



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:31 am GMT

PDB ID : 5B1B
Title : Bovine heart cytochrome c oxidase in the fully reduced state at 1.6 angstrom resolution
Authors : Yano, N.; Muramoto, K.; Shimada, A.; Takemura, S.; Baba, J.; Fujisawa, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2015-12-01
Resolution : 1.60 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

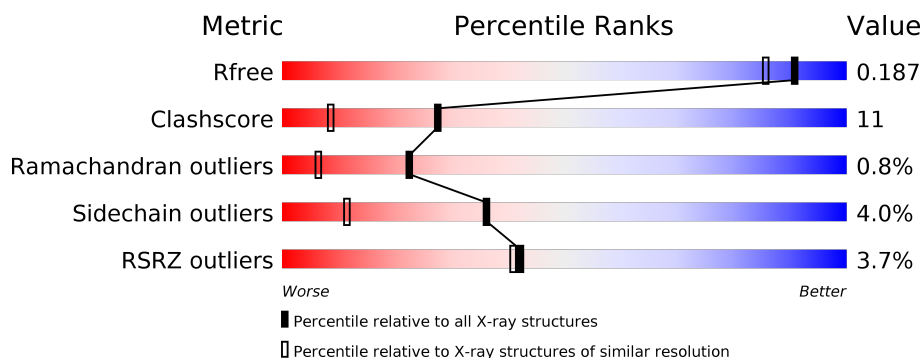
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>66%</div> <div>31%</div> <div>•</div> </div>
1	N	514	<div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
2	B	227	<div> <div>2%</div> <div>63%</div> <div>31%</div> <div>6%</div> </div>
2	O	227	<div> <div>2%</div> <div>68%</div> <div>25%</div> <div>7%</div> </div>
3	C	261	<div> <div>68%</div> <div>26%</div> <div>5%</div> <div>•</div> </div>
3	P	261	<div> <div>67%</div> <div>28%</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	601	X	-	-	-
14	HEA	A	602	X	-	-	-
14	HEA	N	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
16	MG	N	604	-	-	-	X
18	PGV	A	607	-	-	-	X
18	PGV	C	309	-	-	-	X
18	PGV	N	606	-	-	-	X
18	PGV	P	301	-	-	-	X
19	TGL	B	301	-	-	-	X
19	TGL	D	201	-	-	-	X
19	TGL	L	101	-	-	-	X
19	TGL	N	608	-	-	-	X
19	TGL	N	609	-	-	-	X
19	TGL	Q	201	-	-	-	X
2	FME	B	1	-	X	X	-
21	CHD	C	306	-	-	-	X
21	CHD	J	101	-	-	-	X
21	CHD	P	306	-	-	-	X
21	CHD	W	101	-	-	-	X
23	DMU	C	301	-	-	-	X
23	DMU	P	302	-	-	-	X
23	DMU	Z	101	-	-	-	X
26	CDL	C	305	-	-	X	X
26	CDL	G	101	-	-	X	X
26	CDL	P	305	-	-	X	X
26	CDL	T	104	-	-	X	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 34897 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	12	0
			4124	2753	638	693	40			
1	N	514	Total	C	N	O	S	0	13	0
			4131	2757	639	694	41			

- 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	6	0
			1874	1216	289	350	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	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	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	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	1	0
			609	395	108	101	5			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

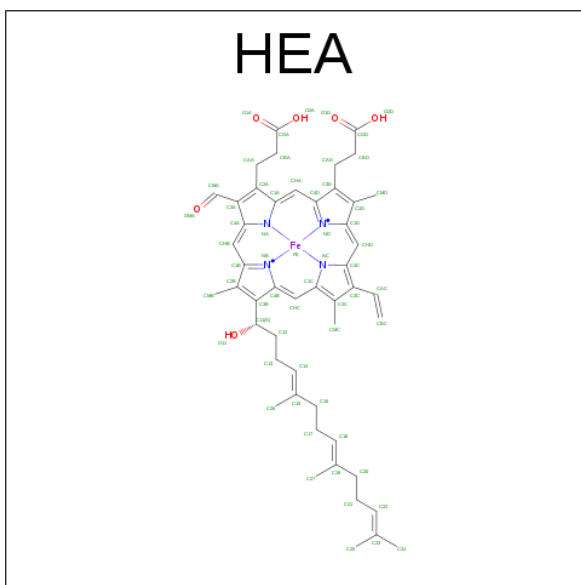
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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, mitochondrial.

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: C₄₉H₅₆FeN₄O₆).



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

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

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

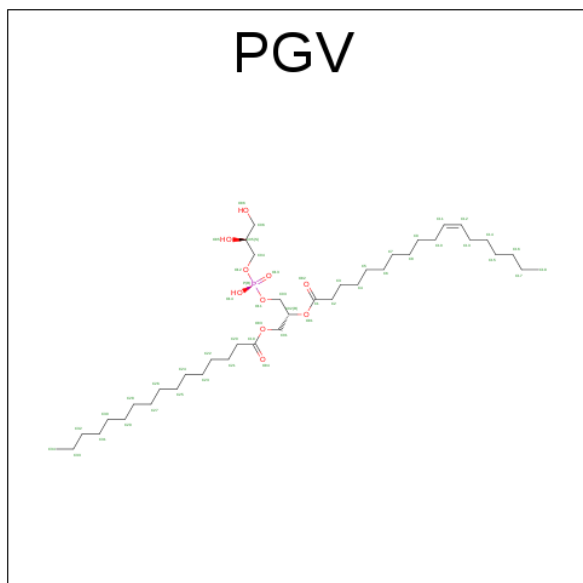
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

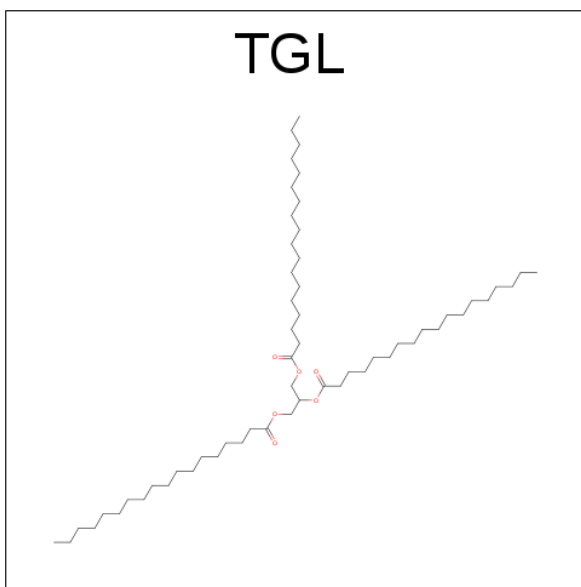
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



