <div>4%</div> <div>75% 19% 5%</div> </div>
3	C	261	<div> <div>8%</div> <div>87% 10% • •</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	A	518	-	-	-	X
18	NA	N	519	-	-	-	X
19	TGL	A	523	-	-	-	X
19	TGL	B	521	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1521	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	N	1523	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	C	268	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	PSC	B	229	-	-	-	X
22	PSC	R	1229	-	-	-	X
23	CHD	B	1085	X	-	-	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	-	-	-	X
23	CHD	W	1059	X	-	-	X
25	CDL	C	270	-	-	X	X
25	CDL	G	269	-	-	X	X
25	CDL	P	1270	-	-	-	X
25	CDL	T	1269	-	-	X	X
26	DMU	C	272	X	-	-	X
26	DMU	M	526	X	-	-	-
26	DMU	T	1272	X	-	-	X
26	DMU	Z	1526	X	-	-	-
27	ZN	F	99	-	-	-	X
28	PEK	G	1263	-	-	-	X
28	PEK	T	263	-	-	-	X

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32105 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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			

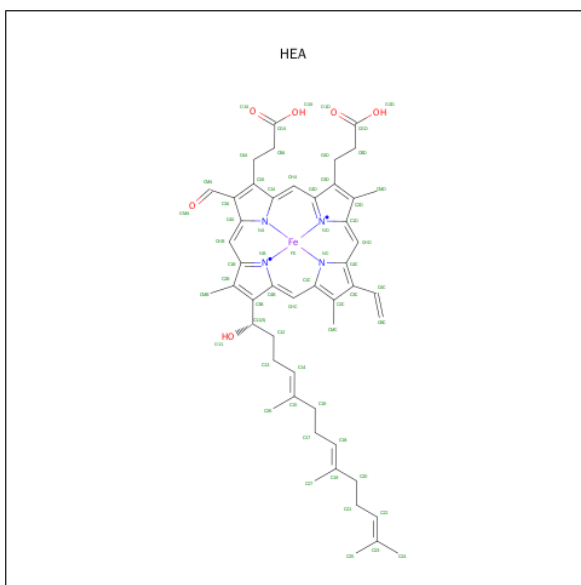
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

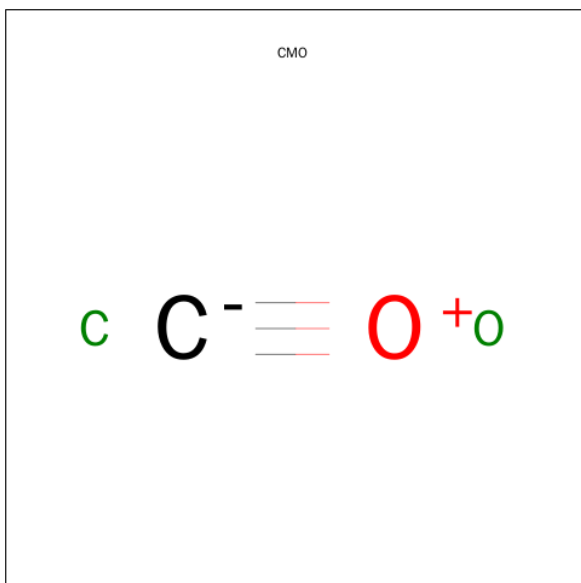
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- 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 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 CARBON MONOXIDE (three-letter code: CMO) (formula: CO).





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

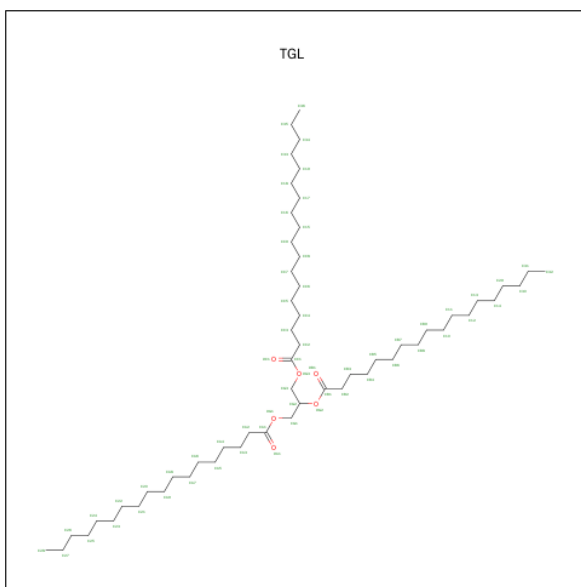
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

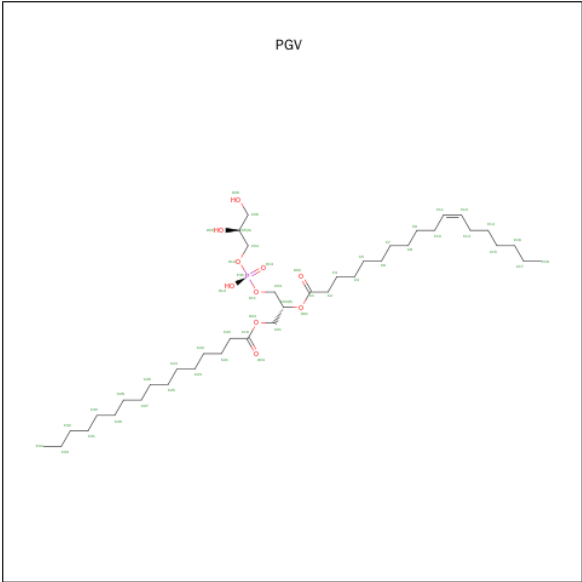
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



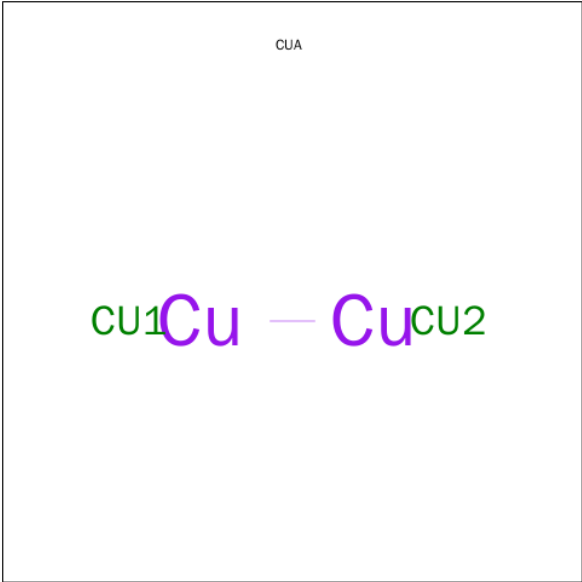
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		

- 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).



