



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:34 am GMT

PDB ID : 3AG2
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

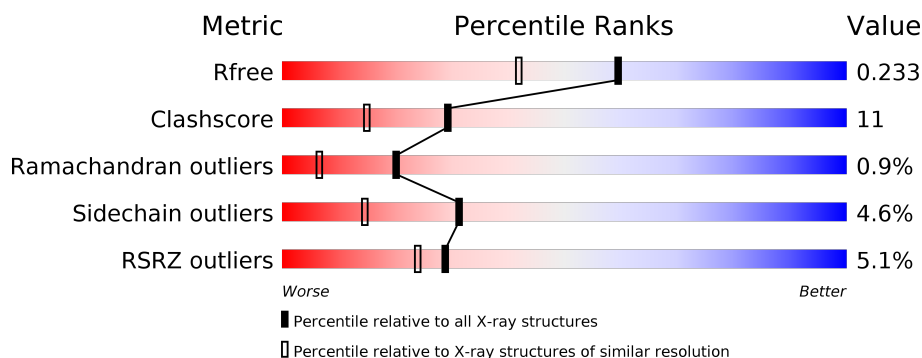
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>30%</div> <div>•</div> </div>
1	N	514	<div> <div>75%</div> <div>22%</div> <div>•</div> </div>
2	B	227	<div> <div>74%</div> <div>21%</div> <div>6%</div> </div>
2	O	227	<div> <div>3%</div> <div>71%</div> <div>25%</div> <div>••</div> </div>
3	C	261	<div> <div>2%</div> <div>78%</div> <div>20%</div> <div>••</div> </div>
3	P	261	<div> <div>4%</div> <div>76%</div> <div>20%</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	TGL	A	523	-	-	-	X
19	TGL	B	521	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	N	1523	-	-	-	X
19	TGL	O	1521	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	C	268	-	-	-	X
20	PGV	N	1524	-	-	-	X
21	CHD	C	271	X	-	-	X
21	CHD	J	60	X	-	-	X
21	CHD	P	1271	X	-	-	X
21	CHD	W	1059	X	-	-	X
23	PSC	B	229	-	-	-	X
23	PSC	R	1229	-	-	-	X
25	PEK	G	1263	-	-	-	X
25	PEK	T	263	-	-	X	-
26	CDL	C	270	-	-	-	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	X	X
26	CDL	T	1269	-	-	X	X
27	DMU	C	272	X	-	-	X
27	DMU	M	526	X	-	-	-
27	DMU	P	1272	X	-	-	X
27	DMU	Z	1526	X	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32400 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 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			

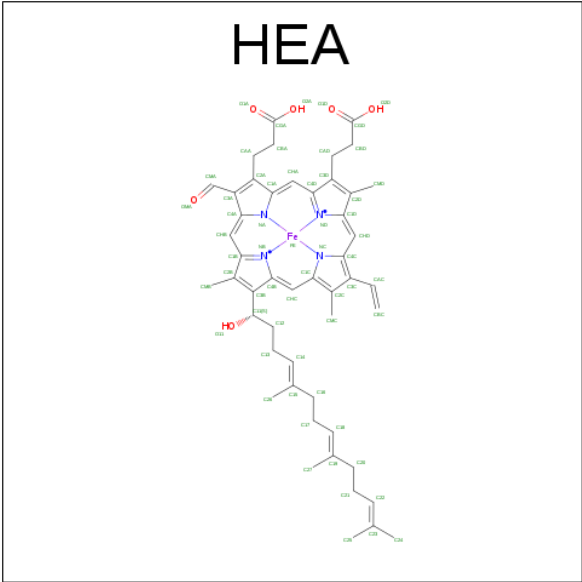
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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: C₄₉H₅₆FeN₄O₆).

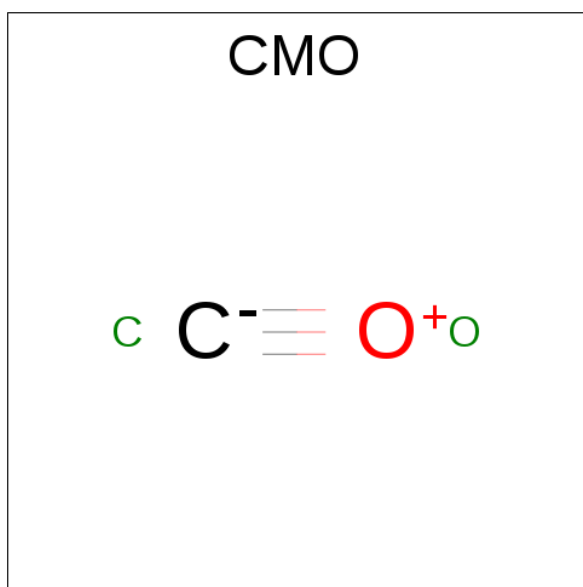


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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

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

- Molecule 16 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

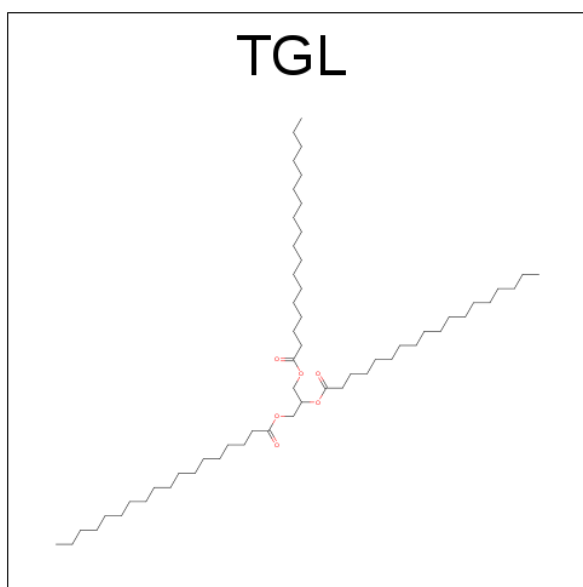
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

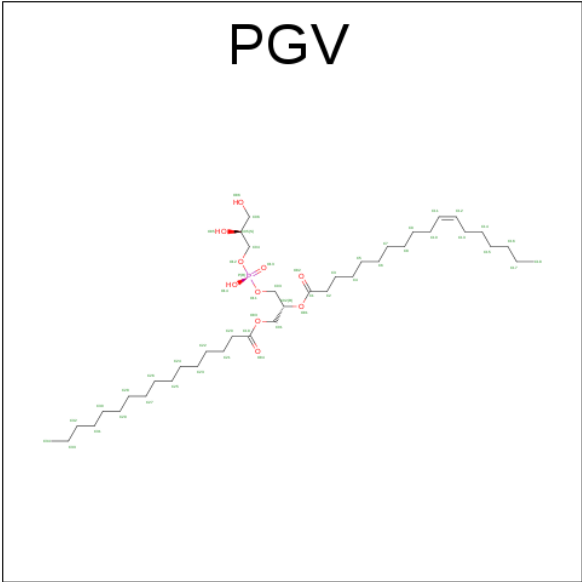
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

