



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 06:58 am GMT

PDB ID : 3ABK  
Title : Bovine heart cytochrome c oxidase at the NO-bound fully reduced state (50K)  
Authors : Ohta, K.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.;  
Tsukihara, T.  
Deposited on : 2009-12-16  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

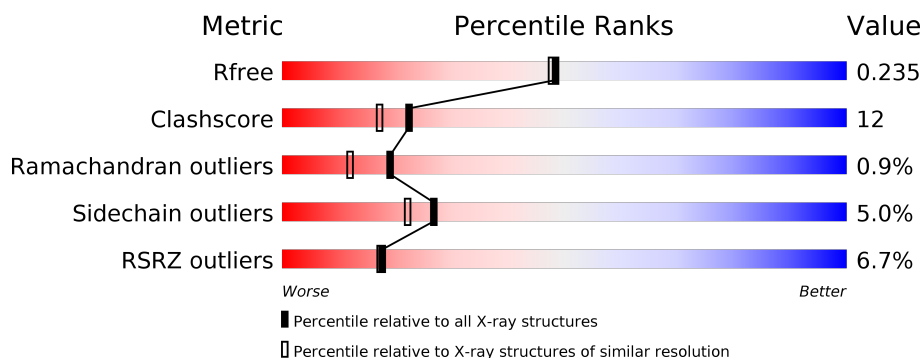
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
1	N	514	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
2	B	227	<div> <div></div> <div> <div></div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
2	O	227	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div>
3	C	261	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>•••</div> </div> </div>
3	P	261	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	-	-	-
14	HEA	N	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	516	X	-	-	-
19	PGV	U	1268	-	-	-	X
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1059	X	-	-	X
24	UNX	C	262	-	-	-	X
24	UNX	P	262	-	-	-	X
25	PEK	G	1263	-	-	-	X
25	PEK	T	263	-	-	-	X
26	CDL	G	269	-	-	X	-
26	CDL	P	1270	-	-	X	-
26	CDL	T	1269	-	-	X	-
27	DMU	C	272	X	-	-	-
27	DMU	M	526	X	-	-	-
27	DMU	P	272	X	-	-	X
27	DMU	Z	1526	X	-	-	-
9	SAC	V	1	-	-	-	X

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32382 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 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

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

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

- Molecule 9 is a protein called Cytochrome c oxidase 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			

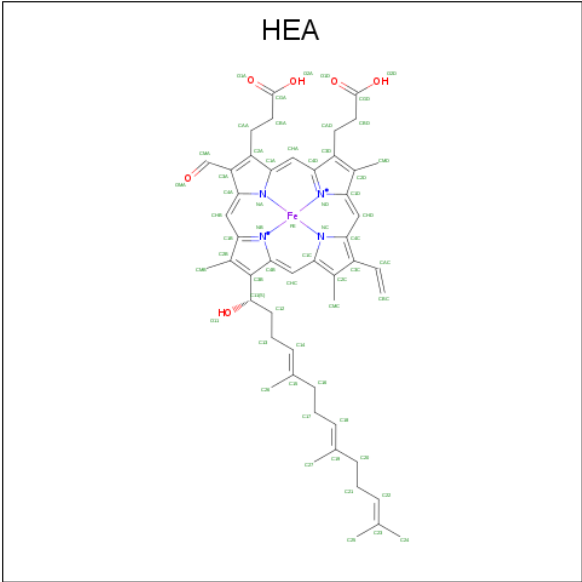
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

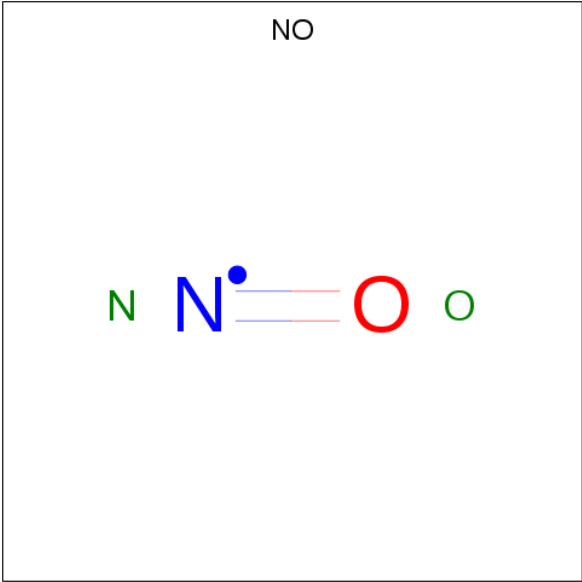
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- 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 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

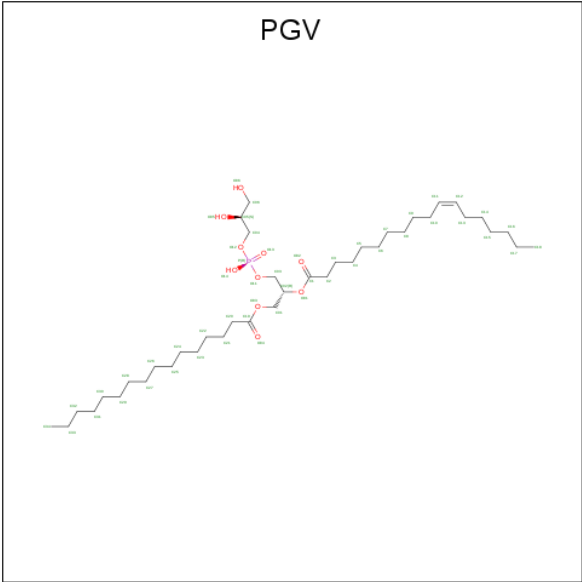
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

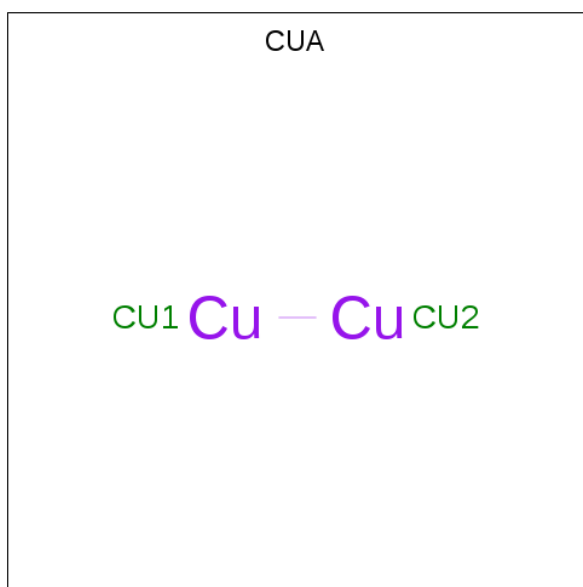
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



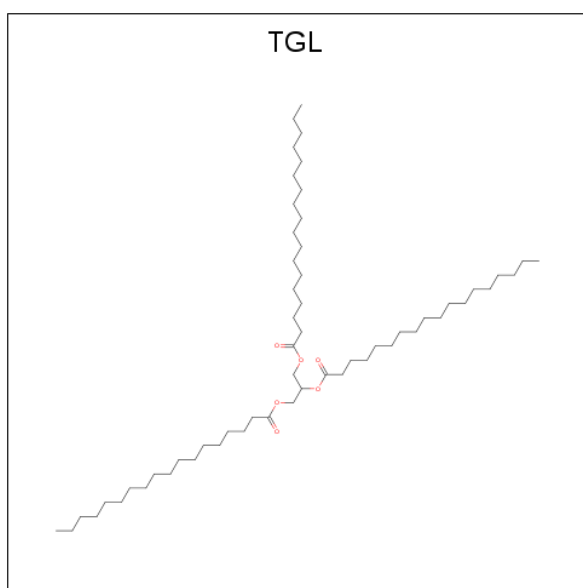
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula:  $C_{57}H_{110}O_6$ ).