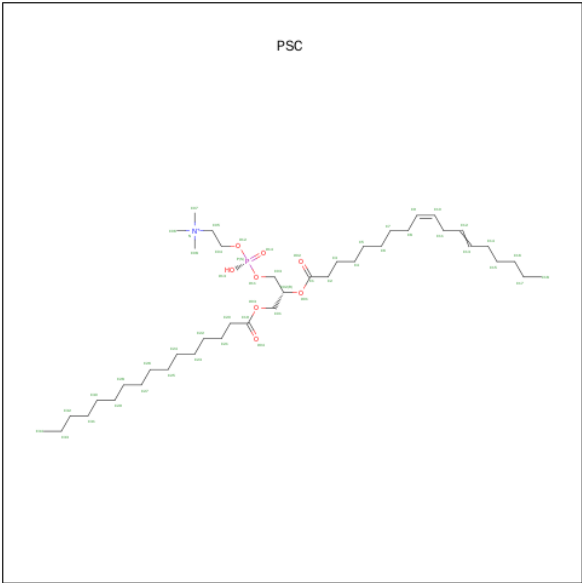
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

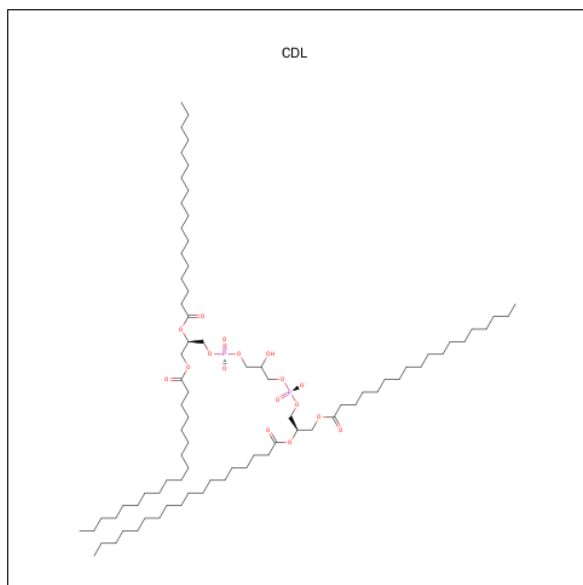
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- ORTEP diagram of the chemical structure of compound 1. The structure is a complex polycyclic molecule with a steroid-like core. The atoms are labeled as follows: Carbon (C1-C26), Oxygen (O1-O3), and Hydrogen (H1-H14). The structure is shown with thermal ellipsoids at the 50% probability level. The molecule features a complex polycyclic system with a central ring system and several side chains. The stereochemistry is indicated by wedged and dashed bonds. The molecule is shown in a perspective view, with the central ring system in the foreground and the side chains extending outwards.

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

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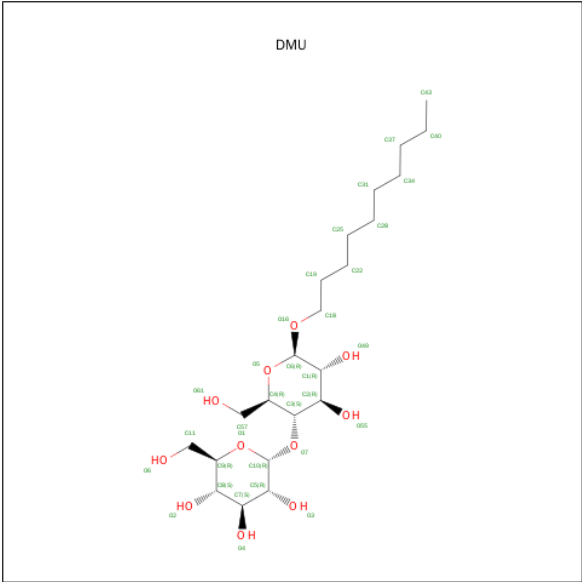
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 26 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).

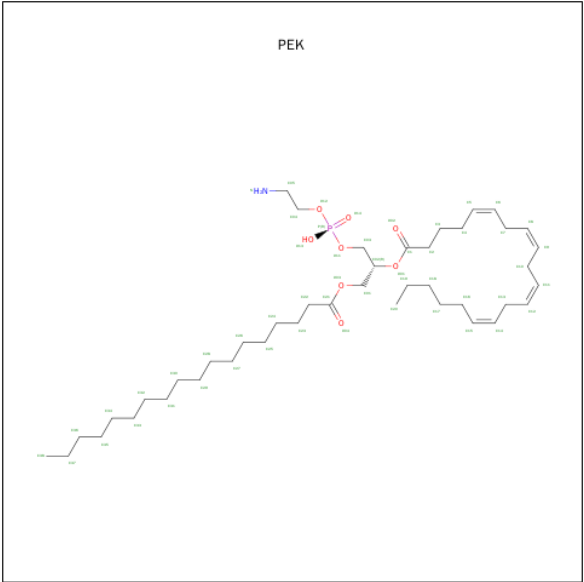


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	M	1	Total	C	O	0	0
			33	22	11		
26	T	1	Total	C	O	0	0
			33	22	11		
26	Z	1	Total	C	O	0	0
			33	22	11		

- 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 (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
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	205	Total	O	0	0
			205	205		
29	B	121	Total	O	0	0
			121	121		
29	C	80	Total	O	0	0
			80	80		
29	D	75	Total	O	0	0
			75	75		
29	E	39	Total	O	0	0
			39	39		
29	F	70	Total	O	0	0
			70	70		

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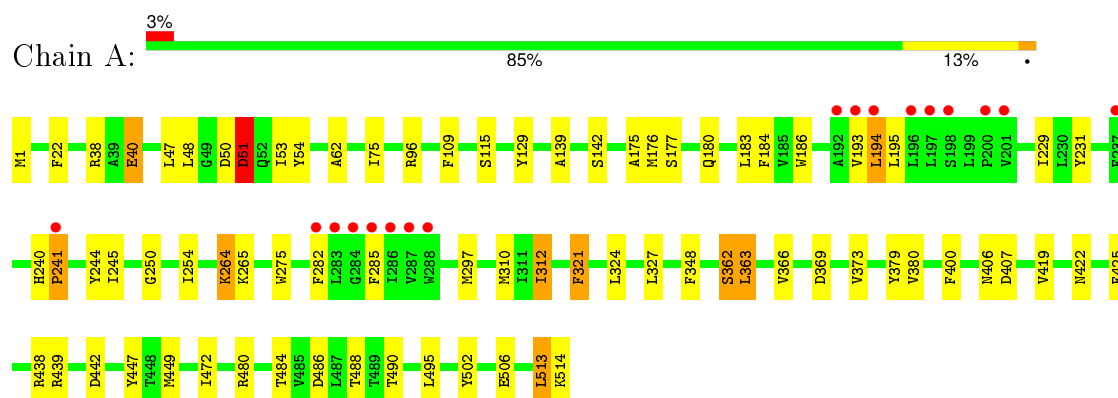
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	G	42	Total 42	O 42	0	0
29	H	33	Total 33	O 33	0	0
29	I	24	Total 24	O 24	0	0
29	J	9	Total 9	O 9	0	0
29	K	17	Total 17	O 17	0	0
29	L	20	Total 20	O 20	0	0
29	M	15	Total 15	O 15	0	0
29	N	184	Total 184	O 184	0	0
29	O	97	Total 97	O 97	0	0
29	P	81	Total 81	O 81	0	0
29	Q	47	Total 47	O 47	0	0
29	R	27	Total 27	O 27	0	0
29	S	52	Total 52	O 52	0	0
29	T	37	Total 37	O 37	0	0
29	U	28	Total 28	O 28	0	0
29	V	17	Total 17	O 17	0	0
29	W	12	Total 12	O 12	0	0
29	X	12	Total 12	O 12	0	0
29	Y	16	Total 16	O 16	0	0
29	Z	9	Total 9	O 9	0	0