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



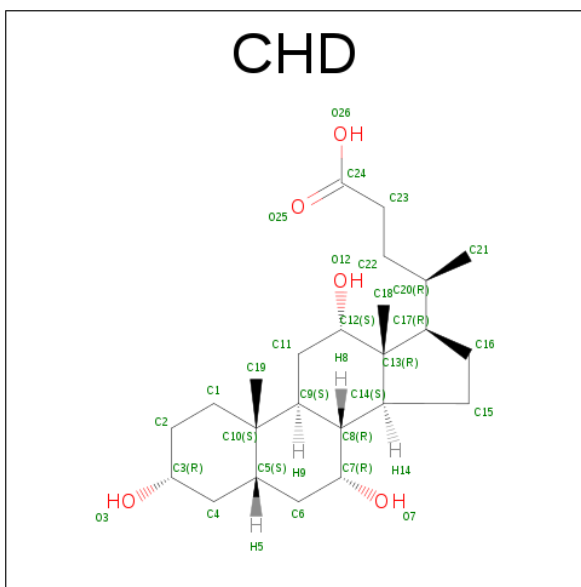
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



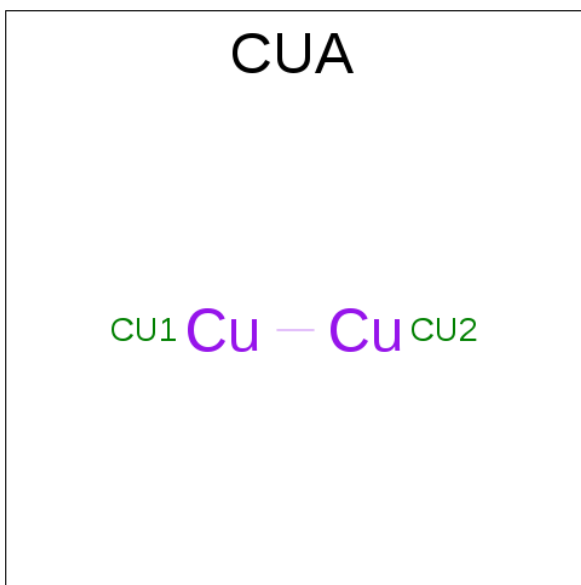
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	G	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0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

- Molecule 21 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



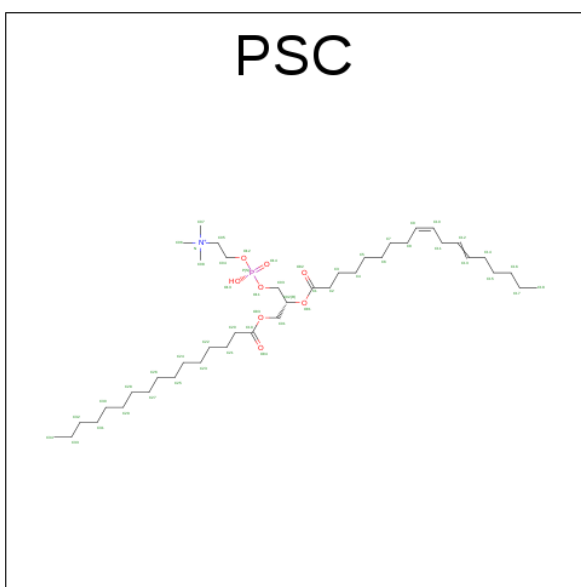
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			29	24	5		
21	B	1	Total	C	O	0	0
			29	24	5		
21	C	1	Total	C	O	0	0
			29	24	5		
21	G	1	Total	C	O	0	0
			29	24	5		
21	J	1	Total	C	O	0	0
			29	24	5		
21	P	1	Total	C	O	0	0
			29	24	5		
21	P	1	Total	C	O	0	0
			29	24	5		
21	W	1	Total	C	O	0	0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

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 23 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
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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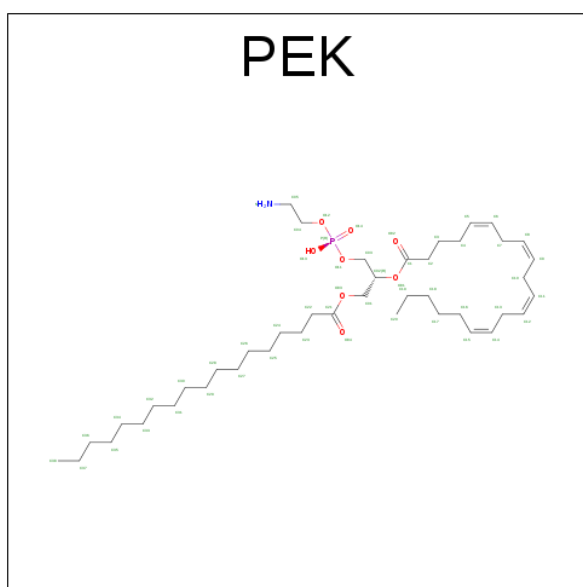
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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: C₄₃H₇₈NO₈P).



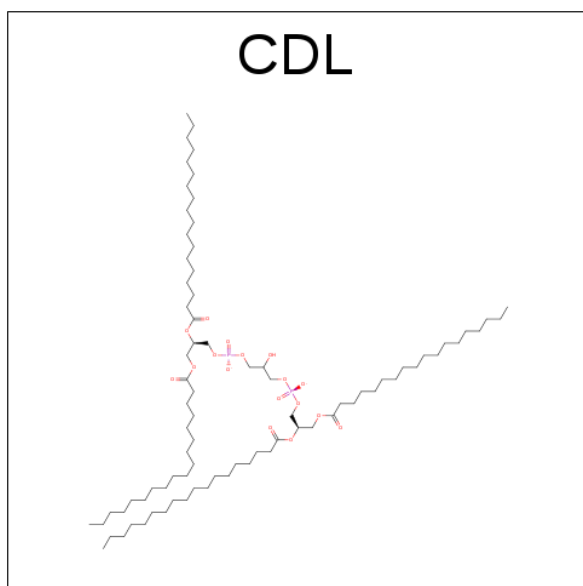
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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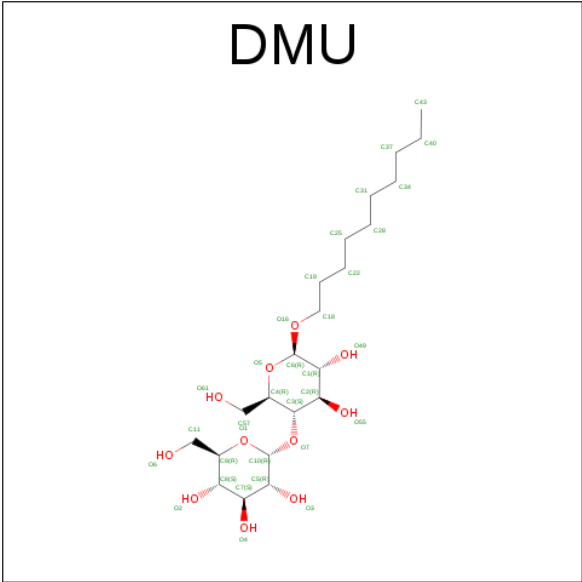
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	213	Total	O	0	0
			213	213		
29	B	135	Total	O	0	0
			135	135		
29	C	109	Total	O	0	0
			109	109		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	D	93	Total 93	O 93	0	0
29	E	61	Total 61	O 61	0	0
29	F	80	Total 80	O 80	0	0
29	G	56	Total 56	O 56	0	0
29	H	53	Total 53	O 53	0	0
29	I	35	Total 35	O 35	0	0
29	J	16	Total 16	O 16	0	0
29	K	21	Total 21	O 21	0	0
29	L	28	Total 28	O 28	0	0
29	M	24	Total 24	O 24	0	0
29	N	205	Total 205	O 205	0	0
29	O	106	Total 106	O 106	0	0
29	P	106	Total 106	O 106	0	0
29	Q	51	Total 51	O 51	0	0
29	R	39	Total 39	O 39	0	0
29	S	62	Total 62	O 62	0	0
29	T	47	Total 47	O 47	0	0
29	U	50	Total 50	O 50	0	0
29	V	21	Total 21	O 21	0	0
29	W	15	Total 15	O 15	0	0
29	X	19	Total 19	O 19	0	0