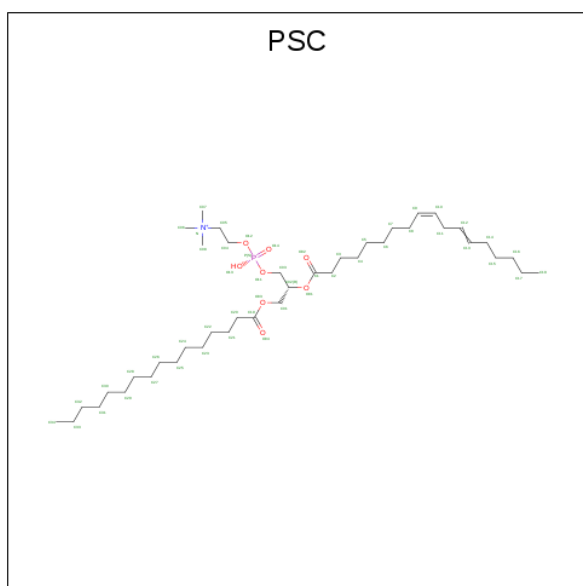
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

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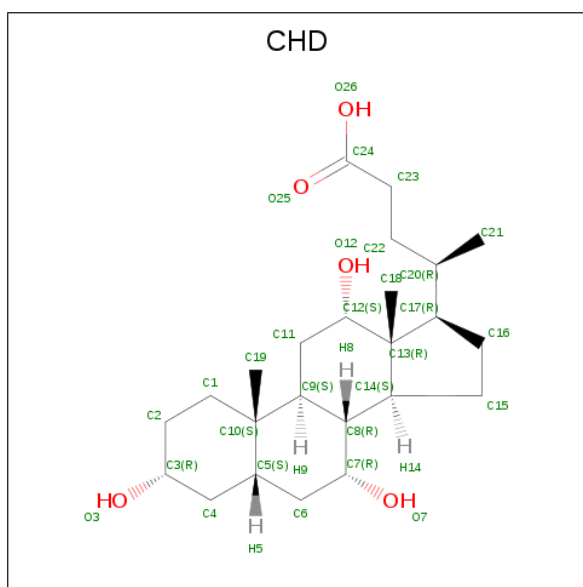
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- 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:  $C_{42}H_{81}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
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:  $C_{24}H_{40}O_5$ ).

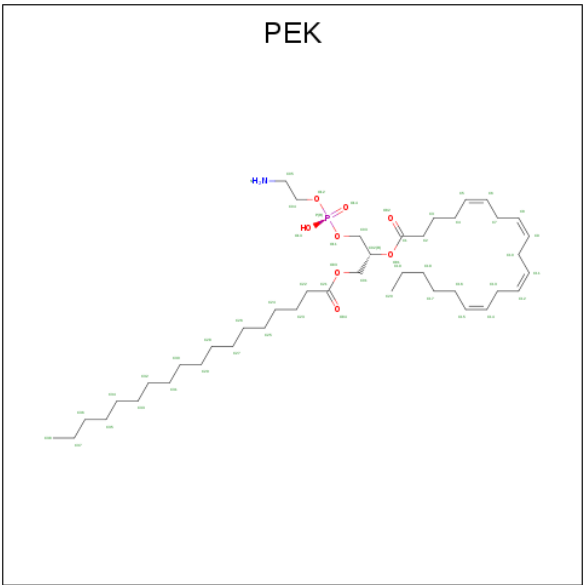


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

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

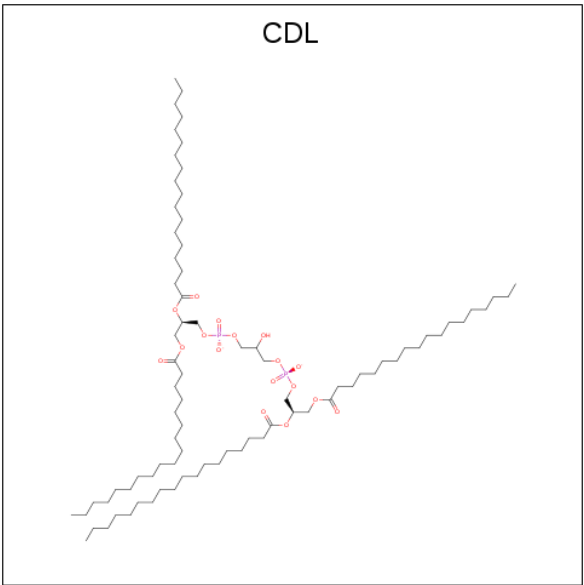
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	X	0	0
			1	1		
24	C	1	Total	X	0	0
			1	1		

- 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).



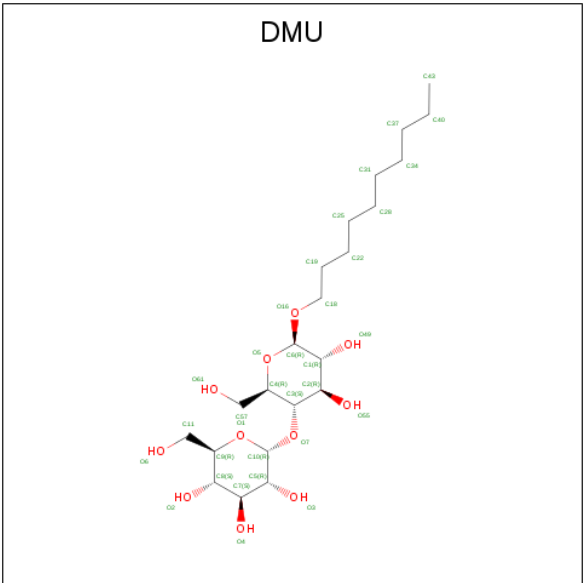
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- 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 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
27	C	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	217	Total O 217 217	0	0
29	B	127	Total O 127 127	0	0
29	C	93	Total O 93 93	0	0
29	D	86	Total O 86 86	0	0
29	E	52	Total O 52 52	0	0
29	F	72	Total O 72 72	0	0
29	G	42	Total O 42 42	0	0
29	H	46	Total O 46 46	0	0
29	I	31	Total O 31 31	0	0
29	J	28	Total O 28 28	0	0
29	K	27	Total O 27 27	0	0
29	L	16	Total O 16 16	0	0