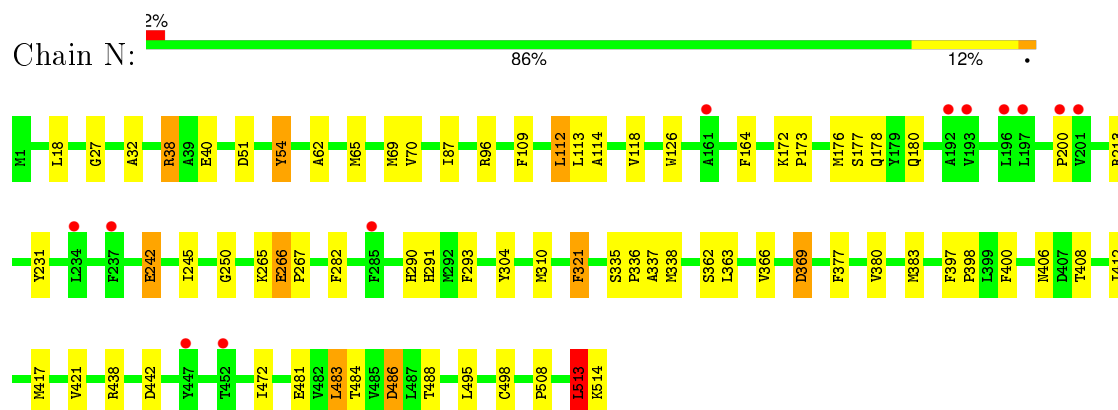
### 3 Residue-property plots [i](#)

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

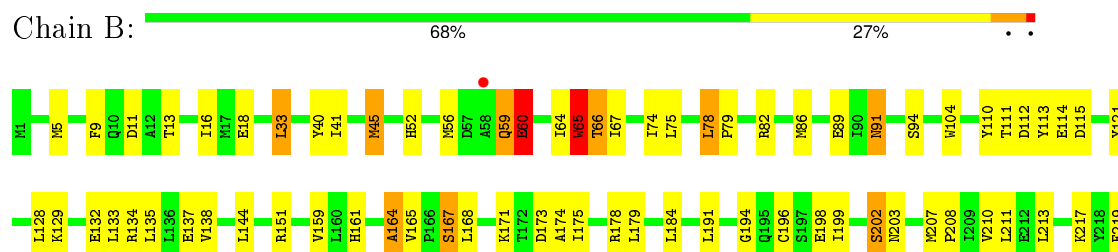
#### • Molecule 1: Cytochrome c oxidase subunit 1



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

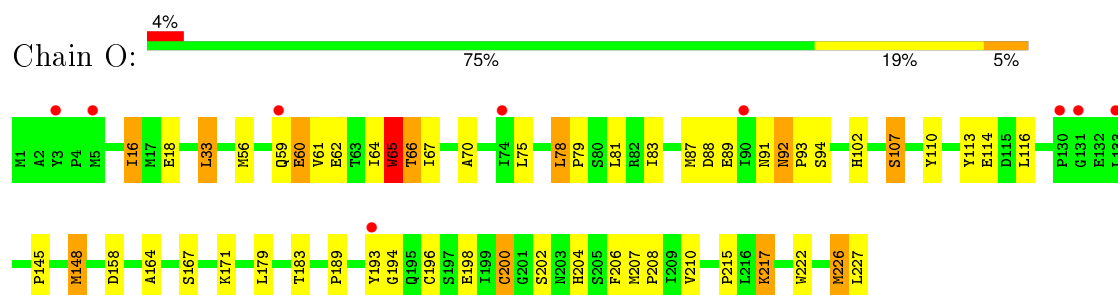


#### • Molecule 2: Cytochrome c oxidase subunit 2

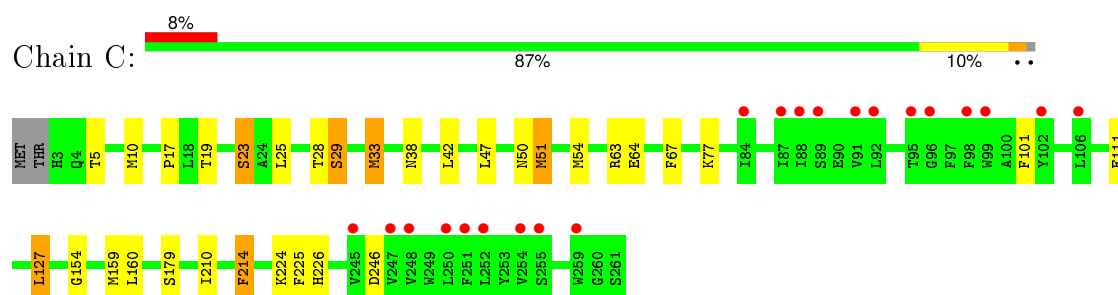




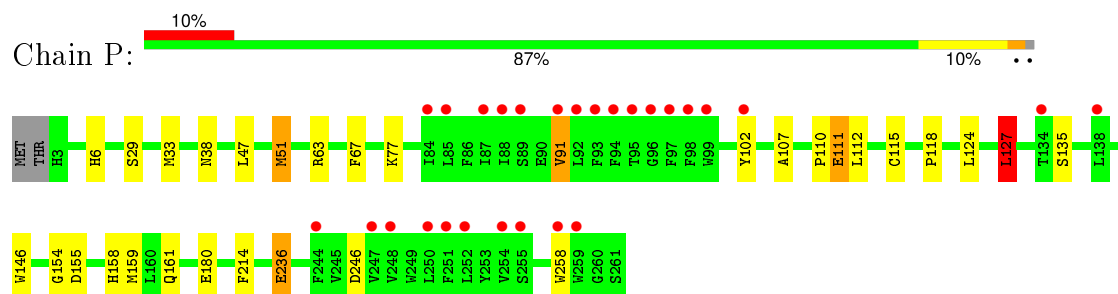
• Molecule 2: Cytochrome c oxidase subunit 2