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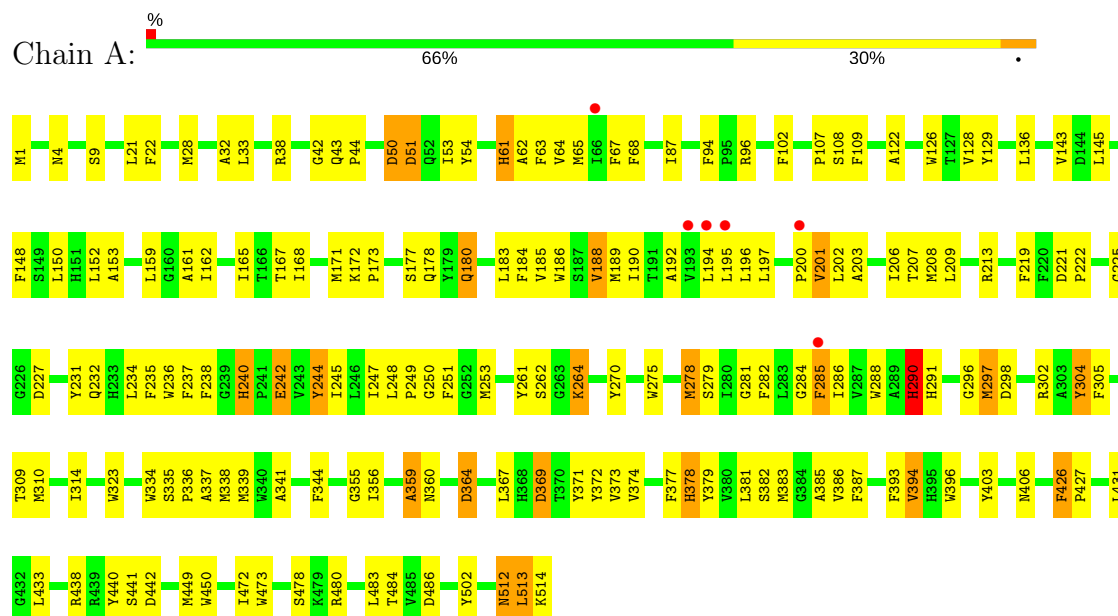
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	12	Total 12	O 12	0	0
29	Z	7	Total 7	O 7	0	0

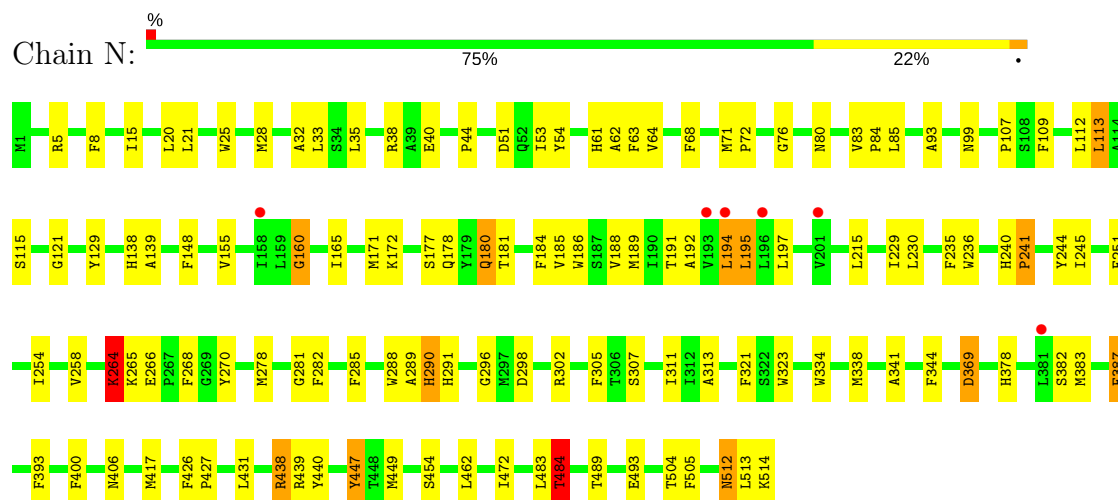
3 Residue-property plots

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

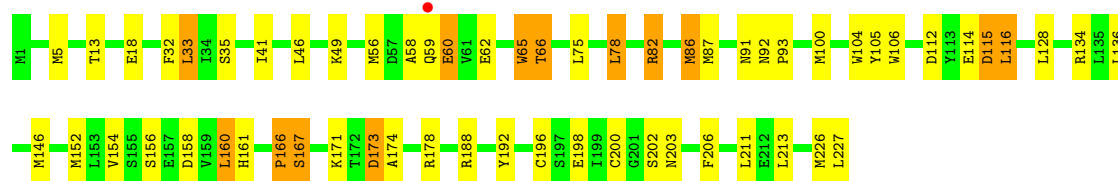


• Molecule 1: Cytochrome c oxidase subunit 1



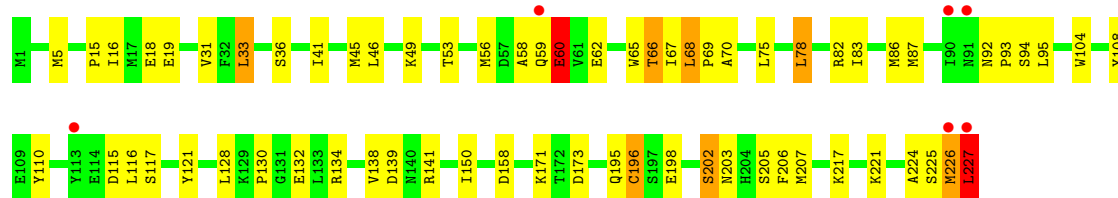
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 