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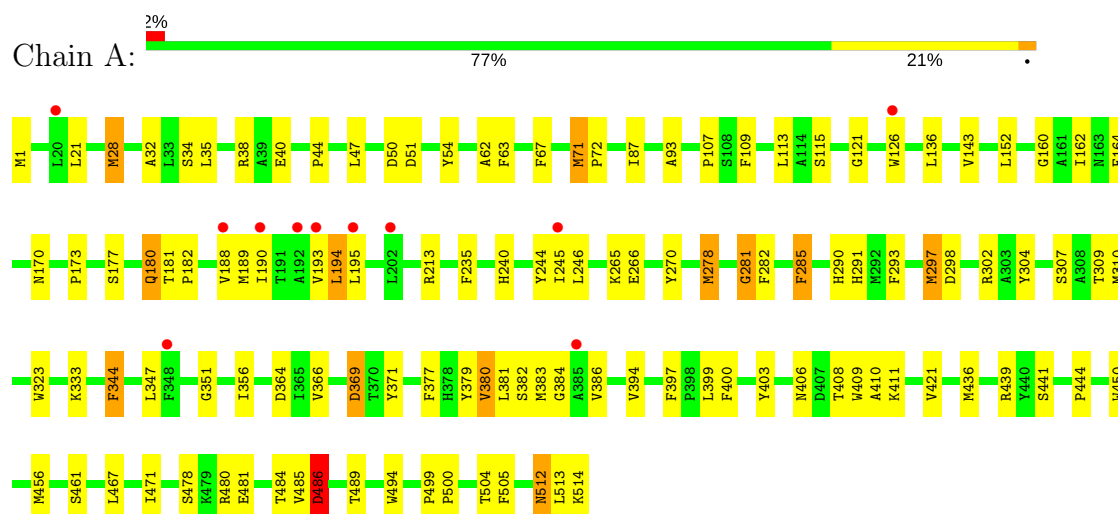
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	M	20	Total 20	O 20	0	0
29	N	207	Total 207	O 207	0	0
29	O	105	Total 105	O 105	0	0
29	P	96	Total 96	O 96	0	0
29	Q	57	Total 57	O 57	0	0
29	R	35	Total 35	O 35	0	0
29	S	63	Total 63	O 63	0	0
29	T	44	Total 44	O 44	0	0
29	U	43	Total 43	O 43	0	0
29	V	20	Total 20	O 20	0	0
29	W	17	Total 17	O 17	0	0
29	X	13	Total 13	O 13	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	11	Total 11	O 11	0	0

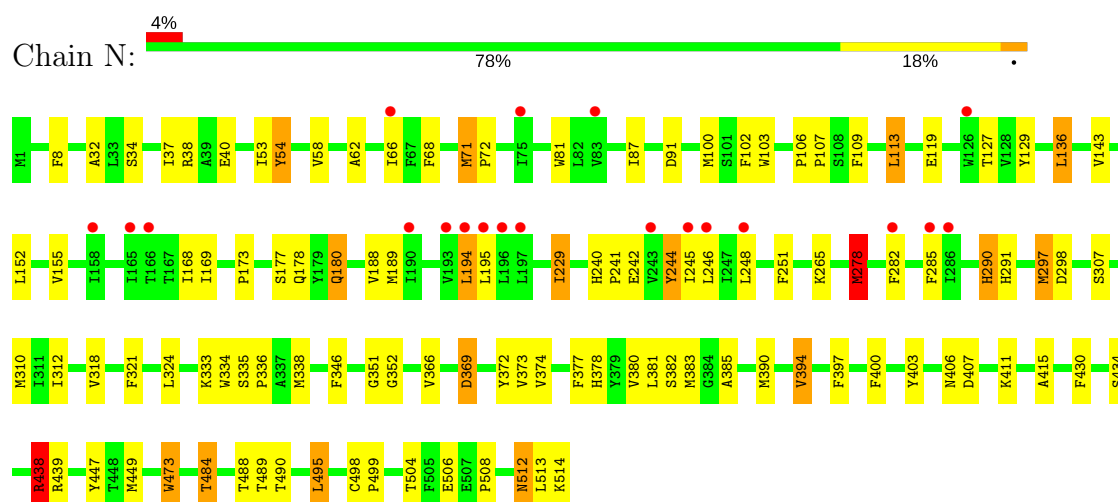
### 3 Residue-property plots [i](#)

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

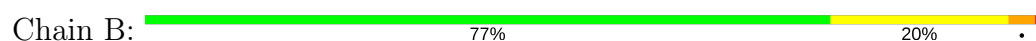
#### • Molecule 1: Cytochrome c oxidase subunit 1

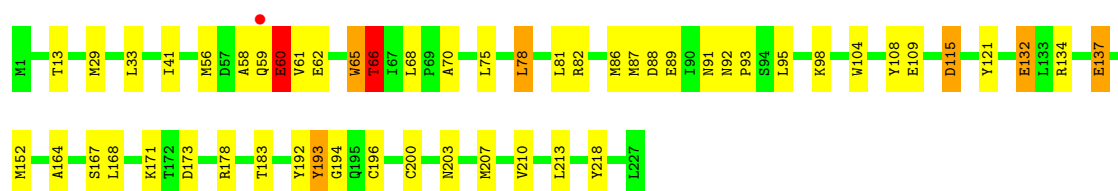


#### • Molecule 1: Cytochrome c oxidase subunit 1

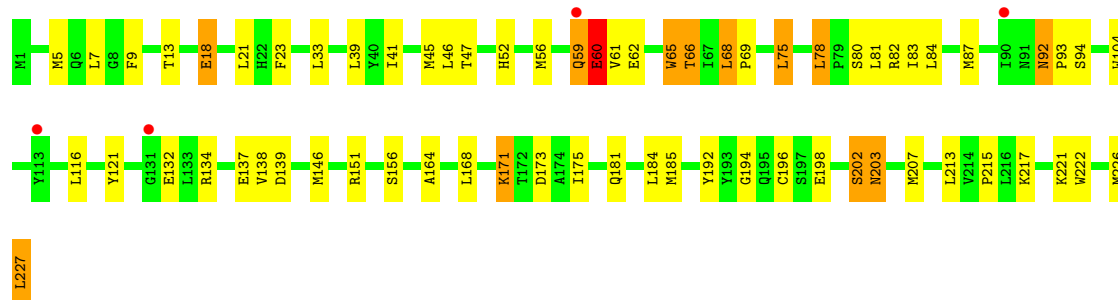


#### • Molecule 2: Cytochrome c oxidase subunit 2

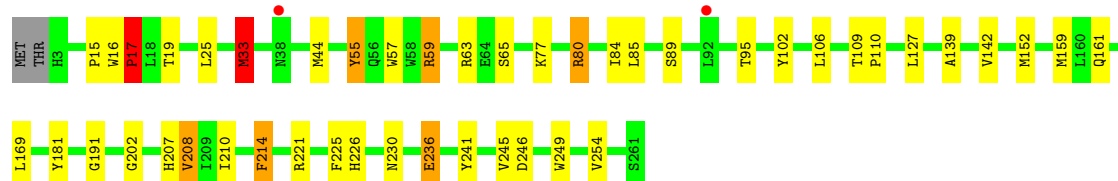
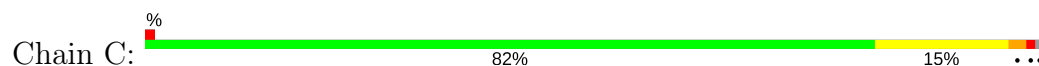