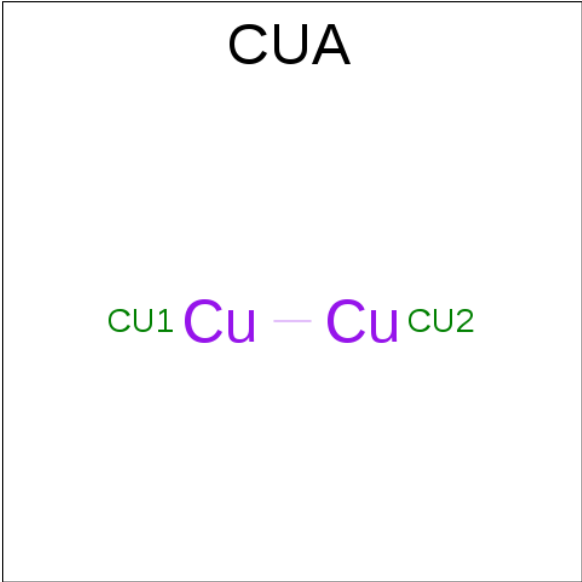
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



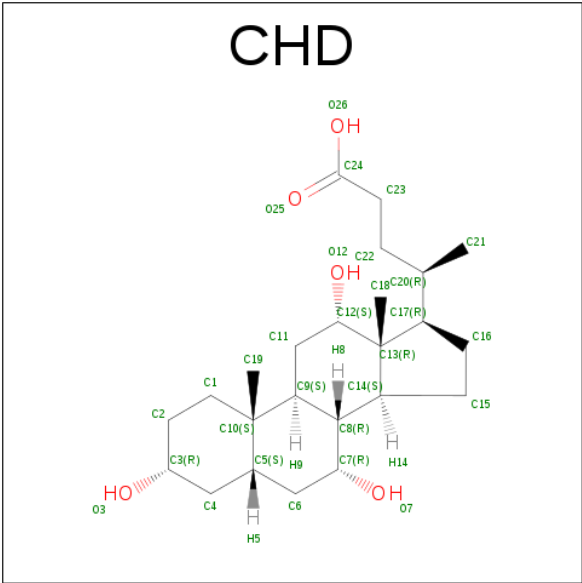
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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 CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



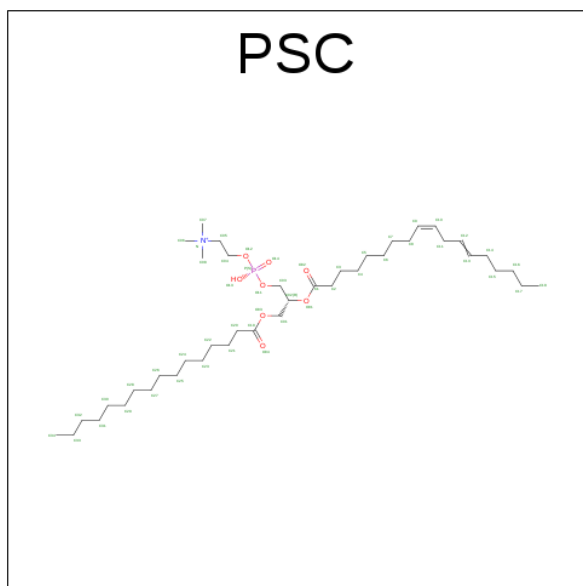
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			29	24	5		
21	C	1	Total	C	O	0	0
			29	24	5		

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

- 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: C₄₂H₈₁NO₈P).



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 DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).

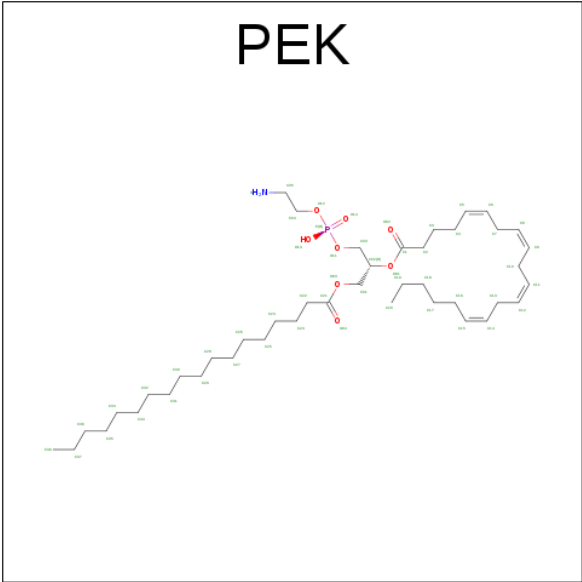


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total 33	C 22	O 11	0	0
23	M	1	Total 33	C 22	O 11	0	0
23	P	1	Total 33	C 22	O 11	0	0
23	Z	1	Total 33	C 22	O 11	0	0

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

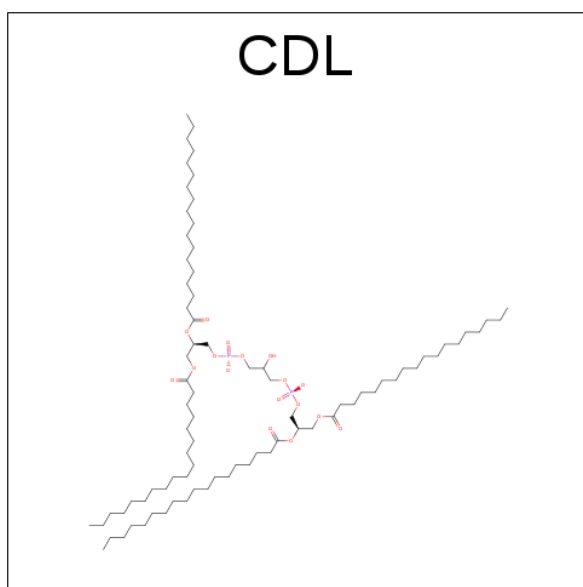
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	289	Total	O	0	0
			289	289		
28	B	254	Total	O	0	1
			255	255		
28	C	181	Total	O	0	0
			181	181		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	256	Total 256	O 256	0	0
28	E	169	Total 169	O 169	0	0
28	F	200	Total 200	O 200	0	0
28	G	108	Total 108	O 108	0	0
28	H	129	Total 129	O 129	0	0
28	I	78	Total 78	O 78	0	0
28	J	64	Total 64	O 64	0	0
28	K	68	Total 68	O 68	0	0
28	L	47	Total 47	O 47	0	0
28	M	50	Total 50	O 50	0	0
28	N	286	Total 286	O 286	0	0
28	O	225	Total 226	O 226	0	1
28	P	194	Total 194	O 194	0	0
28	Q	143	Total 143	O 143	0	0
28	R	156	Total 156	O 156	0	0
28	S	187	Total 187	O 187	0	0
28	T	97	Total 97	O 97	0	0
28	U	113	Total 113	O 113	0	0
28	V	73	Total 73	O 73	0	0
28	W	72	Total 72	O 72	0	0
28	X	48	Total 48	O 48	0	0