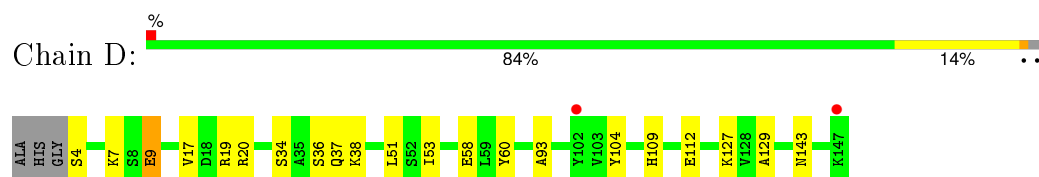
• Molecule 3: Cytochrome c oxidase subunit 3



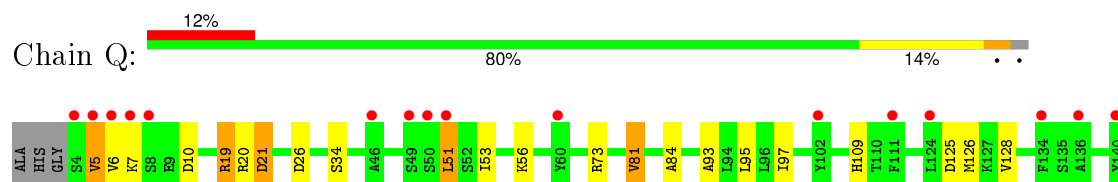
• Molecule 3: Cytochrome c oxidase subunit 3

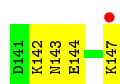


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



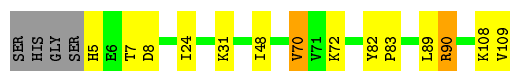
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1





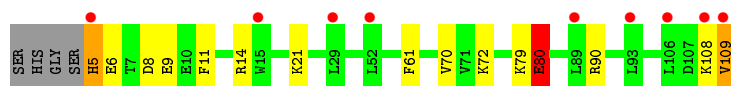
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 83% 11% ..



- Molecule 5: Cytochrome c oxidase subunit 5A

Chain R: 8% 83% 11% ..



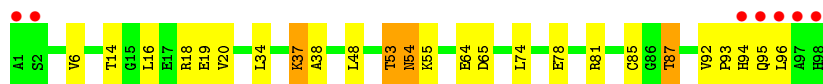
- Molecule 6: Cytochrome c oxidase subunit 5B

Chain F: 7% 80% 17% ..



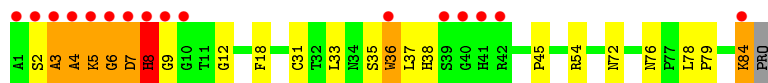
- Molecule 6: Cytochrome c oxidase subunit 5B

Chain S: 7% 74% 21% .



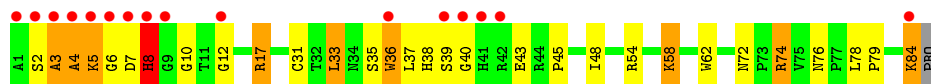
- Molecule 7: Cytochrome c oxidase subunit 6A2

Chain G: 19% 72% 18% 8% ..



- Molecule 7: Cytochrome c oxidase subunit 6A2

Chain T: 19% 64% 24% 11% ..

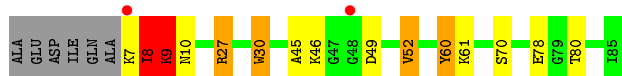
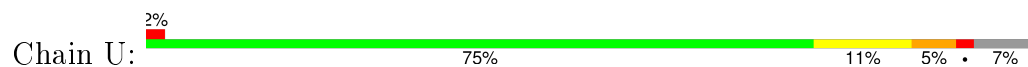


- Molecule 8: Cytochrome c oxidase subunit 6B1

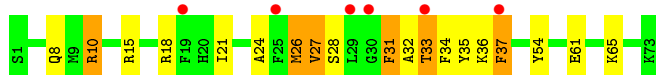
Chain H: 4% 75% 13% . . 7%



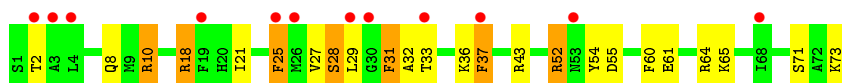
- Molecule 8: Cytochrome c oxidase subunit 6B1



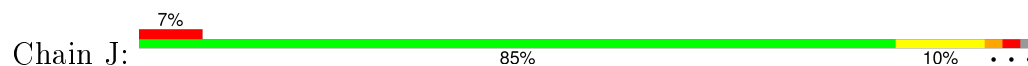
- Molecule 9: Cytochrome c oxidase subunit 6C



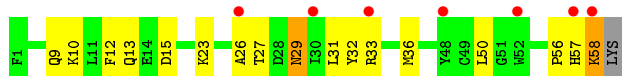
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1