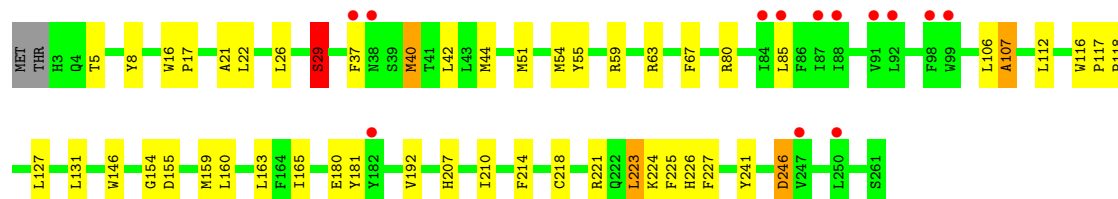
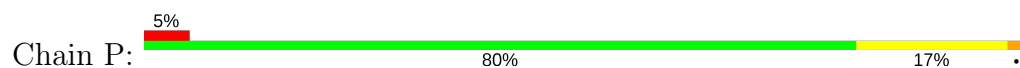
• Molecule 2: Cytochrome c oxidase subunit 2



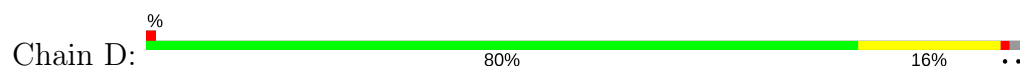
• Molecule 3: Cytochrome c oxidase subunit 3



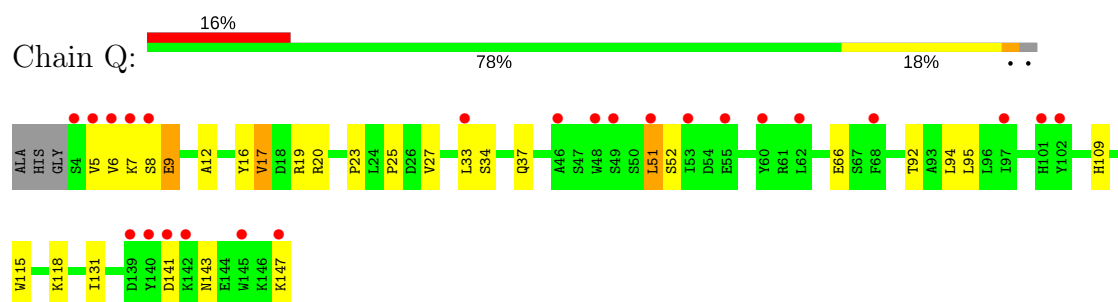
• Molecule 3: Cytochrome c oxidase subunit 3



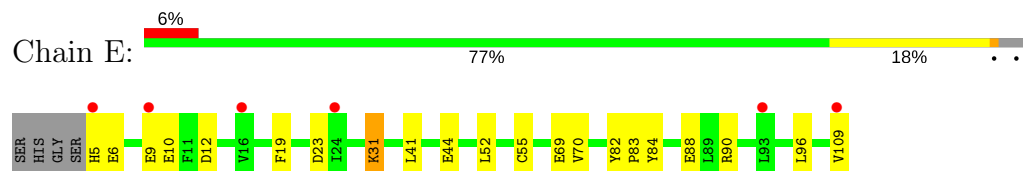
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



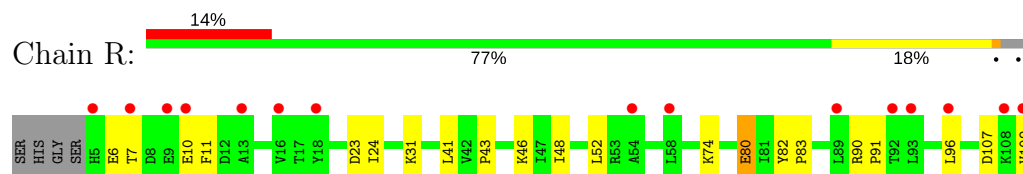
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



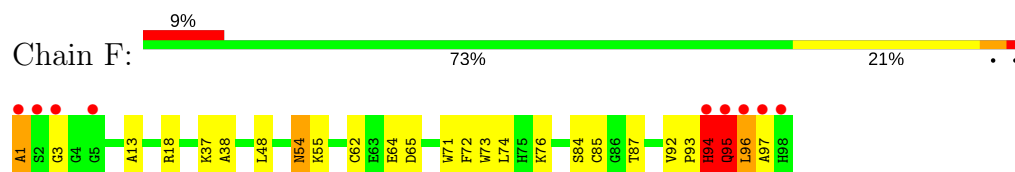
- Molecule 5: Cytochrome c oxidase subunit 5A



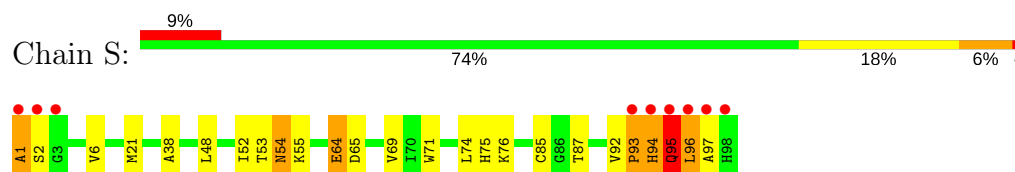
- Molecule 5: Cytochrome c oxidase subunit 5A



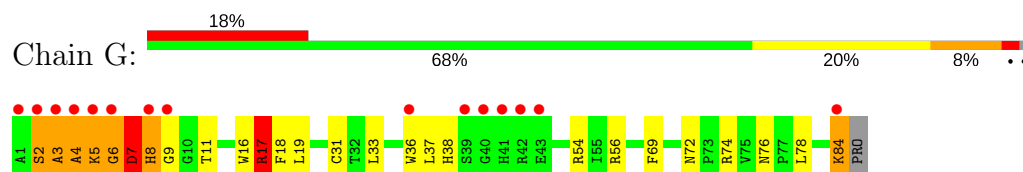
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B

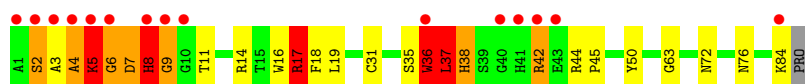


- Molecule 7: Cytochrome c oxidase subunit 6A2

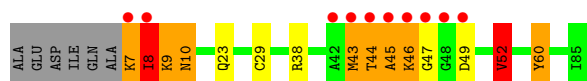
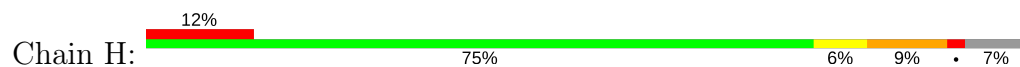


- Molecule 7: Cytochrome c oxidase subunit 6A2

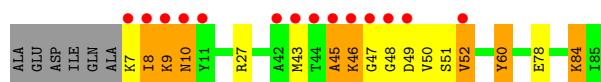
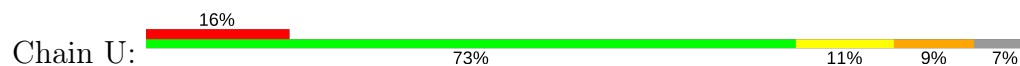




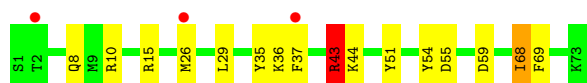
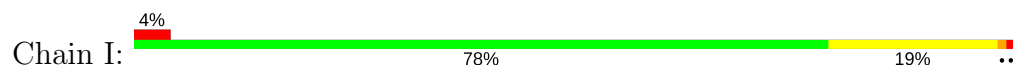
• Molecule 8: Cytochrome c oxidase subunit 6B1