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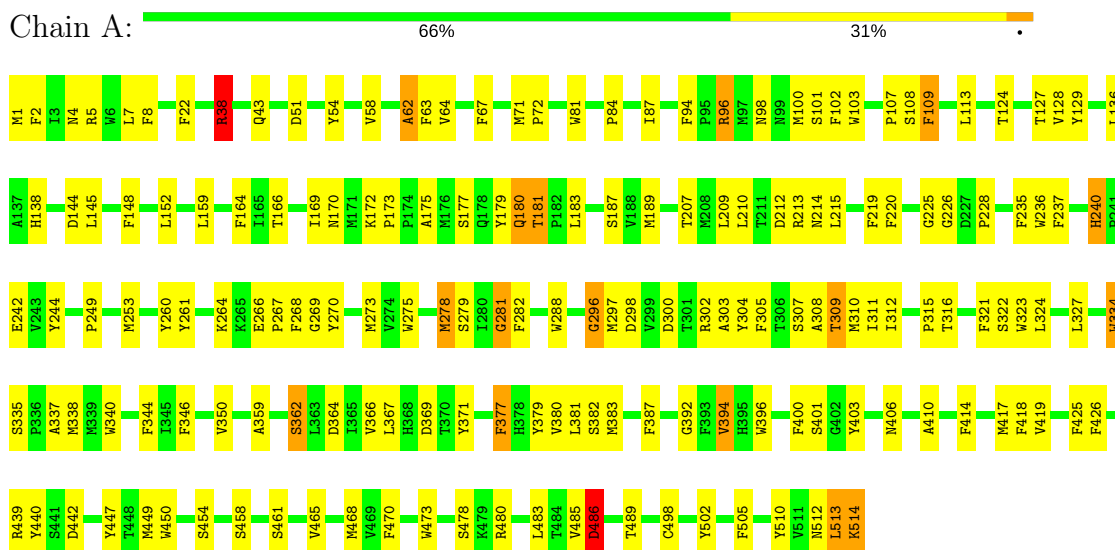
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Y	31	Total 31	O 31	0	0
28	Z	36	Total 36	O 36	0	0

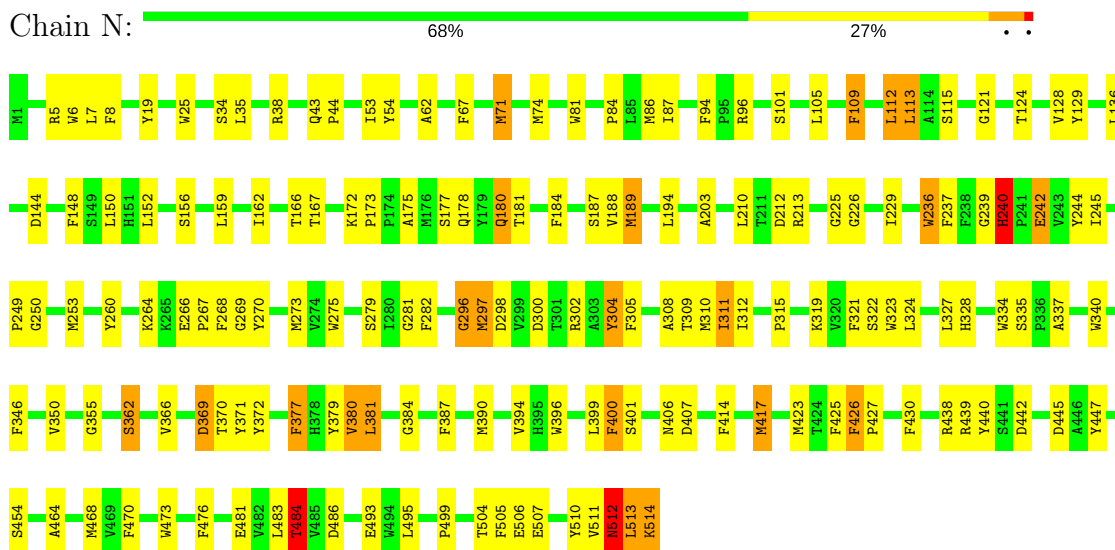
3 Residue-property plots

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

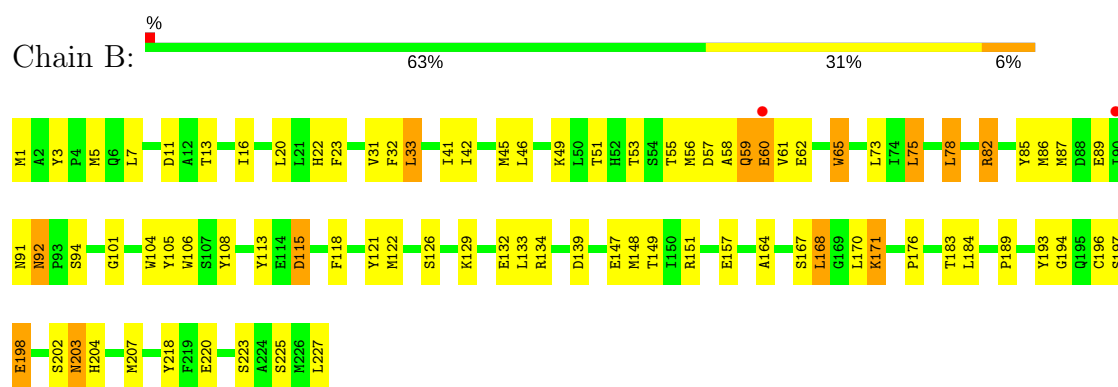
• Molecule 1: Cytochrome c oxidase subunit 1



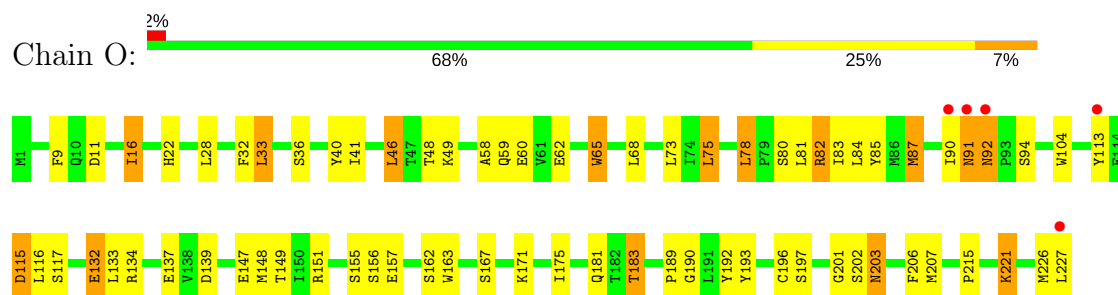
• Molecule 1: Cytochrome c oxidase subunit 1



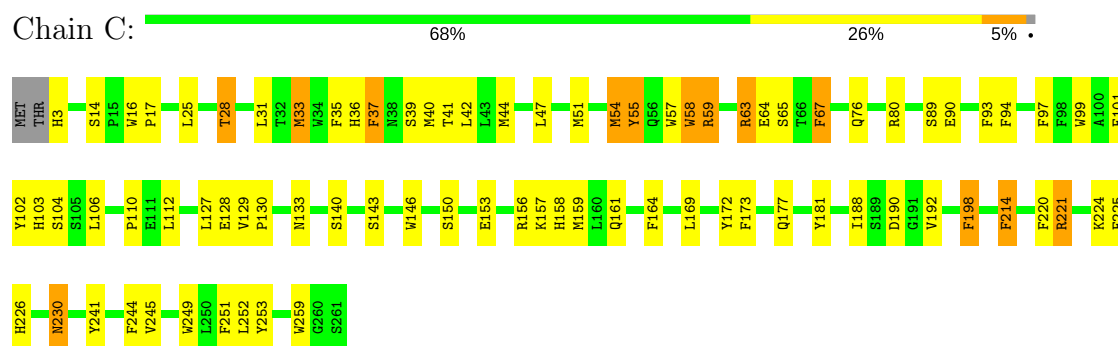
• Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3