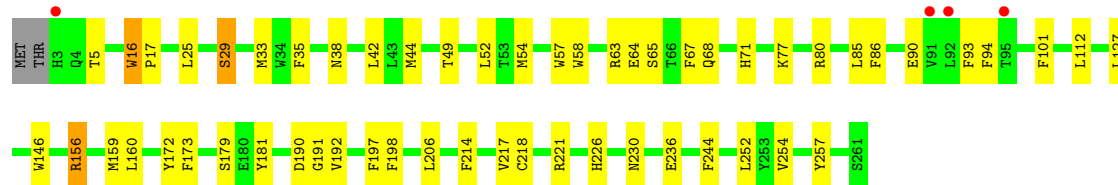
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 



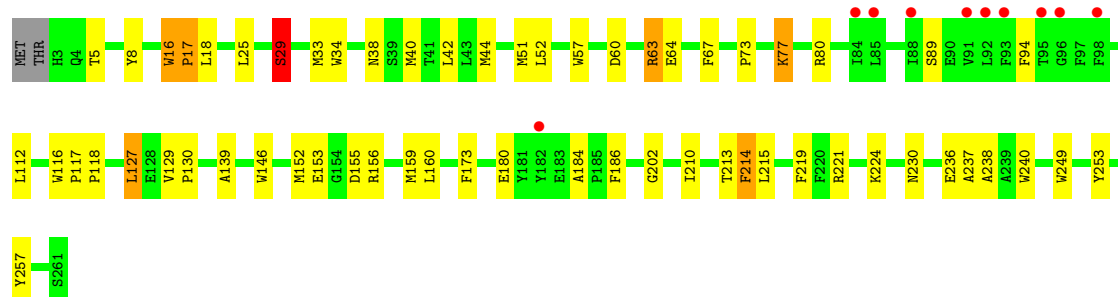
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 




• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 

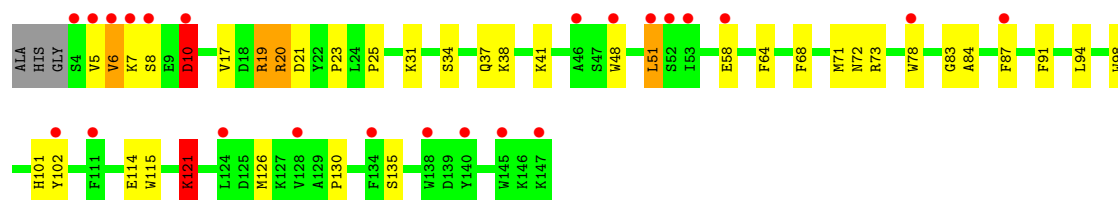
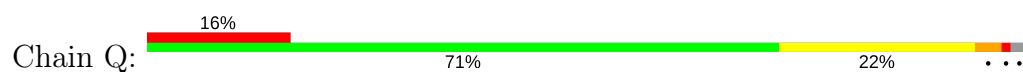


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

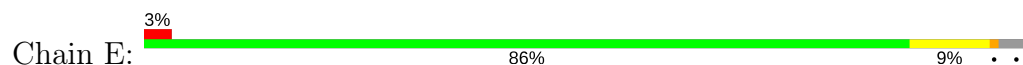
Chain D: 



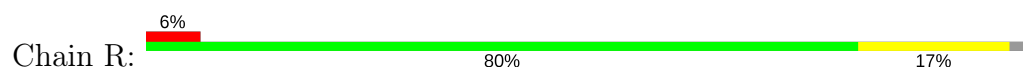
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



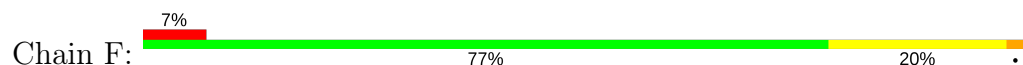
• Molecule 5: Cytochrome c oxidase subunit 5A



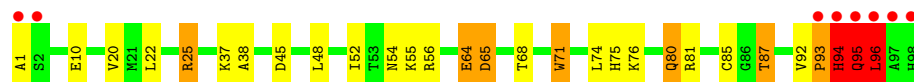
• Molecule 5: Cytochrome c oxidase subunit 5A



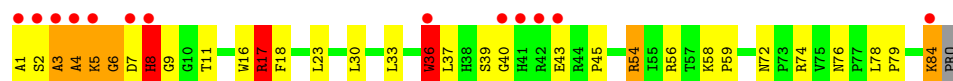
• Molecule 6: Cytochrome c oxidase subunit 5B



• Molecule 6: Cytochrome c oxidase subunit 5B

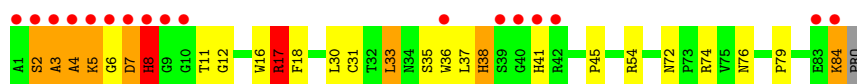


• Molecule 7: Cytochrome c oxidase subunit 6A2

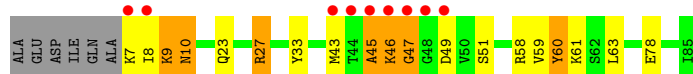


• Molecule 7: Cytochrome c oxidase subunit 6A2

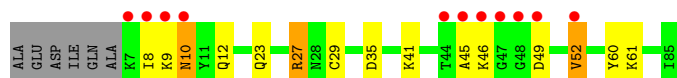
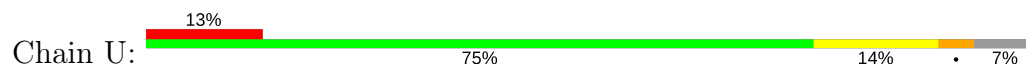




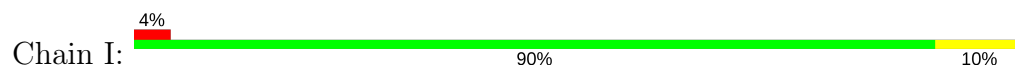
- Molecule 8: Cytochrome c oxidase subunit 6B1



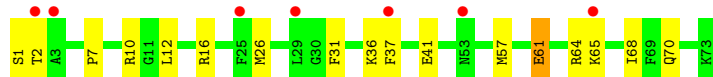
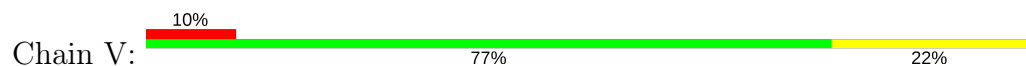
- Molecule 8: Cytochrome c oxidase subunit 6B1