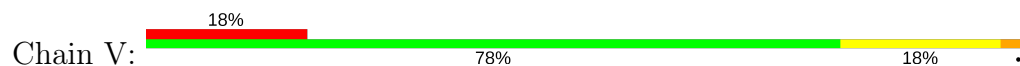
• Molecule 8: Cytochrome c oxidase subunit 6B1



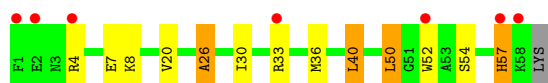
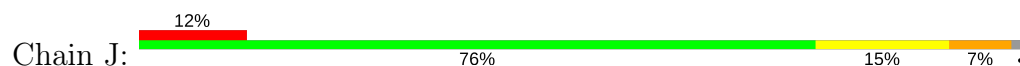
• Molecule 9: Cytochrome c oxidase subunit 6C



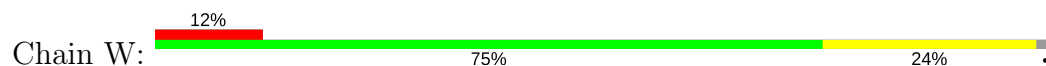
• Molecule 9: Cytochrome c oxidase subunit 6C



• Molecule 10: Cytochrome c oxidase polypeptide 7A1

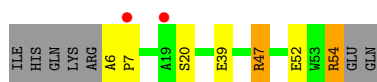


• Molecule 10: Cytochrome c oxidase polypeptide 7A1

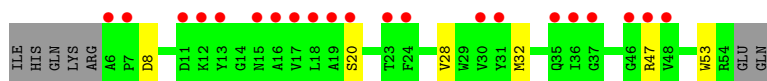
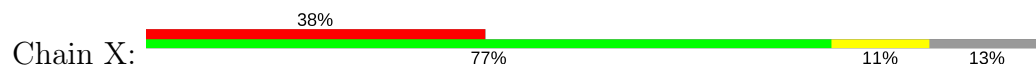


• Molecule 11: Cytochrome c oxidase subunit 7B





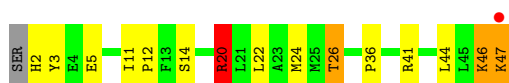
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



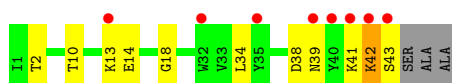
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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, $\alpha$ , $\beta$ , $\gamma$	182.25Å 207.94Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 75.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.00) 98.7 (75.57-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, $R_{free}$	0.183 , 0.219 0.201 , 0.235	Depositor DCC
$R_{free}$ test set	22073 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 69.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.64	40/4189 (1.0%)	1.27	19/5722 (0.3%)
1	N	1.46	26/4189 (0.6%)	1.20	22/5722 (0.4%)
2	B	1.54	15/1860 (0.8%)	1.32	11/2534 (0.4%)
2	O	1.32	7/1860 (0.4%)	1.14	9/2534 (0.4%)
3	C	1.43	15/2197 (0.7%)	1.13	10/3005 (0.3%)
3	P	1.36	9/2197 (0.4%)	1.16	11/3005 (0.4%)
4	D	1.33	2/1229 (0.2%)	1.11	5/1658 (0.3%)
4	Q	1.24	5/1229 (0.4%)	1.04	5/1658 (0.3%)
5	E	1.32	4/871 (0.5%)	0.98	0/1182
5	R	1.15	0/871	0.98	1/1182 (0.1%)
6	F	1.44	6/765 (0.8%)	1.23	1/1038 (0.1%)
6	S	1.33	3/765 (0.4%)	1.17	1/1038 (0.1%)
7	G	1.38	3/690 (0.4%)	1.28	7/937 (0.7%)
7	T	1.36	3/690 (0.4%)	1.21	6/937 (0.6%)
8	H	1.34	0/682	1.12	2/921 (0.2%)
8	U	1.16	0/682	0.97	0/921
9	I	1.32	3/605 (0.5%)	1.20	5/802 (0.6%)
9	V	1.22	1/605 (0.2%)	0.97	1/802 (0.1%)
10	J	1.26	2/471 (0.4%)	1.09	2/636 (0.3%)
10	W	1.25	0/471	1.10	2/636 (0.3%)
11	K	1.36	0/398	1.19	4/546 (0.7%)
11	X	1.11	0/398	0.95	1/546 (0.2%)
12	L	1.42	2/393 (0.5%)	1.09	0/526
12	Y	1.35	1/393 (0.3%)	1.00	1/526 (0.2%)
13	M	1.41	1/345 (0.3%)	1.23	2/470 (0.4%)
13	Z	1.17	0/345	0.99	0/470
All	All	1.41	148/29390 (0.5%)	1.16	128/39954 (0.3%)

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
5	E	0	1
6	F	0	1
6	S	0	2
12	Y	0	1
All	All	0	5

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	10.56	1.69	1.50
7	T	36	TRP	CB-CG	10.45	1.69	1.50
1	A	380[A]	VAL	CB-CG1	-9.14	1.33	1.52
1	A	380[B]	VAL	CB-CG1	-9.14	1.33	1.52
3	P	180	GLU	CD-OE1	8.86	1.35	1.25

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	17	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	A	71	MET	CG-SD-CE	-14.02	77.77	100.20
7	G	17	ARG	NE-CZ-NH1	12.88	126.74	120.30
3	P	246	ASP	CB-CG-OD1	-12.27	107.26	118.30
1	N	278	MET	CG-SD-CE	-11.92	81.12	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	5	HIS	Peptide
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide
6	S	95	GLN	Peptide
12	Y	46	LYS	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	74	0
1	N	4060	0	4037	86	0
2	B	1824	0	1833	25	0
2	O	1824	0	1833	50	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	35	0
4	D	1195	0	1183	19	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	10	0
5	R	852	0	845	19	0
6	F	748	0	728	22	0
6	S	748	0	728	40	0
7	G	675	0	643	45	0
7	T	675	0	643	43	0
8	H	662	0	623	19	0
8	U	662	0	623	20	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	460	0	459	13	0
10	W	460	0	459	12	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	16	0
12	Y	380	0	380	20	0
13	M	335	0	352	13	0
13	Z	335	0	352	6	0
14	A	120	0	108	16	0
14	N	120	0	108	9	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	102	0	152	16	0
19	C	102	0	152	10	0
19	N	102	0	152	7	0
19	P	51	0	76	3	0
19	U	51	0	76	4	0
20	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	2	0	0	0	0
21	B	63	0	110	4	0
21	D	63	0	110	10	0
21	L	63	0	110	15	0
21	N	63	0	110	14	0
21	O	63	0	110	5	0
21	Y	63	0	110	20	0
22	B	52	0	80	20	0
22	R	52	0	80	20	0
23	B	29	0	37	4	0
23	C	58	0	71	4	0
23	J	29	0	36	8	0
23	O	29	0	37	3	0
23	P	58	0	72	5	0
23	W	29	0	35	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	22	0
25	G	53	0	77	19	0
25	P	53	0	77	6	0
25	T	106	0	154	34	0
26	C	100	0	156	20	0
26	G	100	0	156	33	0
26	P	100	0	156	27	0
26	T	100	0	156	30	0
27	C	33	0	39	4	0
27	M	33	0	39	0	0
27	P	33	0	38	1	0
27	Z	33	0	38	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	217	0	0	5	0
29	B	127	0	0	3	0
29	C	93	0	0	4	0
29	D	86	0	0	6	0
29	E	52	0	0	0	0
29	F	72	0	0	3	0
29	G	42	0	0	7	0
29	H	46	0	0	1	0
29	I	31	0	0	3	0
29	J	28	0	0	4	0
29	K	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	L	16	0	0	1	0
29	M	20	0	0	0	0
29	N	207	0	0	6	0
29	O	105	0	0	2	0
29	P	96	0	0	3	0
29	Q	57	0	0	4	0
29	R	35	0	0	1	0
29	S	63	0	0	5	0
29	T	44	0	0	5	0
29	U	43	0	0	5	0
29	V	20	0	0	0	0
29	W	17	0	0	2	0
29	X	13	0	0	0	0
29	Y	12	0	0	1	0
29	Z	11	0	0	1	0
All	All	32382	0	31350	777	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 12.