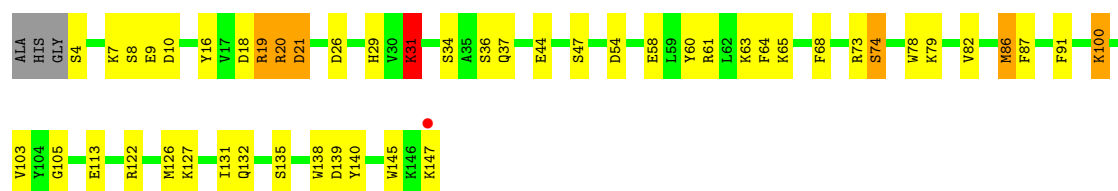


- Molecule 3: Cytochrome c oxidase subunit 3

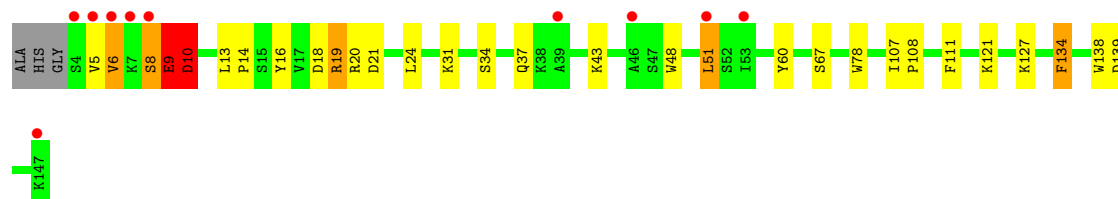
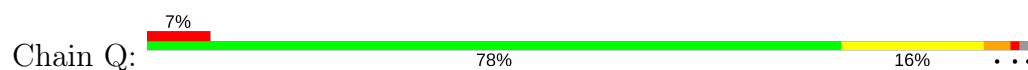


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

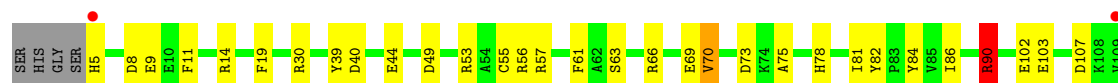




- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



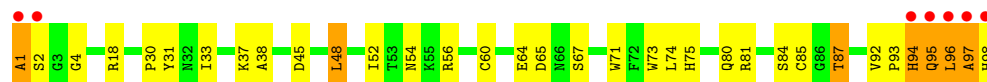
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



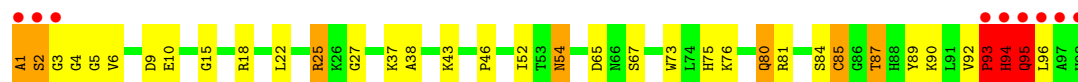
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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

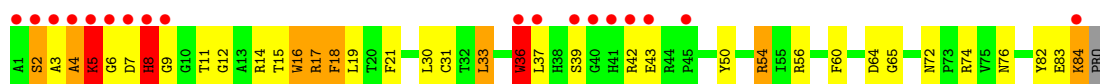


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

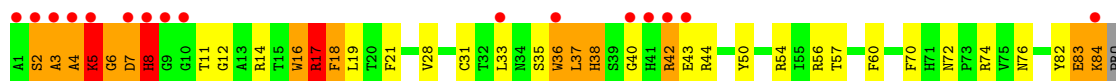


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

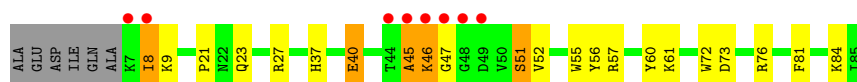




- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



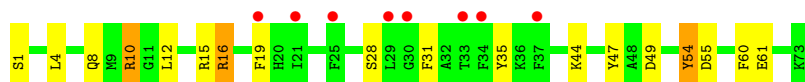
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 8: Cytochrome c oxidase subunit 6B1

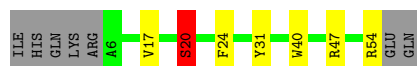


- Molecule 9: Cytochrome c oxidase subunit 6C

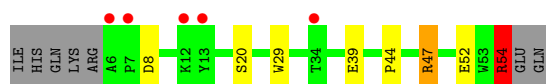




- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



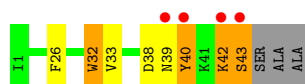
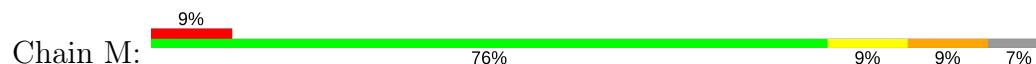
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.61Å 204.14Å 177.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60 88.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-1.60) 96.5 (88.98-1.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.161 , 0.186 0.162 , 0.187	Depositor DCC
R_{free} test set	41997 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34897	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.03	91/4253 (2.1%)	1.92	121/5805 (2.1%)
1	N	2.02	93/4260 (2.2%)	1.80	93/5814 (1.6%)
2	B	1.98	42/1912 (2.2%)	1.70	36/2603 (1.4%)
2	O	1.77	26/1908 (1.4%)	1.52	27/2599 (1.0%)
3	C	1.96	45/2261 (2.0%)	1.77	39/3090 (1.3%)
3	P	1.99	54/2260 (2.4%)	1.79	48/3088 (1.6%)
4	D	2.07	36/1284 (2.8%)	2.16	25/1730 (1.4%)
4	Q	1.64	11/1237 (0.9%)	1.67	16/1668 (1.0%)
5	E	2.03	23/882 (2.6%)	2.13	31/1196 (2.6%)
5	R	1.88	19/871 (2.2%)	1.69	19/1182 (1.6%)
6	F	1.75	13/806 (1.6%)	1.65	16/1093 (1.5%)
6	S	1.89	19/772 (2.5%)	1.65	11/1048 (1.0%)
7	G	2.08	19/702 (2.7%)	1.73	15/953 (1.6%)
7	T	1.94	16/724 (2.2%)	2.18	20/984 (2.0%)
8	H	1.72	4/682 (0.6%)	1.51	8/921 (0.9%)
8	U	1.63	7/682 (1.0%)	1.24	1/921 (0.1%)
9	I	1.84	10/605 (1.7%)	1.63	11/802 (1.4%)
9	V	1.58	2/613 (0.3%)	1.65	8/812 (1.0%)
10	J	1.85	9/471 (1.9%)	1.61	7/636 (1.1%)
10	W	1.74	8/471 (1.7%)	1.66	10/636 (1.6%)
11	K	1.80	7/405 (1.7%)	1.49	4/556 (0.7%)
11	X	1.66	4/405 (1.0%)	1.57	5/556 (0.9%)
12	L	2.08	6/393 (1.5%)	2.28	12/526 (2.3%)
12	Y	2.03	11/393 (2.8%)	1.70	3/526 (0.6%)
13	M	1.74	5/345 (1.4%)	1.53	2/470 (0.4%)
13	Z	1.72	5/345 (1.4%)	1.36	0/470
All	All	1.92	585/29942 (2.0%)	1.78	588/40685 (1.4%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	N	0	4
2	B	0	1
2	O	0	1
3	C	0	1
4	D	0	1
4	Q	0	2
5	E	0	1
6	F	0	1
6	S	0	4
7	T	0	1
8	U	0	1
9	V	0	1
10	W	0	1
12	L	0	1
All	All	0	26