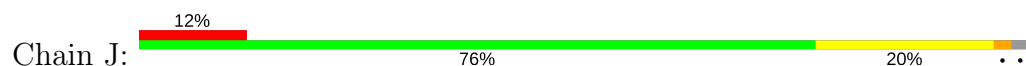
- Molecule 9: Cytochrome c oxidase subunit 6C



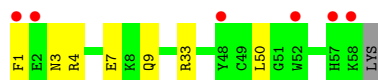
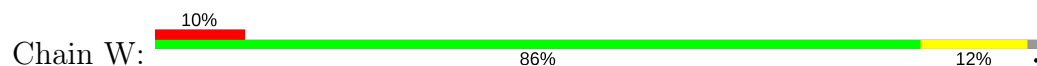
- Molecule 9: Cytochrome c oxidase subunit 6C



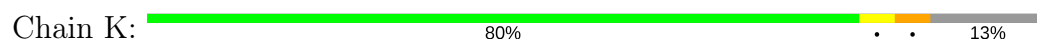
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1

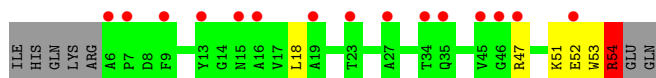
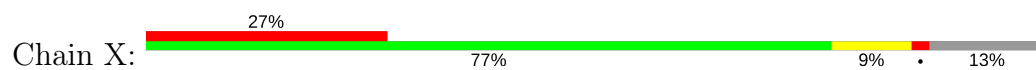


- Molecule 11: Cytochrome c oxidase subunit 7B

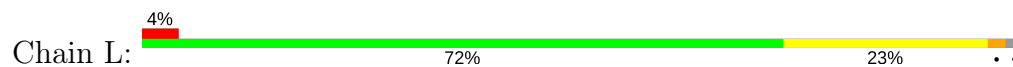




- Molecule 11: Cytochrome c oxidase subunit 7B



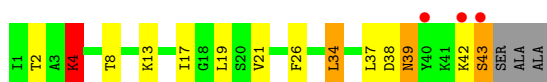
- Molecule 12: Cytochrome c oxidase subunit 7C



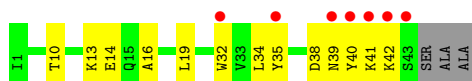
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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, α , β , γ	182.83Å 206.93Å 178.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 80.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 99.6 (80.36-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.192 , 0.223 0.204 , 0.233	Depositor DCC
R_{free} test set	30375 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32400	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: CMO, ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CU, DMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.97	92/4156 (2.2%)	1.70	92/5678 (1.6%)
1	N	1.62	41/4156 (1.0%)	1.37	33/5678 (0.6%)
2	B	1.61	20/1860 (1.1%)	1.41	19/2534 (0.7%)
2	O	1.31	9/1860 (0.5%)	1.20	11/2534 (0.4%)
3	C	1.62	22/2197 (1.0%)	1.31	19/3005 (0.6%)
3	P	1.52	17/2197 (0.8%)	1.29	19/3005 (0.6%)
4	D	1.46	6/1229 (0.5%)	1.22	7/1658 (0.4%)
4	Q	1.24	8/1229 (0.7%)	1.01	3/1658 (0.2%)
5	E	1.29	2/871 (0.2%)	1.04	2/1182 (0.2%)
5	R	1.16	0/871	0.97	3/1182 (0.3%)
6	F	1.43	4/765 (0.5%)	1.19	3/1038 (0.3%)
6	S	1.37	4/765 (0.5%)	1.29	8/1038 (0.8%)
7	G	1.38	3/690 (0.4%)	1.29	8/937 (0.9%)
7	T	1.41	3/690 (0.4%)	1.37	5/937 (0.5%)
8	H	1.37	1/682 (0.1%)	1.18	4/921 (0.4%)
8	U	1.19	0/682	1.04	1/921 (0.1%)
9	I	1.26	0/605	1.03	0/802
9	V	1.20	0/605	1.02	2/802 (0.2%)
10	J	1.30	2/471 (0.4%)	1.08	1/636 (0.2%)
10	W	1.22	2/471 (0.4%)	1.06	0/636
11	K	1.42	1/398 (0.3%)	1.14	1/546 (0.2%)
11	X	1.17	1/398 (0.3%)	0.98	1/546 (0.2%)
12	L	1.53	1/393 (0.3%)	1.19	0/526
12	Y	1.45	2/393 (0.5%)	1.14	1/526 (0.2%)
13	M	1.46	2/345 (0.6%)	1.31	2/470 (0.4%)
13	Z	1.12	0/345	1.01	0/470
All	All	1.53	243/29324 (0.8%)	1.31	245/39866 (0.6%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	2
6	S	0	2
10	J	0	1
All	All	0	10

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	TYR	CD2-CE2	14.73	1.61	1.39
1	A	394	VAL	CB-CG2	-11.76	1.28	1.52
1	A	438	ARG	CB-CG	-10.50	1.24	1.52
1	A	371	TYR	CE1-CZ	-10.20	1.25	1.38
1	A	203	ALA	N-CA	9.97	1.66	1.46