The worst 5 of 777 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:T:1265:PEK:H383	26:T:1269:CDL:C27	1.34	1.51
1:N:297:MET:CE	1:N:297:MET:SD	2.10	1.40
25:T:1265:PEK:C38	26:T:1269:CDL:H273	1.51	1.36
10:W:2:GLU:HB2	10:W:4:ARG:NH1	1.50	1.26
25:T:1265:PEK:C38	26:T:1269:CDL:C27	2.12	1.18

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	517/514 (101%)	502 (97%)	15 (3%)	0	100	100
1	N	517/514 (101%)	495 (96%)	22 (4%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	36	31
2	O	225/227 (99%)	219 (97%)	5 (2%)	1 (0%)	36	31
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	8 (6%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	2 (2%)	1 (1%)	17	10
6	F	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	1
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	4	1
7	G	81/85 (95%)	68 (84%)	7 (9%)	6 (7%)	1	0
7	T	81/85 (95%)	67 (83%)	6 (7%)	8 (10%)	1	0
8	H	77/85 (91%)	68 (88%)	3 (4%)	6 (8%)	1	0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2	0
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	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%)	44 (94%)	3 (6%)	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%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3514/3614 (97%)	3356 (96%)	125 (4%)	33 (1%)	19	12

5 of 33 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	49	50
1	N	430/426 (101%)	414 (96%)	16 (4%)	37	35
2	B	210/210 (100%)	200 (95%)	10 (5%)	28	24
2	O	210/210 (100%)	196 (93%)	14 (7%)	18	13
3	C	224/226 (99%)	217 (97%)	7 (3%)	43	42
3	P	224/226 (99%)	219 (98%)	5 (2%)	55	58
4	D	128/129 (99%)	124 (97%)	4 (3%)	43	42
4	Q	128/129 (99%)	121 (94%)	7 (6%)	24	19
5	E	92/95 (97%)	88 (96%)	4 (4%)	32	28
5	R	92/95 (97%)	89 (97%)	3 (3%)	41	39
6	F	81/81 (100%)	76 (94%)	5 (6%)	20	15
6	S	81/81 (100%)	77 (95%)	4 (5%)	27	23
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	3
7	T	67/68 (98%)	58 (87%)	9 (13%)	4	2
8	H	71/75 (95%)	65 (92%)	6 (8%)	12	7
8	U	71/75 (95%)	66 (93%)	5 (7%)	16	11
9	I	57/57 (100%)	50 (88%)	7 (12%)	5	3
9	V	57/57 (100%)	48 (84%)	9 (16%)	3	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	58	61
10	W	49/50 (98%)	48 (98%)	1 (2%)	58	61
11	K	39/46 (85%)	36 (92%)	3 (8%)	14	9
11	X	39/46 (85%)	37 (95%)	2 (5%)	26	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	38 (97%)	1 (3%)	49	50
12	Y	39/40 (98%)	36 (92%)	3 (8%)	14	9
13	M	37/38 (97%)	33 (89%)	4 (11%)	7	4
13	Z	37/38 (97%)	33 (89%)	4 (11%)	7	4
All	All	3048/3082 (99%)	2895 (95%)	153 (5%)	27	22