The worst 5 of 585 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	TRP	CB-CG	-18.39	1.17	1.50
1	N	512	ASN	CA-CB	17.27	1.98	1.53
12	L	5	GLU	CD-OE2	-15.61	1.08	1.25
2	O	65	TRP	CB-CG	-14.85	1.23	1.50
4	D	100	LYS	CE-NZ	14.62	1.85	1.49

The worst 5 of 588 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-43.20	98.70	120.30
7	T	17	ARG	NE-CZ-NH1	35.11	137.86	120.30
4	D	20	ARG	NE-CZ-NH1	32.62	136.61	120.30
4	Q	20	ARG	NE-CZ-NH2	-29.37	105.62	120.30
7	T	17	ARG	NE-CZ-NH2	-25.91	107.34	120.30

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	296	GLY	Mainchain
1	A	304	TYR	Sidechain
1	A	38	ARG	Sidechain
1	A	96	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	4124	0	4102	50	0
1	N	4131	0	4107	97	0
2	B	1874	0	1869	51	0
2	O	1870	0	1867	51	0
3	C	2174	0	2082	54	0
3	P	2173	0	2083	43	0
4	D	1249	0	1242	25	0
4	Q	1203	0	1191	15	0
5	E	863	0	857	8	0
5	R	852	0	845	5	0
6	F	789	0	769	24	0
6	S	755	0	734	30	0
7	G	686	0	651	31	0
7	T	706	0	664	46	0
8	H	662	0	623	10	0
8	U	662	0	623	15	0
9	I	601	0	613	9	0
9	V	609	0	621	18	0
10	J	460	0	459	7	0
10	W	460	0	459	8	0
11	K	391	0	374	1	0
11	X	391	0	374	5	0
12	L	380	0	380	14	0
12	Y	380	0	380	7	0
13	M	335	0	352	4	0
13	Z	335	0	352	6	0
14	A	120	0	108	10	0
14	N	120	0	108	9	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	102	0	152	10	0
18	C	102	0	152	7	0
18	N	102	0	152	7	0
18	P	102	0	152	8	0
19	B	63	0	110	4	0
19	D	63	0	110	10	0
19	L	63	0	110	12	0
19	N	126	0	218	18	0
19	Q	63	0	110	10	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	0	0
21	C	58	0	77	3	0
21	G	29	0	39	1	0
21	J	29	0	38	5	0
21	P	58	0	77	4	0
21	W	29	0	37	2	0
22	B	52	0	80	14	0
22	R	52	0	80	17	0
23	C	33	0	42	12	0
23	M	33	0	42	0	0
23	P	33	0	42	4	0
23	Z	33	0	42	0	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	23	0
25	G	53	0	77	12	0
25	T	159	0	231	29	0
26	C	100	0	156	25	0
26	G	100	0	156	27	0
26	P	100	0	156	29	0
26	T	100	0	156	26	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	289	0	0	11	0
28	B	255	0	0	9	0
28	C	181	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	256	0	0	11	0
28	E	169	0	0	1	0
28	F	200	0	0	10	0
28	G	108	0	0	4	0
28	H	129	0	0	4	0
28	I	78	0	0	1	0
28	J	64	0	0	2	0
28	K	68	0	0	0	0
28	L	47	0	0	4	0
28	M	50	0	0	0	0
28	N	286	0	0	14	0
28	O	226	0	0	6	0
28	P	194	0	0	6	0
28	Q	143	0	0	3	0
28	R	156	0	0	2	0
28	S	187	0	0	8	0
28	T	97	0	0	3	0
28	U	113	0	0	5	0
28	V	73	0	0	4	0
28	W	72	0	0	2	0
28	X	48	0	0	1	0
28	Y	31	0	0	1	0
28	Z	36	0	0	1	0
All	All	34897	0	31876	713	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 11.

The worst 5 of 713 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:FME:CB	2:B:1:FME:CG	1.76	1.61
1:N:71:MET:CE	1:N:71:MET:CG	1.86	1.53
1:N:512:ASN:CA	1:N:512:ASN:ND2	1.72	1.49
1:N:512:ASN:CA	1:N:512:ASN:HD22	1.26	1.48
1:N:71:MET:CG	1:N:71:MET:HE3	1.41	1.47

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	525/514 (102%)	510 (97%)	15 (3%)	0	100	100
2	B	231/227 (102%)	224 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	222 (96%)	6 (3%)	2 (1%)	20	4
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/261 (102%)	259 (98%)	6 (2%)	0	100	100
4	D	148/147 (101%)	143 (97%)	5 (3%)	0	100	100
4	Q	143/147 (97%)	134 (94%)	8 (6%)	1 (1%)	25	7
5	E	104/109 (95%)	104 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	101/98 (103%)	97 (96%)	1 (1%)	3 (3%)	5	0
6	S	97/98 (99%)	90 (93%)	5 (5%)	2 (2%)	8	1
7	G	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	2	0
7	T	84/85 (99%)	71 (84%)	6 (7%)	7 (8%)	1	0
8	H	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	0
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	72/73 (99%)	70 (97%)	1 (1%)	1 (1%)	13	2
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	44 (100%)	0	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	7	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3577/3614 (99%)	3447 (96%)	102 (3%)	28 (1%)	22	6

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	97	ALA
7	G	5	LYS
7	G	8	HIS
8	H	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/426 (103%)	430 (98%)	8 (2%)	64	40
1	N	439/426 (103%)	431 (98%)	8 (2%)	64	40
2	B	216/210 (103%)	208 (96%)	8 (4%)	39	13
2	O	215/210 (102%)	202 (94%)	13 (6%)	22	4
3	C	232/226 (103%)	228 (98%)	4 (2%)	66	42
3	P	232/226 (103%)	228 (98%)	4 (2%)	66	42
4	D	134/129 (104%)	130 (97%)	4 (3%)	46	18
4	Q	129/129 (100%)	126 (98%)	3 (2%)	56	28
5	E	93/95 (98%)	90 (97%)	3 (3%)	44	17
5	R	92/95 (97%)	89 (97%)	3 (3%)	43	16
6	F	86/81 (106%)	83 (96%)	3 (4%)	41	15
6	S	82/81 (101%)	74 (90%)	8 (10%)	9	1
7	G	68/68 (100%)	57 (84%)	11 (16%)	3	0
7	T	70/68 (103%)	56 (80%)	14 (20%)	1	0
8	H	71/75 (95%)	67 (94%)	4 (6%)	25	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/75 (95%)	64 (90%)	7 (10%)	9	1
9	I	57/57 (100%)	56 (98%)	1 (2%)	64	40
9	V	58/57 (102%)	53 (91%)	5 (9%)	12	1
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	60	34
11	K	40/46 (87%)	39 (98%)	1 (2%)	53	25
11	X	40/46 (87%)	38 (95%)	2 (5%)	28	7
12	L	39/40 (98%)	38 (97%)	1 (3%)	51	23
12	Y	39/40 (98%)	37 (95%)	2 (5%)	28	7
13	M	37/38 (97%)	34 (92%)	3 (8%)	14	2
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	0
All	All	3113/3082 (101%)	2987 (96%)	126 (4%)	36	11