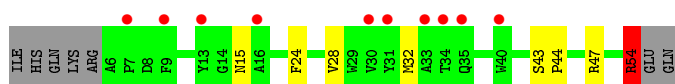


- Molecule 11: Cytochrome c oxidase subunit 7B

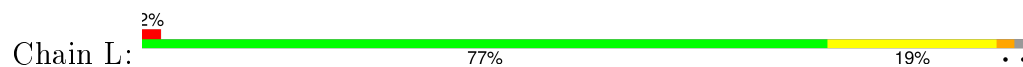


- Molecule 11: Cytochrome c oxidase subunit 7B

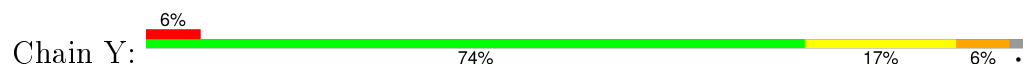




- Molecule 12: Cytochrome c oxidase subunit 7C



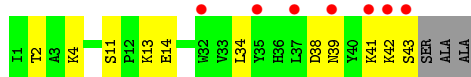
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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, $\alpha$ , $\beta$ , $\gamma$	189.49Å 210.89Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 94.75 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 99.2 (94.75-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, $R_{free}$	0.162 , 0.192 0.178 , 0.206	Depositor DCC
$R_{free}$ test set	17411 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 352235 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: CMO, ZN, CHD, HEA, SAC, CDL, PSC, PEK, 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	1.52	24/4156 (0.6%)	1.14	17/5678 (0.3%)
1	N	1.30	13/4156 (0.3%)	1.00	9/5678 (0.2%)
2	B	1.52	17/1860 (0.9%)	1.22	15/2534 (0.6%)
2	O	1.19	5/1860 (0.3%)	1.02	3/2534 (0.1%)
3	C	1.44	6/2197 (0.3%)	1.00	2/3005 (0.1%)
3	P	1.26	7/2197 (0.3%)	0.96	4/3005 (0.1%)
4	D	1.42	8/1229 (0.7%)	1.12	1/1658 (0.1%)
4	Q	1.10	2/1229 (0.2%)	0.98	6/1658 (0.4%)
5	E	1.26	2/871 (0.2%)	1.07	3/1182 (0.3%)
5	R	1.03	2/871 (0.2%)	0.93	1/1182 (0.1%)
6	F	1.47	3/765 (0.4%)	1.25	4/1038 (0.4%)
6	S	1.25	2/765 (0.3%)	1.09	3/1038 (0.3%)
7	G	1.38	2/690 (0.3%)	1.12	3/937 (0.3%)
7	T	1.43	4/690 (0.6%)	1.09	4/937 (0.4%)
8	H	1.29	1/682 (0.1%)	1.01	1/921 (0.1%)
8	U	1.09	1/682 (0.1%)	0.94	0/921
9	I	1.45	3/605 (0.5%)	1.13	3/802 (0.4%)
9	V	1.31	2/605 (0.3%)	1.10	4/802 (0.5%)
10	J	1.35	0/471	1.12	2/636 (0.3%)
10	W	1.10	1/471 (0.2%)	0.98	0/636
11	K	1.34	3/398 (0.8%)	1.16	2/546 (0.4%)
11	X	0.97	0/398	0.93	1/546 (0.2%)
12	L	1.49	1/393 (0.3%)	1.07	1/526 (0.2%)
12	Y	1.10	0/393	0.98	1/526 (0.2%)
13	M	1.20	0/345	1.15	2/470 (0.4%)
13	Z	0.98	0/345	0.97	0/470
All	All	1.33	109/29324 (0.4%)	1.06	92/39866 (0.2%)

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
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	4

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	36	TRP	CB-CG	12.12	1.72	1.50
7	G	36	TRP	CB-CG	10.31	1.68	1.50
7	T	58	LYS	CE-NZ	9.32	1.72	1.49
2	O	198	GLU	C-O	8.13	1.38	1.23
2	B	198	GLU	C-O	7.69	1.38	1.23

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	32	MET	CG-SD-CE	8.85	114.36	100.20
6	F	18	ARG	NE-CZ-NH2	-8.74	115.93	120.30
4	D	20	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	176	MET	CG-SD-CE	-8.47	86.66	100.20
2	B	112	ASP	CB-CG-OD2	-8.21	110.91	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	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	4027	0	4001	38	0
1	N	4027	0	4001	48	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	22	0
3	P	2110	0	2027	22	0
4	D	1195	0	1183	9	0
4	Q	1195	0	1183	15	0
5	E	852	0	845	11	0
5	R	852	0	845	9	0
6	F	748	0	728	10	0
6	S	748	0	728	14	0
7	G	675	0	643	26	0
7	T	675	0	644	41	0
8	H	662	0	623	8	0
8	U	662	0	623	12	0
9	I	601	0	613	22	0
9	V	601	0	613	25	0
10	J	460	0	459	5	0
10	W	460	0	459	12	0
11	K	384	0	366	3	0
11	X	384	0	366	6	0
12	L	380	0	380	14	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0
14	A	120	0	108	4	0
14	N	120	0	108	7	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	3	0
19	B	63	0	109	9	0
19	L	63	0	110	19	0
19	N	189	0	330	21	0
20	A	102	0	152	13	0
20	C	102	0	152	7	0
20	N	102	0	152	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	102	0	152	7	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	17	0
22	R	52	0	80	16	0
23	B	29	0	37	3	0
23	C	58	0	71	3	0
23	J	29	0	36	2	0
23	O	29	0	37	1	0
23	P	58	0	72	4	0
23	W	29	0	36	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	100	0	156	22	0
25	G	100	0	156	24	0
25	P	100	0	156	16	0
25	T	100	0	156	23	0
26	C	33	0	38	2	0
26	M	33	0	38	0	0
26	T	33	0	39	6	0
26	Z	33	0	39	1	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	22	0
28	S	53	0	77	6	0
28	T	106	0	154	19	0
29	A	205	0	0	3	0
29	B	121	0	0	3	0
29	C	80	0	0	2	0
29	D	75	0	0	1	0
29	E	39	0	0	1	0
29	F	70	0	0	2	0
29	G	42	0	0	5	0
29	H	33	0	0	5	0
29	I	24	0	0	1	0
29	J	9	0	0	0	0
29	K	17	0	0	0	0
29	L	20	0	0	2	0
29	M	15	0	0	0	0
29	N	184	0	0	6	0
29	O	97	0	0	2	0
29	P	81	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Q	47	0	0	2	0
29	R	27	0	0	0	0
29	S	52	0	0	1	0
29	T	37	0	0	8	0
29	U	28	0	0	4	0
29	V	17	0	0	4	0
29	W	12	0	0	2	0
29	X	12	0	0	1	0
29	Y	16	0	0	0	0
29	Z	9	0	0	0	0
All	All	32105	0	31279	581	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 9.

The worst 5 of 581 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)
1:A:75:ILE:CG1	1:A:75:ILE:CD1	1.76	1.62
28:G:265:PEK:C6	28:G:265:PEK:C7	1.81	1.53
7:T:58:LYS:NZ	7:T:58:LYS:CE	1.72	1.47
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.40	1.36
7:T:45:PRO:CD	29:T:3099:HOH:O	1.75	1.35

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
1	N	512/514 (100%)	495 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	39	42
2	O	225/227 (99%)	212 (94%)	12 (5%)	1 (0%)	39	42
3	C	257/261 (98%)	253 (98%)	3 (1%)	1 (0%)	39	42
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	39	42
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	132 (93%)	9 (6%)	1 (1%)	26	25
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%)	88 (92%)	5 (5%)	3 (3%)	5	2
6	S	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	9	5
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2	0
7	T	81/85 (95%)	65 (80%)	11 (14%)	5 (6%)	2	0
8	H	77/85 (91%)	66 (86%)	5 (6%)	6 (8%)	1	0
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	1
9	I	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	6	3
9	V	71/73 (97%)	64 (90%)	4 (6%)	3 (4%)	3	1
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	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%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	7	4
All	All	3504/3614 (97%)	3339 (95%)	129 (4%)	36 (1%)	19	16