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	17	ARG	NE-CZ-NH1	15.38	127.99	120.30
7	T	17	ARG	NE-CZ-NH2	-12.64	113.98	120.30
3	P	63	ARG	NE-CZ-NH1	12.31	126.45	120.30
4	D	20	ARG	NE-CZ-NH2	-12.09	114.25	120.30
3	C	221	ARG	NE-CZ-NH1	-12.06	114.27	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	VAL	Mainchain
1	A	201	VAL	Mainchain
1	A	232	GLN	Mainchain
1	A	247	ILE	Mainchain
1	A	65	MET	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	65	0
1	N	4027	0	4001	79	0
2	B	1824	0	1833	23	0
2	O	1824	0	1833	37	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	6	0
4	Q	1195	0	1183	27	0
5	E	852	0	845	3	0
5	R	852	0	845	11	0
6	F	748	0	728	17	0
6	S	748	0	728	28	0
7	G	675	0	643	38	0
7	T	675	0	643	56	0
8	H	662	0	623	11	0
8	U	662	0	623	9	0
9	I	601	0	613	6	0
9	V	601	0	613	13	0
10	J	460	0	459	7	0
10	W	460	0	459	4	0
11	K	384	0	366	2	0
11	X	384	0	366	7	0
12	L	380	0	380	12	0
12	Y	380	0	380	9	0
13	M	335	0	352	8	0
13	Z	335	0	352	6	0
14	A	120	0	109	14	0
14	N	120	0	108	3	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	2	0	0	1	0
16	N	2	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	12	0
19	B	63	0	110	7	0
19	L	63	0	110	12	0
19	N	126	0	220	18	0
19	O	63	0	110	9	0
20	A	102	0	152	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	102	0	152	7	0
20	G	51	0	76	2	0
20	N	102	0	152	10	0
20	P	51	0	76	6	0
21	A	29	0	37	0	0
21	B	29	0	35	1	0
21	C	29	0	35	8	0
21	G	29	0	37	1	0
21	J	29	0	35	1	0
21	P	58	0	71	10	0
21	W	29	0	35	2	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	17	0
23	R	52	0	80	15	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	53	0	77	5	0
25	G	106	0	154	29	0
25	P	106	0	154	21	0
25	T	53	0	77	24	0
26	C	100	0	156	20	0
26	G	100	0	156	39	0
26	P	100	0	156	21	0
26	T	100	0	156	35	0
27	C	33	0	38	2	0
27	M	33	0	38	0	0
27	P	33	0	38	4	0
27	Z	33	0	39	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	213	0	0	2	0
29	B	135	0	0	5	0
29	C	109	0	0	1	0
29	D	93	0	0	2	0
29	E	61	0	0	1	0
29	F	80	0	0	2	0
29	G	56	0	0	6	0
29	H	53	0	0	1	0
29	I	35	0	0	1	0
29	J	16	0	0	1	0
29	K	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	L	28	0	0	3	0
29	M	24	0	0	1	0
29	N	205	0	0	6	0
29	O	106	0	0	1	0
29	P	106	0	0	3	0
29	Q	51	0	0	3	0
29	R	39	0	0	0	0
29	S	62	0	0	4	0
29	T	47	0	0	10	0
29	U	50	0	0	1	0
29	V	21	0	0	0	0
29	W	15	0	0	0	0
29	X	19	0	0	0	0
29	Y	12	0	0	0	0
29	Z	7	0	0	0	0
All	All	32400	0	31275	668	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 668 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:THR:CG2	1:N:484:THR:CB	1.77	1.63
26:G:269:CDL:C15	26:G:269:CDL:C16	1.76	1.62
7:T:5:LYS:CG	7:T:5:LYS:CB	1.75	1.56
1:A:297:MET:SD	1:A:297:MET:CE	2.02	1.46
7:G:5:LYS:HD2	25:G:1263:PEK:C38	1.50	1.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	496 (97%)	16 (3%)	0	100	100
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	38	23
2	O	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	20	6
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	38	23
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	101 (98%)	1 (1%)	1 (1%)	18	5
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	18	5
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	0
7	G	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	1	0
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2	0
8	H	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	0
8	U	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	3 (4%)	1 (1%)	13	3
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	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%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	7	1
All	All	3504/3614 (97%)	3352 (96%)	121 (4%)	31 (1%)	20	6

5 of 31 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
7	G	39	SER
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	426/426 (100%)	418 (98%)	8 (2%)	62	50
1	N	426/426 (100%)	414 (97%)	12 (3%)	49	34
2	B	210/210 (100%)	200 (95%)	10 (5%)	30	13
2	O	210/210 (100%)	194 (92%)	16 (8%)	15	4
3	C	224/226 (99%)	218 (97%)	6 (3%)	50	35
3	P	224/226 (99%)	216 (96%)	8 (4%)	40	23
4	D	128/129 (99%)	126 (98%)	2 (2%)	68	58
4	Q	128/129 (99%)	121 (94%)	7 (6%)	25	10
5	E	92/95 (97%)	90 (98%)	2 (2%)	57	44
5	R	92/95 (97%)	91 (99%)	1 (1%)	78	72
6	F	81/81 (100%)	78 (96%)	3 (4%)	39	22
6	S	81/81 (100%)	74 (91%)	7 (9%)	12	3
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	1
7	T	67/68 (98%)	61 (91%)	6 (9%)	11	3
8	H	71/75 (95%)	64 (90%)	7 (10%)	9	2
8	U	71/75 (95%)	64 (90%)	7 (10%)	9	2
9	I	57/57 (100%)	52 (91%)	5 (9%)	12	3
9	V	57/57 (100%)	54 (95%)	3 (5%)	26	11
10	J	49/50 (98%)	48 (98%)	1 (2%)	60	48
10	W	49/50 (98%)	47 (96%)	2 (4%)	35	18
11	K	39/46 (85%)	37 (95%)	2 (5%)	28	12
11	X	39/46 (85%)	37 (95%)	2 (5%)	28	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	38 (97%)	1 (3%)	51	36
12	Y	39/40 (98%)	37 (95%)	2 (5%)	28	12
13	M	37/38 (97%)	30 (81%)	7 (19%)	2	0
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	1
All	All	3040/3082 (99%)	2900 (95%)	140 (5%)	31	15

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	109	PHE
2	O	75	LEU
10	W	4	ARG
1	N	180	GLN
1	N	484	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	180	GLN
2	O	181	GLN
9	V	8	GLN
1	N	512	ASN
2	O	52	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	1.40	2 (22%)	7,9,11	6.13	5 (71%)
2	FME	B	1	2	9,9,10	1.93	3 (33%)	7,9,11	6.21	4 (57%)
7	TPO	G	11	7	9,10,11	3.22	5 (55%)	10,14,16	1.53	2 (20%)
9	SAC	I	1	9	8,8,9	2.61	3 (37%)	6,9,11	0.98	0
1	FME	N	1	1	9,9,10	1.22	1 (11%)	7,9,11	6.01	2 (28%)
2	FME	O	1	2	9,9,10	1.24	1 (11%)	7,9,11	6.24	3 (42%)
7	TPO	T	11	7	9,10,11	2.97	5 (55%)	10,14,16	1.89	3 (30%)
9	SAC	V	1	9	8,8,9	4.18	3 (37%)	6,9,11	2.70	5 (83%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.08	1.10	1.22
2	O	1	FME	O1-CN	-2.71	1.14	1.22
2	B	1	FME	CG-SD	-2.43	1.67	1.81
1	N	1	FME	O1-CN	-2.22	1.15	1.22
1	A	1	FME	O1-CN	-2.14	1.16	1.22