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

Mol	Chain	Res	Type
1	N	495	LEU
2	O	221	LYS
10	W	50	LEU
1	N	512	ASN
2	O	75	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	31	GLN
1	N	98	ASN
7	T	76	ASN
8	H	37	HIS
10	J	57	HIS

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	1.46	2 (22%)	7,9,11	2.16	2 (28%)
2	FME	B	1	2	9,9,10	5.98	6 (66%)	7,9,11	10.97	5 (71%)
7	TPO	G	11	7	9,10,11	3.92	5 (55%)	10,14,16	2.38	4 (40%)
9	SAC	I	1	9	8,8,9	2.62	4 (50%)	6,9,11	2.51	2 (33%)
1	FME	N	1	1	9,9,10	0.76	0	7,9,11	2.56	4 (57%)
2	FME	O	1	2	9,9,10	1.68	2 (22%)	7,9,11	2.00	3 (42%)
7	TPO	T	11	7	9,10,11	3.09	3 (33%)	10,14,16	1.44	2 (20%)
9	SAC	V	1	9	8,8,9	3.22	3 (37%)	6,9,11	1.54	1 (16%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.54	1.62	1.81
2	O	1	FME	CG-SD	-2.58	1.67	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O-C	2.03	1.28	1.19
9	I	1	SAC	CB-CA	2.13	1.57	1.53
1	A	1	FME	O-C	2.54	1.30	1.19

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O1-CN-N	-23.88	58.59	125.20
2	B	1	FME	CA-N-CN	-15.31	99.27	122.82
7	G	11	TPO	C-CA-N	-4.95	99.88	109.86
9	I	1	SAC	CB-CA-N	-4.79	99.44	110.60
1	N	1	FME	O-C-CA	-3.90	116.06	125.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
2	B	1	FME	11	0
7	G	11	TPO	2	0
9	I	1	SAC	1	0
7	T	11	TPO	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 44 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	HEA	A	601	1	44,67,67	2.31	20 (45%)	37,103,103	3.40	19 (51%)
14	HEA	A	602	1	44,67,67	1.68	13 (29%)	37,103,103	2.35	15 (40%)
18	PGV	A	606	-	50,50,50	1.41	5 (10%)	51,56,56	1.52	8 (15%)
18	PGV	A	607	-	50,50,50	1.60	5 (10%)	51,56,56	2.06	13 (25%)
19	TGL	B	301	-	62,62,62	1.42	7 (11%)	65,65,65	2.63	17 (26%)
20	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
21	CHD	B	303	-	29,32,32	2.93	18 (62%)	47,51,51	2.93	25 (53%)
22	PSC	B	304	-	51,51,51	1.35	3 (5%)	56,59,59	1.57	11 (19%)
23	DMU	C	301	-	34,34,34	0.69	1 (2%)	45,45,45	2.37	17 (37%)
25	PEK	C	303	-	52,52,52	1.32	6 (11%)	54,57,57	2.01	17 (31%)
18	PGV	C	304	-	50,50,50	1.02	2 (4%)	51,56,56	1.28	6 (11%)
26	CDL	C	305	-	99,99,99	1.66	21 (21%)	101,111,111	2.01	27 (26%)
21	CHD	C	306	-	29,32,32	1.22	4 (13%)	47,51,51	3.82	25 (53%)
21	CHD	C	307	-	29,32,32	2.84	14 (48%)	47,51,51	3.18	27 (57%)
25	PEK	C	308	-	52,52,52	1.58	4 (7%)	54,57,57	1.84	12 (22%)
18	PGV	C	309	-	50,50,50	1.32	4 (8%)	51,56,56	2.09	11 (21%)
19	TGL	D	201	-	62,62,62	2.12	9 (14%)	65,65,65	3.00	17 (26%)
26	CDL	G	101	-	99,99,99	1.55	15 (15%)	101,111,111	1.84	25 (24%)
25	PEK	G	102	-	52,52,52	1.22	2 (3%)	54,57,57	1.62	7 (12%)
21	CHD	G	103	-	29,32,32	2.77	14 (48%)	47,51,51	3.10	24 (51%)
21	CHD	J	101	-	29,32,32	1.89	8 (27%)	47,51,51	4.07	31 (65%)
19	TGL	L	101	-	62,62,62	1.97	11 (17%)	65,65,65	2.81	22 (33%)
23	DMU	M	101	-	34,34,34	1.09	2 (5%)	45,45,45	1.90	11 (24%)
14	HEA	N	601	1	44,67,67	1.63	10 (22%)	37,103,103	3.21	19 (51%)
14	HEA	N	602	1	44,67,67	1.82	14 (31%)	37,103,103	2.18	12 (32%)
18	PGV	N	606	-	50,50,50	1.31	2 (4%)	51,56,56	2.01	9 (17%)
18	PGV	N	607	-	50,50,50	1.46	8 (16%)	51,56,56	1.62	12 (23%)
19	TGL	N	608	-	62,62,62	1.50	8 (12%)	65,65,65	2.63	18 (27%)
19	TGL	N	609	-	62,62,62	1.72	9 (14%)	65,65,65	2.26	18 (27%)
20	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
18	PGV	P	301	-	50,50,50	1.22	3 (6%)	51,56,56	1.77	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	DMU	P	302	-	34,34,34	0.81	1 (2%)	45,45,45	1.48	7 (15%)
18	PGV	P	304	-	50,50,50	1.10	2 (4%)	51,56,56	1.46	10 (19%)
26	CDL	P	305	-	99,99,99	1.72	17 (17%)	101,111,111	2.14	27 (26%)
21	CHD	P	306	-	29,32,32	1.40	5 (17%)	47,51,51	3.11	23 (48%)
21	CHD	P	307	-	29,32,32	2.12	12 (41%)	47,51,51	2.73	20 (42%)
19	TGL	Q	201	-	62,62,62	1.89	7 (11%)	65,65,65	2.35	13 (20%)
22	PSC	R	201	-	51,51,51	1.62	5 (9%)	56,59,59	1.85	10 (17%)
25	PEK	T	101	-	52,52,52	1.13	3 (5%)	54,57,57	1.61	13 (24%)
25	PEK	T	102	-	52,52,52	1.26	3 (5%)	54,57,57	1.36	8 (14%)
25	PEK	T	103	-	52,52,52	1.91	9 (17%)	54,57,57	2.25	14 (25%)
26	CDL	T	104	-	99,99,99	1.42	14 (14%)	101,111,111	1.89	23 (22%)
21	CHD	W	101	-	29,32,32	1.73	9 (31%)	47,51,51	4.37	26 (55%)
23	DMU	Z	101	-	34,34,34	1.22	5 (14%)	45,45,45	1.73	14 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1	2/2/7/16	0/24/76/76	0/0/8/8
18	PGV	A	606	-	-	0/55/55/55	0/0/0/0
18	PGV	A	607	-	-	1/55/55/55	0/0/0/0
19	TGL	B	301	-	-	0/65/65/65	0/0/0/0
20	CUA	B	302	2	-	0/0/0/0	0/0/0/0
21	CHD	B	303	-	-	0/7/74/74	0/4/4/4
22	PSC	B	304	-	-	0/55/55/55	0/0/0/0
23	DMU	C	301	-	-	0/19/59/59	0/2/2/2
25	PEK	C	303	-	-	0/56/56/56	0/0/0/0
18	PGV	C	304	-	-	0/55/55/55	0/0/0/0
26	CDL	C	305	-	-	0/110/110/110	0/0/0/0
21	CHD	C	306	-	-	0/7/74/74	0/4/4/4
21	CHD	C	307	-	-	0/7/74/74	0/4/4/4
25	PEK	C	308	-	-	0/56/56/56	0/0/0/0
18	PGV	C	309	-	-	1/55/55/55	0/0/0/0
19	TGL	D	201	-	-	0/65/65/65	0/0/0/0
26	CDL	G	101	-	-	0/110/110/110	0/0/0/0
25	PEK	G	102	-	-	0/56/56/56	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHD	G	103	-	-	0/7/74/74	0/4/4/4
21	CHD	J	101	-	-	0/7/74/74	0/4/4/4
19	TGL	L	101	-	-	0/65/65/65	0/0/0/0
23	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	HEA	N	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1	3/3/7/16	0/24/76/76	0/0/8/8
18	PGV	N	606	-	-	3/55/55/55	0/0/0/0
18	PGV	N	607	-	-	0/55/55/55	0/0/0/0
19	TGL	N	608	-	-	0/65/65/65	0/0/0/0
19	TGL	N	609	-	-	0/65/65/65	0/0/0/0
20	CUA	O	301	2	-	0/0/0/0	0/0/0/0
18	PGV	P	301	-	-	1/55/55/55	0/0/0/0
23	DMU	P	302	-	-	0/19/59/59	0/2/2/2
18	PGV	P	304	-	-	0/55/55/55	0/0/0/0
26	CDL	P	305	-	-	2/110/110/110	0/0/0/0
21	CHD	P	306	-	-	0/7/74/74	0/4/4/4
21	CHD	P	307	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	201	-	-	0/65/65/65	0/0/0/0
22	PSC	R	201	-	-	0/55/55/55	0/0/0/0
25	PEK	T	101	-	-	0/56/56/56	0/0/0/0
25	PEK	T	102	-	-	0/56/56/56	0/0/0/0
25	PEK	T	103	-	-	2/56/56/56	0/0/0/0
26	CDL	T	104	-	-	0/110/110/110	0/0/0/0
21	CHD	W	101	-	-	0/7/74/74	1/4/4/4
23	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