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	39	ASN
1	N	508	PRO
9	V	70	GLN
1	N	109	PHE
1	N	290	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	57	HIS
1	N	512	ASN
7	T	8	HIS
1	N	80	ASN
1	N	178	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	A	1	1	9,9,10	1.05	1 (11%)	7,9,11	5.42	3 (42%)
2	FME	B	1	2	9,9,10	2.06	3 (33%)	7,9,11	8.14	4 (57%)
7	TPO	G	11	7	9,10,11	2.72	5 (55%)	11,14,16	1.49	2 (18%)
9	SAC	I	1	9	8,8,9	2.53	2 (25%)	7,9,11	2.04	2 (28%)
1	FME	N	1	1	9,9,10	0.67	0	7,9,11	6.28	3 (42%)
2	FME	O	1	2	9,9,10	1.33	2 (22%)	7,9,11	5.22	3 (42%)
7	TPO	T	11	7	9,10,11	3.33	4 (44%)	11,14,16	1.92	4 (36%)
9	SAC	V	1	9	8,8,9	3.38	3 (37%)	7,9,11	1.96	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	-	0/5/9/11	0/0/0/0
2	FME	B	1	2	-	0/5/9/11	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	-	0/5/9/11	0/0/0/0
2	FME	O	1	2	-	0/5/9/11	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 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.57	1.08	1.22
2	B	1	FME	CG-SD	-2.31	1.68	1.81
2	O	1	FME	CA-C	-2.22	1.47	1.50
2	O	1	FME	O1-CN	-2.20	1.15	1.22
7	G	11	TPO	CG2-CB	2.02	1.56	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.70	90.98	122.82
1	N	1	FME	CA-N-CN	-15.77	98.57	122.82
1	A	1	FME	CA-N-CN	-13.36	102.27	122.82
2	O	1	FME	CA-N-CN	-13.30	102.36	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.09	101.51	112.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
7	G	11	TPO	4	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	43,67,67	1.42	9 (20%)	37,103,103	2.07	13 (35%)
14	HEA	A	516	1	43,67,67	1.36	7 (16%)	37,103,103	2.21	11 (29%)
15	NO	A	520	16	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	A	521	-	50,50,50	1.27	6 (12%)	53,56,56	1.75	12 (22%)
19	PGV	A	524	-	50,50,50	1.35	4 (8%)	53,56,56	1.70	11 (20%)
23	CHD	B	1085	-	29,32,32	1.84	5 (17%)	47,51,51	5.73	34 (72%)
20	CUA	B	228	2	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
22	PSC	B	229	-	51,51,51	1.22	3 (5%)	57,59,59	1.38	10 (17%)
21	TGL	B	521	-	62,62,62	1.30	6 (9%)	65,65,65	1.97	13 (20%)
25	PEK	C	264	-	52,52,52	0.93	2 (3%)	55,57,57	1.84	16 (29%)
25	PEK	C	265	-	52,52,52	1.62	6 (11%)	55,57,57	1.68	8 (14%)
19	PGV	C	267	-	50,50,50	0.88	3 (6%)	53,56,56	1.36	8 (15%)
19	PGV	C	268	-	50,50,50	1.41	4 (8%)	53,56,56	1.70	7 (13%)
26	CDL	C	270	-	99,99,99	1.48	13 (13%)	105,111,111	1.46	15 (14%)
23	CHD	C	271	-	29,32,32	0.73	0	47,51,51	5.03	33 (70%)
27	DMU	C	272	-	34,34,34	1.49	4 (11%)	45,45,45	3.37	25 (55%)
23	CHD	C	525	-	29,32,32	1.57	6 (20%)	47,51,51	5.57	37 (78%)
21	TGL	D	523	-	62,62,62	1.61	8 (12%)	65,65,65	1.56	15 (23%)
25	PEK	G	1263	-	52,52,52	1.34	4 (7%)	55,57,57	1.51	7 (12%)
26	CDL	G	269	-	99,99,99	1.43	12 (12%)	105,111,111	1.54	19 (18%)
23	CHD	J	60	-	29,32,32	0.96	0	47,51,51	5.35	35 (74%)
21	TGL	L	522	-	62,62,62	1.57	8 (12%)	65,65,65	2.14	16 (24%)
27	DMU	M	526	-	34,34,34	1.10	4 (11%)	45,45,45	3.32	25 (55%)
19	PGV	N	1266	-	50,50,50	0.98	2 (4%)	53,56,56	1.55	9 (16%)
21	TGL	N	1523	-	62,62,62	1.40	7 (11%)	65,65,65	1.47	10 (15%)
19	PGV	N	1524	-	50,50,50	1.10	2 (4%)	53,56,56	1.34	6 (11%)
14	HEA	N	515	1	43,67,67	1.12	4 (9%)	37,103,103	1.84	9 (24%)
14	HEA	N	516	1,15	43,67,67	1.14	5 (11%)	37,103,103	2.44	14 (37%)
15	NO	N	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
21	TGL	O	1521	-	62,62,62	1.36	6 (9%)	65,65,65	1.65	11 (16%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.62	5 (17%)	47,51,51	5.71	32 (68%)
25	PEK	P	1264	-	52,52,52	0.93	3 (5%)	55,57,57	1.84	14 (25%)
19	PGV	P	1267	-	50,50,50	0.93	3 (6%)	53,56,56	1.54	8 (15%)
26	CDL	P	1270	-	99,99,99	1.45	12 (12%)	105,111,111	1.71	20 (19%)
23	CHD	P	1271	-	29,32,32	0.80	1 (3%)	47,51,51	5.12	33 (70%)
23	CHD	P	1525	-	29,32,32	1.68	6 (20%)	47,51,51	5.60	38 (80%)
27	DMU	P	272	-	34,34,34	1.65	6 (17%)	45,45,45	3.32	25 (55%)
22	PSC	R	1229	-	51,51,51	1.35	3 (5%)	57,59,59	1.34	5 (8%)
25	PEK	T	1265	-	52,52,52	1.43	6 (11%)	55,57,57	1.59	6 (10%)
26	CDL	T	1269	-	99,99,99	1.42	13 (13%)	105,111,111	1.55	16 (15%)
25	PEK	T	263	-	52,52,52	1.47	4 (7%)	55,57,57	1.42	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	PGV	U	1268	-	50,50,50	1.56	3 (6%)	53,56,56	1.91	7 (13%)
23	CHD	W	1059	-	29,32,32	1.24	3 (10%)	47,51,51	5.45	32 (68%)
21	TGL	Y	1522	-	62,62,62	1.69	10 (16%)	65,65,65	2.25	17 (26%)
27	DMU	Z	1526	-	34,34,34	1.11	2 (5%)	45,45,45	3.11	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	3/3/7/16	0/24/76/76	0/0/8/8
15	NO	A	520	16	-	0/0/0/0	0/0/0/0
19	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	PGV	A	524	-	-	0/55/55/55	0/0/0/0
23	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	229	-	-	0/55/55/55	0/0/0/0
21	TGL	B	521	-	-	0/65/65/65	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	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
27	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
21	TGL	D	523	-	-	0/65/65/65	0/0/0/0
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
23	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
21	TGL	L	522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
21	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	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	NO	N	520	14,16	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
20	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
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	2/110/110/110	0/0/0/0
23	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	P	1525	-	1/1/12/12	0/7/74/74	0/4/4/4
27	DMU	P	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
25	PEK	T	1265	-	-	0/56/56/56	0/0/0/0
26	CDL	T	1269	-	-	3/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
19	PGV	U	1268	-	-	0/55/55/55	0/0/0/0
23	CHD	W	1059	-	1/1/12/12	0/7/74/74	0/4/4/4
21	TGL	Y	1522	-	-	2/65/65/65	0/0/0/0
27	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 220 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1085	CHD	C10-C5	-4.73	1.47	1.55
23	P	1525	CHD	C13-C12	-4.51	1.47	1.54
23	O	229	CHD	C13-C14	-3.98	1.48	1.55
21	L	522	TGL	C20-CA9	-3.53	1.31	1.51
23	B	1085	CHD	C13-C14	-3.47	1.49	1.55

The worst 5 of 714 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C18-C13-C12	-13.70	94.92	109.07
23	P	1525	CHD	C18-C13-C12	-11.80	96.87	109.07
23	B	1085	CHD	C18-C13-C12	-11.00	97.70	109.07
23	C	525	CHD	C23-C22-C20	-10.23	100.94	114.72
23	W	1059	CHD	C6-C5-C4	-9.84	99.98	111.13

5 of 39 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA

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Mol	Chain	Res	Type	Atom
14	N	515	HEA	NB
27	Z	1526	DMU	C2
27	Z	1526	DMU	C4

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	Y	1522	TGL	CG2-OG2-CB1-OB1
19	N	1524	PGV	C02-O01-C1-C2
26	T	1269	CDL	PB2-OB2-CB2-C1
21	Y	1522	TGL	CG2-OG2-CB1-CB2
26	T	1269	CDL	CA4-OA6-CA5-OA7

There are no ring outliers.