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-15.70	98.67	122.82
1	N	1	FME	CA-N-CN	-15.42	99.10	122.82
2	B	1	FME	CA-N-CN	-15.42	99.11	122.82
1	A	1	FME	CA-N-CN	-14.65	100.30	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O1-CN-N	-3.66	115.00	125.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1	SAC	CB-CA-N-C1A
2	B	1	FME	O1-CN-N-CA
1	N	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
7	G	11	TPO	2	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, 8 are monoatomic and 2 are unknown - 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	44,67,67	1.48	9 (20%)	37,103,103	3.91	18 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	516	1	44,67,67	2.55	8 (18%)	37,103,103	3.14	14 (37%)
16	CMO	A	520	15	0,1,1	0.00	-	0,0,0	0.00	-
20	PGV	A	521	-	50,50,50	1.32	5 (10%)	51,56,56	1.70	13 (25%)
19	TGL	A	523	-	62,62,62	1.45	7 (11%)	65,65,65	1.47	11 (16%)
20	PGV	A	524	-	50,50,50	1.41	4 (8%)	51,56,56	1.55	9 (17%)
21	CHD	A	525	-	29,32,32	1.62	7 (24%)	47,51,51	5.64	34 (72%)
21	CHD	B	1085	-	29,32,32	1.76	8 (27%)	47,51,51	5.79	32 (68%)
22	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	PSC	B	229	-	51,51,51	1.36	3 (5%)	56,59,59	1.32	6 (10%)
19	TGL	B	521	-	62,62,62	1.34	6 (9%)	65,65,65	2.06	15 (23%)
25	PEK	C	264	-	52,52,52	1.01	1 (1%)	54,57,57	1.84	14 (25%)
20	PGV	C	267	-	50,50,50	0.97	2 (4%)	51,56,56	1.60	10 (19%)
20	PGV	C	268	-	50,50,50	1.34	2 (4%)	51,56,56	1.63	7 (13%)
26	CDL	C	270	-	99,99,99	1.44	12 (12%)	101,111,111	1.57	17 (16%)
21	CHD	C	271	-	29,32,32	0.84	0	47,51,51	5.02	28 (59%)
27	DMU	C	272	-	34,34,34	1.99	5 (14%)	45,45,45	3.41	24 (53%)
25	PEK	G	1263	-	52,52,52	1.39	4 (7%)	54,57,57	1.56	5 (9%)
20	PGV	G	1268	-	50,50,50	1.41	3 (6%)	51,56,56	1.89	9 (17%)
25	PEK	G	265	-	52,52,52	1.46	5 (9%)	54,57,57	1.52	6 (11%)
26	CDL	G	269	-	99,99,99	1.62	16 (16%)	101,111,111	1.70	20 (19%)
21	CHD	G	86	-	29,32,32	1.50	6 (20%)	47,51,51	5.49	35 (74%)
21	CHD	J	60	-	29,32,32	1.41	5 (17%)	47,51,51	5.17	31 (65%)
19	TGL	L	522	-	62,62,62	1.60	10 (16%)	65,65,65	2.23	18 (27%)
27	DMU	M	526	-	34,34,34	0.91	1 (2%)	45,45,45	3.51	29 (64%)
20	PGV	N	1266	-	50,50,50	1.26	5 (10%)	51,56,56	1.73	12 (23%)
19	TGL	N	1522	-	62,62,62	1.83	10 (16%)	65,65,65	2.04	18 (27%)
19	TGL	N	1523	-	62,62,62	1.46	6 (9%)	65,65,65	1.67	12 (18%)
20	PGV	N	1524	-	50,50,50	1.22	2 (4%)	51,56,56	1.53	8 (15%)
14	HEA	N	515	1	44,67,67	1.31	4 (9%)	37,103,103	3.19	19 (51%)
14	HEA	N	516	1	44,67,67	1.42	9 (20%)	37,103,103	2.69	13 (35%)
16	CMO	N	520	15	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	O	1521	-	62,62,62	1.36	6 (9%)	65,65,65	1.89	10 (15%)
22	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
25	PEK	P	1264	-	52,52,52	0.95	4 (7%)	54,57,57	1.84	11 (20%)
25	PEK	P	1265	-	52,52,52	1.38	4 (7%)	54,57,57	1.51	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	P	1267	-	50,50,50	0.92	2 (4%)	51,56,56	1.52	8 (15%)
26	CDL	P	1270	-	99,99,99	1.42	15 (15%)	101,111,111	1.61	22 (21%)
21	CHD	P	1271	-	29,32,32	0.85	1 (3%)	47,51,51	4.90	33 (70%)
27	DMU	P	1272	-	34,34,34	2.38	7 (20%)	45,45,45	3.45	23 (51%)
21	CHD	P	1525	-	29,32,32	1.27	5 (17%)	47,51,51	5.93	37 (78%)
23	PSC	R	1229	-	51,51,51	1.39	5 (9%)	56,59,59	1.31	5 (8%)
26	CDL	T	1269	-	99,99,99	1.41	13 (13%)	101,111,111	1.62	18 (17%)
25	PEK	T	263	-	52,52,52	1.50	6 (11%)	54,57,57	1.55	9 (16%)
21	CHD	W	1059	-	29,32,32	1.43	6 (20%)	47,51,51	5.37	32 (68%)
27	DMU	Z	1526	-	34,34,34	1.07	2 (5%)	45,45,45	3.31	22 (48%)

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
16	CMO	A	520	15	-	0/0/0/0	0/0/0/0
20	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	TGL	A	523	-	-	0/65/65/65	0/0/0/0
20	PGV	A	524	-	-	1/55/55/55	0/0/0/0
21	CHD	A	525	-	-	0/7/74/74	0/4/4/4
21	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
22	CUA	B	228	2	-	0/0/0/0	0/0/0/0
23	PSC	B	229	-	-	0/55/55/55	0/0/0/0
19	TGL	B	521	-	-	0/65/65/65	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
21	CHD	C	271	-	2/2/12/12	0/7/74/74	0/4/4/4
27	DMU	C	272	-	5/5/10/10	0/19/59/59	0/2/2/2
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
20	PGV	G	1268	-	-	0/55/55/55	0/0/0/0
25	PEK	G	265	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
21	CHD	G	86	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHD	J	60	-	1/1/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
16	CMO	N	520	15	-	0/0/0/0	0/0/0/0
19	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
22	CUA	O	228	2	-	0/0/0/0	0/0/0/0
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
21	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
27	DMU	P	1272	-	5/5/10/10	0/19/59/59	0/2/2/2
21	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
23	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
21	CHD	W	1059	-	1/1/12/12	0/7/74/74	0/4/4/4
27	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 241 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1085	CHD	C10-C5	-4.33	1.48	1.55
14	N	515	HEA	C1A-NA	-4.19	1.31	1.36
14	A	516	HEA	CAA-C2A	-3.72	1.45	1.52
21	B	1085	CHD	C13-C14	-3.67	1.49	1.55
19	L	522	TGL	C10-CB9	-3.61	1.31	1.51

The worst 5 of 723 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	C13-C12-C11	-15.12	91.56	114.46
21	B	1085	CHD	C18-C13-C12	-11.59	97.29	109.08
21	A	525	CHD	C19-C10-C9	-11.30	94.99	111.16
21	G	86	CHD	C18-C13-C12	-11.17	97.71	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1085	CHD	C19-C10-C9	-11.04	95.36	111.16

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
21	P	1271	CHD	C9
21	C	271	CHD	C14

All (3) torsion outliers are listed below:

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

There are no ring outliers.