The worst 5 of 334 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	307	CHD	C13-C12	-5.09	1.46	1.54
14	A	601	HEA	C3C-C2C	-5.03	1.33	1.40
14	A	601	HEA	C4B-NB	-4.16	1.31	1.36
21	B	303	CHD	C10-C5	-4.13	1.48	1.55
21	G	103	CHD	C10-C5	-3.96	1.48	1.55

The worst 5 of 694 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	201	TGL	OG2-CB1-CB2	-14.69	81.04	111.55
21	W	101	CHD	C18-C13-C12	-12.41	96.45	109.08
19	Q	201	TGL	OG2-CB1-CB2	-12.07	86.49	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C13-C12-C11	-11.12	97.63	114.46
19	L	101	TGL	CC4-CC3-CC2	-10.89	73.35	113.24

5 of 9 chirality outliers are listed below:

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

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	309	PGV	C02-O01-C1-C2
18	A	607	PGV	C02-O01-C1-C2
25	T	103	PEK	C02-O01-C1-O02
18	P	301	PGV	P-O11-C03-C02
18	N	606	PGV	P-O11-C03-C02

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	W	101	CHD	C11-C12-C13-C14-C8-C9

39 monomers are involved in 319 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	3	0
14	A	602	HEA	7	0
18	A	606	PGV	2	0
18	A	607	PGV	8	0
19	B	301	TGL	4	0
22	B	304	PSC	14	0
23	C	301	DMU	12	0
25	C	303	PEK	9	0
18	C	304	PGV	4	0
26	C	305	CDL	25	0
21	C	306	CHD	2	0
21	C	307	CHD	1	0
25	C	308	PEK	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	309	PGV	3	0
19	D	201	TGL	10	0
26	G	101	CDL	27	0
25	G	102	PEK	12	0
21	G	103	CHD	1	0
21	J	101	CHD	5	0
19	L	101	TGL	12	0
14	N	601	HEA	3	0
14	N	602	HEA	6	0
18	N	606	PGV	6	0
18	N	607	PGV	1	0
19	N	608	TGL	7	0
19	N	609	TGL	11	0
18	P	301	PGV	1	0
23	P	302	DMU	4	0
18	P	304	PGV	7	0
26	P	305	CDL	29	0
21	P	306	CHD	3	0
21	P	307	CHD	1	0
19	Q	201	TGL	10	0
22	R	201	PSC	17	0
25	T	101	PEK	5	0
25	T	102	PEK	17	0
25	T	103	PEK	7	0
26	T	104	CDL	26	0
21	W	101	CHD	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.65	0 100 100	16, 20, 28, 70	0
1	N	513/514 (99%)	-0.61	0 100 100	17, 24, 31, 63	0
2	B	226/227 (99%)	-0.62	2 (0%) 84 85	19, 28, 48, 90	0
2	O	226/227 (99%)	-0.52	5 (2%) 62 63	23, 34, 61, 99	0
3	C	259/261 (99%)	-0.86	0 100 100	19, 24, 36, 77	0
3	P	259/261 (99%)	-0.81	1 (0%) 92 92	19, 24, 37, 65	0
4	D	144/147 (97%)	-0.84	1 (0%) 87 88	23, 29, 42, 72	0
4	Q	144/147 (97%)	0.36	10 (6%) 18 17	28, 42, 74, 152	0
5	E	105/109 (96%)	-0.70	2 (1%) 67 67	23, 29, 51, 123	0
5	R	105/109 (96%)	-0.14	3 (2%) 52 51	26, 36, 58, 130	0
6	F	98/98 (100%)	-0.09	7 (7%) 17 16	20, 31, 98, 153	0
6	S	98/98 (100%)	-0.08	9 (9%) 10 9	20, 29, 72, 146	0
7	G	83/85 (97%)	0.41	18 (21%) 1 1	22, 31, 92, 134	0
7	T	83/85 (97%)	0.21	16 (19%) 1 1	22, 33, 103, 143	0
8	H	79/85 (92%)	-0.14	8 (10%) 8 7	25, 35, 95, 127	0
8	U	79/85 (92%)	-0.24	9 (11%) 6 5	30, 39, 95, 118	0
9	I	72/73 (98%)	0.25	8 (11%) 6 6	26, 41, 62, 79	0
9	V	72/73 (98%)	0.32	8 (11%) 6 6	26, 46, 68, 86	0
10	J	58/59 (98%)	0.22	5 (8%) 11 11	25, 33, 64, 120	0
10	W	58/59 (98%)	-0.10	4 (6%) 18 17	24, 35, 68, 141	0
11	K	49/56 (87%)	-0.41	0 100 100	27, 34, 50, 61	0
11	X	49/56 (87%)	0.71	5 (10%) 7 7	34, 43, 65, 81	0
12	L	46/47 (97%)	-0.91	0 100 100	21, 26, 41, 89	0
12	Y	46/47 (97%)	-0.76	1 (2%) 62 63	25, 32, 53, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.43	4 (9%) 9 9	23, 27, 64, 116	0
13	Z	43/46 (93%)	-0.16	6 (13%) 3 3	30, 36, 78, 136	0
All	All	3550/3614 (98%)	-0.43	132 (3%) 42 41	16, 28, 60, 153	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	35.6