38 monomers are involved in 373 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	8	0
14	A	516	HEA	8	0
19	A	521	PGV	2	0
19	A	524	PGV	14	0
23	B	1085	CHD	4	0
22	B	229	PSC	20	0
21	B	521	TGL	4	0
25	C	264	PEK	9	0
25	C	265	PEK	13	0
19	C	267	PGV	4	0
19	C	268	PGV	6	0
26	C	270	CDL	20	0
23	C	271	CHD	2	0
27	C	272	DMU	4	0
23	C	525	CHD	2	0
21	D	523	TGL	10	0
25	G	1263	PEK	19	0
26	G	269	CDL	33	0
23	J	60	CHD	8	0
21	L	522	TGL	15	0
21	N	1523	TGL	14	0
19	N	1524	PGV	7	0
14	N	515	HEA	6	0
14	N	516	HEA	3	0
21	O	1521	TGL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	O	229	CHD	3	0
25	P	1264	PEK	6	0
19	P	1267	PGV	3	0
26	P	1270	CDL	27	0
23	P	1271	CHD	5	0
27	P	272	DMU	1	0
22	R	1229	PSC	20	0
25	T	1265	PEK	20	0
26	T	1269	CDL	30	0
25	T	263	PEK	14	0
19	U	1268	PGV	4	0
23	W	1059	CHD	3	0
21	Y	1522	TGL	20	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%)	0.30	11 (2%) 63 62	23, 29, 38, 65	0
1	N	513/514 (99%)	0.23	20 (3%) 39 39	29, 35, 44, 71	0
2	B	226/227 (99%)	-0.25	1 (0%) 92 92	24, 33, 53, 72	0
2	O	226/227 (99%)	-0.14	4 (1%) 68 67	31, 42, 64, 81	0
3	C	259/261 (99%)	-0.17	2 (0%) 86 85	26, 32, 43, 66	0
3	P	259/261 (99%)	0.05	13 (5%) 29 28	30, 36, 48, 67	0
4	D	144/147 (97%)	-0.17	1 (0%) 87 87	30, 40, 53, 66	0
4	Q	144/147 (97%)	1.06	24 (16%) 1 1	39, 50, 71, 105	0
5	E	105/109 (96%)	0.36	6 (5%) 24 23	33, 40, 64, 97	0
5	R	105/109 (96%)	0.97	15 (14%) 2 2	36, 46, 70, 97	0
6	F	98/98 (100%)	0.44	9 (9%) 9 8	30, 41, 80, 117	0
6	S	98/98 (100%)	0.30	9 (9%) 9 8	34, 46, 80, 113	0
7	G	83/85 (97%)	0.83	15 (18%) 1 1	29, 38, 90, 106	0
7	T	83/85 (97%)	1.00	15 (18%) 1 1	32, 41, 91, 106	0
8	H	79/85 (92%)	0.27	10 (12%) 3 3	29, 41, 81, 101	0
8	U	79/85 (92%)	0.62	14 (17%) 1 1	37, 47, 85, 106	0
9	I	72/73 (98%)	0.25	3 (4%) 36 35	31, 46, 65, 70	0
9	V	72/73 (98%)	0.96	13 (18%) 1 1	36, 52, 67, 77	0
10	J	58/59 (98%)	0.52	7 (12%) 4 4	32, 41, 66, 95	0
10	W	58/59 (98%)	0.54	7 (12%) 4 4	36, 45, 67, 97	0
11	K	49/56 (87%)	0.03	2 (4%) 37 37	31, 39, 54, 64	0
11	X	49/56 (87%)	1.79	21 (42%) 0 0	42, 50, 66, 78	0
12	L	46/47 (97%)	-0.24	2 (4%) 35 34	29, 34, 51, 77	0
12	Y	46/47 (97%)	-0.06	1 (2%) 62 60	35, 43, 60, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.04	4 (9%) 8 8	31, 34, 72, 96	0
13	Z	43/46 (93%)	0.74	8 (18%) 1 1	39, 44, 81, 104	0
All	All	3550/3614 (98%)	0.27	237 (6%) 18 17	23, 38, 64, 117	0

The worst 5 of 237 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	14.9
6	F	1	ALA	10.4
6	S	98	HIS	9.8
6	S	1	ALA	9.6
6	S	97	ALA	9.1

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.44	0.47	83,84,85,86	0
7	TPO	T	11	11/12	0.61	0.28	75,82,102,103	0
9	SAC	I	1	9/10	0.67	0.28	73,76,78,80	0
7	TPO	G	11	11/12	0.68	0.27	69,76,102,102	0
1	FME	A	1	10/11	0.91	0.18	44,51,71,75	0
1	FME	N	1	10/11	0.93	0.18	46,53,78,82	0
2	FME	O	1	10/11	0.96	0.11	40,42,47,55	0
2	FME	B	1	10/11	0.97	0.12	33,33,41,48	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
24	UNX	C	262	1/1	0.08	0.56	80,80,80,80	0
27	DMU	P	272	33/33	0.33	0.44	77,107,124,124	0
27	DMU	C	272	33/33	0.35	0.39	68,100,115,116	0
25	PEK	T	1265	53/53	0.52	0.32	49,79,110,118	0
24	UNX	P	262	1/1	0.55	0.53	79,79,79,79	0
25	PEK	C	265	53/53	0.58	0.31	49,83,106,107	0
26	CDL	G	269	100/100	0.58	0.31	62,86,116,120	0
25	PEK	G	1263	53/53	0.62	0.51	52,103,133,134	0
22	PSC	R	1229	52/52	0.63	0.33	48,99,136,139	0
21	TGL	Y	1522	63/63	0.64	0.30	51,73,89,92	0
26	CDL	T	1269	100/100	0.65	0.30	58,86,114,118	0
23	CHD	W	1059	29/29	0.65	0.45	101,109,113,115	0
25	PEK	T	263	53/53	0.65	0.42	52,103,125,127	0
22	PSC	B	229	52/52	0.68	0.34	43,92,139,143	0
19	PGV	U	1268	51/51	0.69	0.41	60,84,103,105	0
21	TGL	N	1523	63/63	0.72	0.24	61,79,97,99	0
19	PGV	C	268	51/51	0.72	0.38	53,81,98,102	0
19	PGV	N	1524	51/51	0.72	0.28	54,74,103,105	0
26	CDL	P	1270	100/100	0.74	0.30	36,94,119,119	0
23	CHD	J	60	29/29	0.74	0.46	99,105,108,110	0
21	TGL	L	522	63/63	0.76	0.26	43,66,82,89	0
21	TGL	D	523	63/63	0.76	0.22	48,69,91,91	0
19	PGV	A	524	51/51	0.76	0.23	44,72,112,114	0
27	DMU	Z	1526	33/33	0.79	0.28	49,57,70,70	0
26	CDL	C	270	100/100	0.79	0.33	41,91,129,130	0
21	TGL	O	1521	63/63	0.80	0.21	58,80,95,96	0
23	CHD	C	271	29/29	0.86	0.25	79,83,85,85	0
21	TGL	B	521	63/63	0.86	0.22	53,74,88,90	0
23	CHD	P	1271	29/29	0.87	0.29	78,92,94,95	0
27	DMU	M	526	33/33	0.90	0.15	33,47,65,71	0
25	PEK	P	1264	53/53	0.92	0.16	35,50,86,88	0
17	MG	N	518	1/1	0.93	0.17	34,34,34,34	0
19	PGV	P	1267	51/51	0.93	0.17	29,40,82,87	0
25	PEK	C	264	53/53	0.94	0.14	30,46,78,80	0
18	NA	N	519	1/1	0.95	0.11	39,39,39,39	0
19	PGV	C	267	51/51	0.95	0.14	28,40,73,76	0
15	NO	N	520	2/2	0.95	0.14	39,39,39,42	0
19	PGV	N	1266	51/51	0.95	0.20	30,42,65,69	0
23	CHD	C	525	29/29	0.96	0.19	26,33,39,41	0
23	CHD	P	1525	29/29	0.96	0.18	32,37,43,47	0
18	NA	A	519	1/1	0.97	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	PGV	A	521	51/51	0.97	0.14	23,35,63,67	0
20	CUA	O	228	2/2	0.97	0.09	34,34,34,36	0
15	NO	A	520	2/2	0.97	0.10	32,32,32,36	0
23	CHD	O	229	29/29	0.97	0.10	27,32,38,40	0
23	CHD	B	1085	29/29	0.97	0.10	27,31,36,42	0
14	HEA	N	515	60/60	0.97	0.14	28,36,45,49	0
17	MG	A	518	1/1	0.98	0.18	23,23,23,23	0
14	HEA	N	516	60/60	0.98	0.18	27,33,37,40	0
14	HEA	A	515	60/60	0.98	0.15	22,28,41,42	0
28	ZN	F	99	1/1	0.99	0.08	37,37,37,37	0
20	CUA	B	228	2/2	0.99	0.13	27,27,27,28	0
16	CU	N	517	1/1	0.99	0.15	35,35,35,35	0
28	ZN	S	99	1/1	0.99	0.08	43,43,43,43	0
14	HEA	A	516	60/60	0.99	0.17	18,26,31,36	0
16	CU	A	517	1/1	1.00	0.15	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.