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	3	ALA
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	426/426 (100%)	416 (98%)	10 (2%)	58	71
1	N	426/426 (100%)	414 (97%)	12 (3%)	51	63
2	B	210/210 (100%)	199 (95%)	11 (5%)	29	33
2	O	210/210 (100%)	191 (91%)	19 (9%)	12	11
3	C	224/226 (99%)	216 (96%)	8 (4%)	42	52
3	P	224/226 (99%)	220 (98%)	4 (2%)	66	79
4	D	128/129 (99%)	122 (95%)	6 (5%)	32	39
4	Q	128/129 (99%)	121 (94%)	7 (6%)	27	30
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	56
5	R	92/95 (97%)	84 (91%)	8 (9%)	13	12
6	F	81/81 (100%)	76 (94%)	5 (6%)	23	25
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	17
7	G	67/68 (98%)	60 (90%)	7 (10%)	9	8
7	T	67/68 (98%)	59 (88%)	8 (12%)	6	5
8	H	71/75 (95%)	66 (93%)	5 (7%)	19	19
8	U	71/75 (95%)	64 (90%)	7 (10%)	10	9
9	I	57/57 (100%)	50 (88%)	7 (12%)	6	5
9	V	57/57 (100%)	48 (84%)	9 (16%)	3	2
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	76
10	W	49/50 (98%)	43 (88%)	6 (12%)	6	5
11	K	39/46 (85%)	36 (92%)	3 (8%)	16	16
11	X	39/46 (85%)	36 (92%)	3 (8%)	16	16
12	L	39/40 (98%)	37 (95%)	2 (5%)	29	34
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16	16
13	M	37/38 (97%)	32 (86%)	5 (14%)	5	3
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3040/3082 (99%)	2871 (94%)	169 (6%)	26	29

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	112	LEU
2	O	107	SER
10	W	29	ASN
1	N	338	MET
2	O	16	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	2	HIS
1	N	180	GLN
8	U	22	ASN
1	N	178	GLN
1	N	512	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	0.76	0	6,9,11	5.94	5 (83%)
2	FME	B	1	2	8,9,10	1.32	1 (12%)	6,9,11	7.17	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	TPO	G	11	7	8,10,11	2.23	4 (50%)	7,14,16	2.37	2 (28%)
9	SAC	I	1	9	7,8,9	3.70	2 (28%)	7,9,11	3.57	3 (42%)
1	FME	N	1	1	8,9,10	0.90	0	6,9,11	5.05	3 (50%)
2	FME	O	1	2	8,9,10	0.84	0	6,9,11	4.49	3 (50%)
7	TPO	T	11	7	8,10,11	2.26	5 (62%)	7,14,16	2.31	2 (28%)
9	SAC	V	1	9	7,8,9	3.70	3 (42%)	7,9,11	2.78	4 (57%)

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 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.19	1.12	1.22
7	T	11	TPO	P-O2P	2.08	1.62	1.54
7	G	11	TPO	P-O3P	2.14	1.62	1.54
7	T	11	TPO	CG2-CB	2.32	1.57	1.51
7	G	11	TPO	P-O2P	2.32	1.63	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.81	96.98	122.82
1	A	1	FME	CA-N-CN	-12.33	103.86	122.82
1	N	1	FME	CA-N-CN	-10.28	107.00	122.82
2	O	1	FME	CA-N-CN	-9.32	108.49	122.82
9	I	1	SAC	CB-CA-N	-7.68	93.78	110.60

There are no chirality outliers.



All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	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	1.52	8 (20%)	41,103,103	2.82	13 (31%)
14	HEA	A	516	1	40,67,67	1.36	6 (15%)	41,103,103	2.37	13 (31%)
15	CMO	A	520	-	0,1,1	0.00	-	0,0,0	0.00	-
20	PGV	A	521	-	50,50,50	0.81	2 (4%)	51,56,56	1.75	8 (15%)
19	TGL	A	523	-	62,62,62	1.38	6 (9%)	65,65,65	1.73	11 (16%)
20	PGV	A	524	-	50,50,50	1.30	4 (8%)	51,56,56	1.46	7 (13%)
23	CHD	B	1085	-	29,32,32	1.54	4 (13%)	48,51,51	5.60	36 (75%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	229	-	51,51,51	1.37	3 (5%)	55,59,59	1.34	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	TGL	B	521	-	62,62,62	1.45	8 (12%)	65,65,65	2.64	16 (24%)
20	PGV	C	267	-	50,50,50	0.88	2 (4%)	51,56,56	1.23	7 (13%)
20	PGV	C	268	-	50,50,50	1.41	2 (4%)	51,56,56	1.76	9 (17%)
25	CDL	C	270	-	99,99,99	1.40	14 (14%)	101,111,111	1.46	15 (14%)
23	CHD	C	271	-	29,32,32	0.83	1 (3%)	48,51,51	5.01	33 (68%)
26	DMU	C	272	-	34,34,34	1.30	5 (14%)	45,45,45	3.46	21 (46%)
23	CHD	C	525	-	29,32,32	1.34	3 (10%)	48,51,51	5.10	37 (77%)
28	PEK	G	1263	-	51,52,52	1.39	5 (9%)	52,57,57	1.58	8 (15%)
28	PEK	G	264	-	51,52,52	1.03	5 (9%)	52,57,57	1.64	11 (21%)
28	PEK	G	265	-	51,52,52	1.70	7 (13%)	52,57,57	1.63	9 (17%)
25	CDL	G	269	-	99,99,99	1.41	13 (13%)	101,111,111	1.46	17 (16%)
23	CHD	J	60	-	29,32,32	0.88	0	48,51,51	5.36	36 (75%)
19	TGL	L	522	-	62,62,62	1.66	10 (16%)	65,65,65	2.01	16 (24%)
26	DMU	M	526	-	34,34,34	1.24	2 (5%)	45,45,45	3.50	22 (48%)
20	PGV	N	1266	-	50,50,50	0.83	2 (4%)	51,56,56	1.41	6 (11%)
19	TGL	N	1521	-	62,62,62	1.39	9 (14%)	65,65,65	2.29	14 (21%)
19	TGL	N	1522	-	62,62,62	1.60	7 (11%)	65,65,65	1.81	17 (26%)
19	TGL	N	1523	-	62,62,62	1.40	7 (11%)	65,65,65	1.46	10 (15%)
20	PGV	N	1524	-	50,50,50	1.22	2 (4%)	51,56,56	1.27	7 (13%)
14	HEA	N	515	1	40,67,67	1.28	5 (12%)	41,103,103	2.63	15 (36%)
14	HEA	N	516	1,15	40,67,67	1.49	6 (15%)	41,103,103	2.39	14 (34%)
15	CMO	N	520	14	0,1,1	0.00	-	0,0,0	0.00	-
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.45	4 (13%)	48,51,51	5.50	35 (72%)
20	PGV	P	1267	-	50,50,50	0.99	2 (4%)	51,56,56	1.03	4 (7%)
20	PGV	P	1268	-	50,50,50	1.37	2 (4%)	51,56,56	1.64	9 (17%)
25	CDL	P	1270	-	99,99,99	1.42	13 (13%)	101,111,111	1.44	12 (11%)
23	CHD	P	1271	-	29,32,32	0.78	1 (3%)	48,51,51	5.24	34 (70%)
23	CHD	P	1525	-	29,32,32	1.03	2 (6%)	48,51,51	5.41	36 (75%)
22	PSC	R	1229	-	51,51,51	1.33	3 (5%)	55,59,59	1.28	4 (7%)
28	PEK	S	1265	-	51,52,52	1.26	2 (3%)	52,57,57	1.39	6 (11%)
28	PEK	T	1264	-	51,52,52	0.91	4 (7%)	52,57,57	1.49	10 (19%)
25	CDL	T	1269	-	99,99,99	1.47	13 (13%)	101,111,111	1.53	13 (12%)
26	DMU	T	1272	-	34,34,34	1.33	3 (8%)	45,45,45	3.22	23 (51%)
28	PEK	T	263	-	51,52,52	1.40	4 (7%)	52,57,57	1.29	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CHD	W	1059	-	29,32,32	0.58	0	48,51,51	5.10	35 (72%)
26	DMU	Z	1526	-	34,34,34	0.98	3 (8%)	45,45,45	3.21	21 (46%)