4	Q	5	VAL	32.0
4	Q	6	VAL	15.9
6	F	97	ALA	14.9
4	Q	4	SER	11.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.97	0.09	-	31,38,64,86	0
9	SAC	I	1	9/10	0.82	0.29	-	63,91,107,108	0
9	SAC	V	1	9/10	0.67	0.53	-	108,123,136,136	0
7	TPO	G	11	11/12	0.49	0.23	-	68,82,133,143	0
2	FME	O	1	10/11	0.97	0.06	-	33,33,40,47	0
2	FME	B	1	10/11	0.96	0.08	-	20,26,38,51	0
1	FME	N	1	10/11	0.97	0.11	-	32,37,56,66	0
7	TPO	T	11	11/12	0.49	0.24	-	74,84,143,151	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
21	CHD	W	101	29/29	0.52	0.43	12.70	62,129,154,158	0
26	CDL	P	305	100/100	0.85	0.30	10.20	34,76,126,142	0
21	CHD	J	101	29/29	0.61	0.45	9.67	54,125,148,152	0
26	CDL	C	305	100/100	0.84	0.35	7.74	33,74,131,147	0
18	PGV	A	607	51/51	0.86	0.17	6.48	34,73,109,140	0
19	TGL	D	201	63/63	0.83	0.15	6.17	29,61,90,99	0
26	CDL	T	104	100/100	0.67	0.26	5.98	50,87,137,163	0
19	TGL	N	608	63/63	0.85	0.20	5.60	47,73,106,120	0
18	PGV	N	606	51/51	0.82	0.25	5.49	39,75,149,165	0
19	TGL	L	101	63/63	0.85	0.18	5.48	28,54,93,94	0
26	CDL	G	101	100/100	0.62	0.28	4.51	49,89,146,161	0
16	MG	N	604	1/1	0.98	0.13	4.20	24,24,24,24	0
19	TGL	N	609	63/63	0.79	0.20	4.02	40,61,94,100	0
23	DMU	C	301	33/33	0.77	0.21	3.60	33,123,149,150	0
21	CHD	P	306	29/29	0.79	0.31	3.38	51,89,103,106	0
19	TGL	Q	201	63/63	0.76	0.18	3.13	41,69,93,97	0
19	TGL	B	301	63/63	0.87	0.15	3.08	38,67,95,99	0
21	CHD	C	306	29/29	0.73	0.38	2.83	52,101,116,126	0
23	DMU	Z	101	33/33	0.80	0.19	2.67	38,44,61,64	0
18	PGV	C	309	51/51	0.85	0.23	2.65	46,78,152,155	0
23	DMU	P	302	33/33	0.75	0.16	2.37	38,103,146,150	0
18	PGV	P	301	51/51	0.79	0.23	2.27	50,79,135,157	0
23	DMU	M	101	33/33	0.89	0.12	1.71	34,37,52,59	0
22	PSC	B	304	52/52	0.82	0.21	1.57	39,93,160,161	0
25	PEK	T	102	53/53	0.77	0.25	1.50	41,91,153,157	0
25	PEK	T	103	53/53	0.76	0.22	1.49	38,73,125,130	0
18	PGV	C	304	51/51	0.98	0.07	1.25	21,26,67,77	0
22	PSC	R	201	52/52	0.84	0.21	1.16	35,80,159,164	0
16	MG	A	604	1/1	0.99	0.09	1.12	19,19,19,19	0
25	PEK	T	101	53/53	0.97	0.08	1.11	26,38,86,89	0
18	PGV	A	606	51/51	0.98	0.07	1.06	18,25,54,62	0
25	PEK	G	102	53/53	0.82	0.24	1.00	43,91,139,153	0
25	PEK	C	308	53/53	0.75	0.18	0.91	43,71,122,155	0
25	PEK	C	303	53/53	0.98	0.07	0.91	23,38,73,95	0
18	PGV	P	304	51/51	0.98	0.06	0.64	20,26,69,77	0
14	HEA	N	601	60/60	0.99	0.07	0.54	20,22,38,41	0
21	CHD	C	307	29/29	0.95	0.09	0.32	23,26,31,34	0
14	HEA	N	602	60/60	0.99	0.08	0.27	18,21,26,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	ZN	F	101	1/1	1.00	0.05	0.26	25,25,25,25	0
18	PGV	N	607	51/51	0.99	0.07	0.24	19,27,59,65	0
21	CHD	P	307	29/29	0.96	0.09	0.06	25,28,31,34	0
21	CHD	G	103	29/29	0.95	0.07	-0.17	22,24,27,31	0
21	CHD	B	303	29/29	0.95	0.07	-0.32	23,25,28,34	0
14	HEA	A	601	60/60	0.99	0.06	-0.48	16,18,31,34	0
14	HEA	A	602	60/60	0.99	0.06	-0.68	16,18,24,28	0
27	ZN	S	101	1/1	0.99	0.05	-0.81	25,25,25,25	0
20	CUA	B	302	2/2	1.00	0.07	-1.03	21,21,21,21	0
20	CUA	O	301	2/2	1.00	0.06	-1.77	26,26,26,26	0
17	NA	N	605	1/1	1.00	0.02	-1.95	30,30,30,30	0
17	NA	A	605	1/1	0.99	0.02	-2.98	24,24,24,24	0
24	UNX	C	302	1/1	0.45	0.81	-	38,38,38,38	1
24	UNX	P	303	1/1	0.42	0.91	-	34,34,34,34	1
15	CU	A	603	1/1	1.00	0.07	-	18,18,18,18	0
15	CU	N	603	1/1	1.00	0.07	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.