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	3/3/7/16	0/24/76/76	0/0/8/8
15	CMO	A	520	-	-	0/0/0/0	0/0/0/0
20	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	TGL	A	523	-	-	0/65/65/65	0/0/0/0
20	PGV	A	524	-	-	2/55/55/55	0/0/0/0
23	CHD	B	1085	-	1/1/12/12	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
19	TGL	B	521	-	-	0/65/65/65	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
25	CDL	C	270	-	-	1/110/110/110	0/0/0/0
23	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
26	DMU	C	272	-	5/5/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
28	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
28	PEK	G	264	-	-	0/56/56/56	0/0/0/0
28	PEK	G	265	-	-	0/56/56/56	0/0/0/0
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
23	CHD	J	60	-	1/1/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
26	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	1/55/55/55	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	CMO	N	520	14	-	0/0/0/0	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	O	229	-	1/1/12/12	0/7/74/74	0/4/4/4
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	1/110/110/110	0/0/0/0
23	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
22	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
28	PEK	S	1265	-	-	0/56/56/56	0/0/0/0
28	PEK	T	1264	-	-	0/56/56/56	0/0/0/0
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
26	DMU	T	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
28	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1059	-	2/2/12/12	0/7/74/74	0/4/4/4
26	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	521	TGL	OC1-CC1	-4.65	1.08	1.22
26	M	526	DMU	C3-C4	-3.83	1.42	1.52
23	O	229	CHD	C13-C14	-3.63	1.49	1.55
14	N	516	HEA	C3A-C2A	-3.54	1.35	1.40
25	T	1269	CDL	C59-C58	-3.53	1.31	1.51

The worst 5 of 683 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C18-C13-C12	-12.07	97.32	109.09
23	O	229	CHD	C18-C13-C12	-12.07	97.32	109.09
23	J	60	CHD	C18-C13-C12	-10.27	99.07	109.09
23	O	229	CHD	C19-C10-C9	-9.69	96.65	111.18
23	C	525	CHD	O12-C12-C13	-9.36	95.93	111.11

5 of 40 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	M	526	DMU	C2
26	M	526	DMU	C4
26	M	526	DMU	C6
26	M	526	DMU	C9
26	M	526	DMU	C5

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C02-O01-C1-C2
25	C	270	CDL	CA4-OA6-CA5-C11
25	P	1270	CDL	CA4-OA6-CA5-C11
20	A	524	PGV	C02-O01-C1-C2
20	A	524	PGV	P-O11-C03-C02

There are no ring outliers.

40 monomers are involved in 272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	3	0
14	A	516	HEA	1	0
20	A	521	PGV	1	0
19	A	523	TGL	3	0
20	A	524	PGV	12	0
23	B	1085	CHD	3	0
22	B	229	PSC	17	0
19	B	521	TGL	9	0
20	C	267	PGV	7	0
25	C	270	CDL	22	0
23	C	271	CHD	2	0
26	C	272	DMU	2	0
23	C	525	CHD	1	0
28	G	1263	PEK	10	0
28	G	264	PEK	4	0
28	G	265	PEK	8	0
25	G	269	CDL	24	0
23	J	60	CHD	2	0
19	L	522	TGL	19	0
20	N	1266	PGV	1	0
19	N	1521	TGL	10	0
19	N	1522	TGL	6	0
19	N	1523	TGL	5	0
20	N	1524	PGV	8	0
14	N	515	HEA	5	0
14	N	516	HEA	2	0
23	O	229	CHD	1	0
20	P	1267	PGV	5	0
20	P	1268	PGV	2	0
25	P	1270	CDL	16	0
23	P	1271	CHD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	1525	CHD	1	0
22	R	1229	PSC	16	0
28	S	1265	PEK	6	0
28	T	1264	PEK	4	0
25	T	1269	CDL	23	0
26	T	1272	DMU	6	0
28	T	263	PEK	15	0
23	W	1059	CHD	3	0
26	Z	1526	DMU	1	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%)	-0.04	17 (3%) 50 49	36, 42, 52, 84	0
1	N	513/514 (99%)	-0.12	12 (2%) 64 63	43, 51, 63, 92	0
2	B	226/227 (99%)	-0.40	1 (0%) 93 93	36, 48, 78, 111	0
2	O	226/227 (99%)	-0.06	9 (3%) 42 41	49, 61, 93, 120	0
3	C	259/261 (99%)	0.09	21 (8%) 15 14	38, 45, 59, 86	0
3	P	259/261 (99%)	0.43	27 (10%) 8 8	44, 51, 68, 88	0
4	D	144/147 (97%)	-0.54	2 (1%) 78 77	43, 51, 75, 91	0
4	Q	144/147 (97%)	0.77	17 (11%) 6 6	55, 69, 96, 132	0
5	E	105/109 (96%)	-0.31	0 100 100	43, 51, 83, 118	0
5	R	105/109 (96%)	0.78	9 (8%) 13 12	51, 63, 92, 123	0
6	F	98/98 (100%)	-0.11	7 (7%) 19 18	40, 53, 112, 143	0
6	S	98/98 (100%)	-0.14	7 (7%) 19 18	49, 61, 113, 144	0
7	G	83/85 (97%)	0.54	16 (19%) 2 1	42, 55, 123, 129	0
7	T	83/85 (97%)	0.74	16 (19%) 2 1	46, 62, 121, 133	0
8	H	79/85 (92%)	0.03	3 (3%) 44 43	46, 58, 119, 129	0
8	U	79/85 (92%)	-0.30	2 (2%) 61 60	54, 69, 120, 127	0
9	I	72/73 (98%)	0.26	6 (8%) 14 13	48, 60, 105, 112	0
9	V	72/73 (98%)	1.01	12 (16%) 2 2	52, 74, 109, 112	0
10	J	58/59 (98%)	0.20	4 (6%) 20 19	45, 58, 86, 119	0
10	W	58/59 (98%)	0.47	7 (12%) 6 5	54, 66, 88, 120	0
11	K	49/56 (87%)	-0.38	0 100 100	45, 57, 75, 83	0
11	X	49/56 (87%)	0.91	10 (20%) 1 1	62, 69, 85, 99	0
12	L	46/47 (97%)	-0.34	1 (2%) 65 64	43, 48, 70, 100	0
12	Y	46/47 (97%)	-0.09	3 (6%) 22 22	53, 61, 82, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.29	1 (2%) 64 63	44, 51, 88, 120	0
13	Z	43/46 (93%)	0.51	7 (16%) 2 2	57, 65, 96, 121	0
All	All	3550/3614 (98%)	0.07	217 (6%) 25 24	36, 53, 92, 144	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	15.2
4	Q	5	VAL	11.5
7	T	1	ALA	10.9
6	F	1	ALA	10.5
4	Q	7	LYS	10.3

## 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
1	FME	N	1	10/11	0.87	0.46	-	77,82,105,107	0
9	SAC	V	1	9/10	0.50	0.62	-	110,112,114,115	0
2	FME	B	1	10/11	0.98	0.10	-	46,48,51,61	0
9	SAC	I	1	9/10	0.58	0.54	-	99,103,106,106	0
2	FME	O	1	10/11	0.94	0.25	-	59,59,64,64	0
7	TPO	T	11	11/12	0.34	0.41	-	97,105,129,130	0
7	TPO	G	11	11/12	0.50	0.46	-	93,102,125,127	0
1	FME	A	1	10/11	0.94	0.21	-	63,70,93,102	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	A	524	51/51	0.78	0.27	12.63	62,101,132,135	0
25	CDL	P	1270	100/100	0.76	0.38	9.59	69,119,136,137	0
25	CDL	C	270	100/100	0.83	0.34	8.36	56,112,137,139	0
26	DMU	C	272	33/33	0.62	0.28	6.61	96,129,132,134	0
26	DMU	T	1272	33/33	0.60	0.37	5.75	111,140,141,141	0
19	TGL	N	1522	63/63	0.64	0.30	5.38	72,95,111,112	0
19	TGL	L	522	63/63	0.77	0.25	4.89	57,89,109,113	0
18	NA	N	519	1/1	0.87	0.24	4.86	58,58,58,58	0
20	PGV	N	1524	51/51	0.73	0.39	4.82	67,106,139,140	0
19	TGL	B	521	63/63	0.86	0.18	4.75	54,96,118,120	0
22	PSC	B	229	52/52	0.63	0.32	4.62	70,117,150,150	0
19	TGL	A	523	63/63	0.78	0.21	4.40	78,102,131,132	0
22	PSC	R	1229	52/52	0.56	0.35	4.38	73,120,150,150	0
23	CHD	J	60	29/29	0.85	0.34	4.03	103,112,119,120	0
19	TGL	N	1523	63/63	0.77	0.34	3.99	84,111,131,133	0
25	CDL	G	269	100/100	0.60	0.40	3.98	89,118,138,141	0
25	CDL	T	1269	100/100	0.58	0.44	3.75	92,117,138,143	0
23	CHD	W	1059	29/29	0.77	0.37	3.41	110,117,120,122	0
28	PEK	G	1263	53/53	0.40	0.68	3.07	83,126,150,150	0
17	MG	A	518	1/1	0.95	0.17	3.03	40,40,40,40	0
19	TGL	N	1521	63/63	0.88	0.22	2.84	69,101,120,123	0
20	PGV	C	268	51/51	0.65	0.66	2.75	78,103,119,120	0
27	ZN	F	99	1/1	0.99	0.15	2.48	48,48,48,48	0
20	PGV	P	1268	51/51	0.73	0.58	2.29	78,108,125,126	0
28	PEK	T	263	53/53	0.55	0.51	2.17	78,123,145,149	0
23	CHD	P	1525	29/29	0.96	0.27	2.14	48,54,57,59	0
23	CHD	C	525	29/29	0.96	0.29	1.85	38,50,57,65	0
26	DMU	Z	1526	33/33	0.90	0.28	1.81	73,80,94,96	0
21	CUA	B	228	2/2	0.99	0.15	1.62	41,41,41,42	0
20	PGV	P	1267	51/51	0.96	0.19	0.98	45,56,102,106	0
14	HEA	N	516	60/60	0.99	0.14	0.87	42,48,69,74	0
14	HEA	N	515	60/60	0.98	0.12	0.74	47,52,65,66	0
23	CHD	C	271	29/29	0.94	0.20	0.65	86,97,99,99	0
28	PEK	T	1264	53/53	0.95	0.17	0.62	49,70,109,111	0
28	PEK	S	1265	53/53	0.72	0.26	0.59	75,112,133,136	0
28	PEK	G	264	53/53	0.96	0.14	0.58	44,65,107,109	0
20	PGV	C	267	51/51	0.97	0.14	0.42	38,52,95,97	0
20	PGV	A	521	51/51	0.97	0.15	0.38	36,53,77,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
17	MG	N	518	1/1	0.92	0.11	0.36	50,50,50,50	0
28	PEK	G	265	53/53	0.74	0.23	0.35	70,109,135,138	0
23	CHD	P	1271	29/29	0.94	0.13	0.35	98,101,103,104	0
27	ZN	S	99	1/1	1.00	0.11	0.22	56,56,56,56	0
26	DMU	M	526	33/33	0.94	0.14	0.16	52,63,87,91	0
20	PGV	N	1266	51/51	0.96	0.15	0.10	45,60,81,84	0
15	CMO	N	520	2/2	1.00	0.14	0.00	47,47,47,48	0
21	CUA	O	228	2/2	0.98	0.11	-0.11	52,52,52,54	0
14	HEA	A	516	60/60	0.99	0.14	-0.24	32,40,56,64	0
14	HEA	A	515	60/60	0.99	0.12	-0.27	33,40,54,68	0
23	CHD	B	1085	29/29	0.97	0.14	-0.27	46,50,53,59	0
23	CHD	O	229	29/29	0.96	0.13	-0.29	45,49,56,62	0
16	CU	A	517	1/1	1.00	0.20	-0.88	40,40,40,40	0
15	CMO	A	520	2/2	0.99	0.15	-1.37	39,39,39,41	0
18	NA	A	519	1/1	0.96	0.06	-4.41	47,47,47,47	0
24	UNX	C	262	1/1	0.39	0.65	-	75,75,75,75	0
24	UNX	P	262	1/1	0.69	0.68	-	75,75,75,75	0
16	CU	N	517	1/1	1.00	0.18	-	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.