40 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	7	0
14	A	516	HEA	7	0
16	A	520	CMO	1	0
20	A	521	PGV	1	0
19	A	523	TGL	12	0
20	A	524	PGV	10	0
21	B	1085	CHD	1	0
23	B	229	PSC	17	0
19	B	521	TGL	7	0
25	C	264	PEK	5	0
20	C	267	PGV	4	0
20	C	268	PGV	3	0
26	C	270	CDL	20	0
21	C	271	CHD	8	0
27	C	272	DMU	2	0
25	G	1263	PEK	12	0
20	G	1268	PGV	2	0
25	G	265	PEK	17	0
26	G	269	CDL	39	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	86	CHD	1	0
21	J	60	CHD	1	0
19	L	522	TGL	12	0
20	N	1266	PGV	2	0
19	N	1522	TGL	14	0
19	N	1523	TGL	4	0
20	N	1524	PGV	8	0
14	N	515	HEA	3	0
19	O	1521	TGL	9	0
25	P	1264	PEK	7	0
25	P	1265	PEK	14	0
20	P	1267	PGV	6	0
26	P	1270	CDL	21	0
21	P	1271	CHD	8	0
27	P	1272	DMU	4	0
21	P	1525	CHD	2	0
23	R	1229	PSC	15	0
26	T	1269	CDL	35	0
25	T	263	PEK	24	0
21	W	1059	CHD	2	0
27	Z	1526	DMU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.12	6 (1%) 79 77	19, 26, 35, 62	0
1	N	513/514 (99%)	0.03	6 (1%) 79 77	23, 31, 39, 66	0
2	B	226/227 (99%)	-0.39	1 (0%) 92 90	19, 31, 55, 77	0
2	O	226/227 (99%)	-0.16	6 (2%) 55 50	28, 38, 66, 85	0
3	C	259/261 (99%)	-0.28	4 (1%) 74 70	23, 29, 41, 64	0
3	P	259/261 (99%)	-0.14	10 (3%) 40 35	25, 31, 43, 67	0
4	D	144/147 (97%)	-0.41	1 (0%) 87 86	27, 35, 52, 69	0
4	Q	144/147 (97%)	1.20	23 (15%) 2 1	35, 47, 73, 118	0
5	E	105/109 (96%)	0.13	3 (2%) 52 47	29, 35, 62, 99	0
5	R	105/109 (96%)	0.63	6 (5%) 24 20	33, 40, 69, 104	0
6	F	98/98 (100%)	0.36	7 (7%) 17 13	27, 37, 82, 128	0
6	S	98/98 (100%)	0.08	8 (8%) 12 10	29, 39, 86, 121	0
7	G	83/85 (97%)	0.78	13 (15%) 2 2	27, 36, 101, 109	0
7	T	83/85 (97%)	0.89	17 (20%) 1 1	26, 36, 98, 111	0
8	H	79/85 (92%)	0.21	9 (11%) 6 4	27, 37, 89, 111	0
8	U	79/85 (92%)	0.28	11 (13%) 3 2	35, 42, 92, 112	0
9	I	72/73 (98%)	0.02	3 (4%) 37 31	28, 44, 66, 73	0
9	V	72/73 (98%)	0.77	7 (9%) 8 7	33, 51, 67, 90	0
10	J	58/59 (98%)	0.54	7 (12%) 5 4	30, 38, 70, 96	0
10	W	58/59 (98%)	0.44	6 (10%) 7 6	31, 39, 72, 108	0
11	K	49/56 (87%)	-0.29	0 100 100	30, 37, 51, 64	0
11	X	49/56 (87%)	1.68	15 (30%) 0 0	39, 46, 64, 79	0
12	L	46/47 (97%)	-0.29	2 (4%) 36 30	25, 32, 46, 77	0
12	Y	46/47 (97%)	-0.17	1 (2%) 62 58	32, 37, 59, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.04	3 (6%) 17 14	28, 31, 75, 106	0
13	Z	43/46 (93%)	0.51	7 (16%) 2 1	35, 39, 92, 117	0
All	All	3550/3614 (98%)	0.12	182 (5%) 29 24	19, 34, 65, 128	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	35.5
4	Q	4	SER	22.2
4	Q	6	VAL	18.1
6	F	98	HIS	12.6
6	F	97	ALA	11.5

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
2	FME	O	1	10/11	0.96	0.16	-	36,38,46,49	0
7	TPO	T	11	11/12	0.46	0.35	-	75,83,108,109	0
2	FME	B	1	10/11	0.96	0.11	-	30,32,39,53	0
9	SAC	I	1	9/10	0.76	0.30	-	81,85,88,89	0
1	FME	N	1	10/11	0.94	0.17	-	45,50,74,74	0
9	SAC	V	1	9/10	0.23	0.66	-	96,98,100,100	0
1	FME	A	1	10/11	0.93	0.15	-	44,48,66,75	0
7	TPO	G	11	11/12	0.51	0.31	-	72,80,107,107	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	1059	29/29	0.41	0.51	16.08	103,122,124,124	0
20	PGV	A	524	51/51	0.78	0.24	11.39	39,75,118,121	0
27	DMU	C	272	33/33	0.48	0.32	10.66	79,115,119,122	0
21	CHD	J	60	29/29	0.47	0.45	10.44	107,123,126,126	0
26	CDL	P	1270	100/100	0.71	0.33	8.41	41,95,114,116	0
20	PGV	N	1524	51/51	0.69	0.32	5.16	50,78,121,124	0
26	CDL	C	270	100/100	0.71	0.34	4.98	45,95,113,114	0
19	TGL	N	1522	63/63	0.64	0.26	4.72	49,72,85,88	0
27	DMU	P	1272	33/33	0.50	0.33	4.62	84,116,120,121	0
19	TGL	L	522	63/63	0.78	0.23	3.73	37,62,79,81	0
21	CHD	P	1271	29/29	0.76	0.34	3.17	95,109,114,115	0
19	TGL	O	1521	63/63	0.83	0.17	3.06	49,74,94,99	0
19	TGL	A	523	63/63	0.80	0.18	3.01	52,75,91,93	0
21	CHD	C	271	29/29	0.76	0.47	2.95	95,110,116,117	0
19	TGL	B	521	63/63	0.83	0.18	2.80	51,70,96,101	0
19	TGL	N	1523	63/63	0.66	0.23	2.70	54,79,93,95	0
23	PSC	R	1229	52/52	0.62	0.33	2.48	48,100,130,134	0
20	PGV	C	268	51/51	0.72	0.36	2.45	54,89,113,114	0
23	PSC	B	229	52/52	0.67	0.29	2.41	52,101,130,132	0
26	CDL	G	269	100/100	0.58	0.29	2.35	60,88,121,127	0
27	DMU	Z	1526	33/33	0.83	0.24	2.29	43,57,73,75	0
26	CDL	T	1269	100/100	0.62	0.28	2.22	58,90,120,122	0
20	PGV	G	1268	51/51	0.69	0.36	1.99	69,93,110,113	0
25	PEK	T	263	53/53	0.52	0.39	1.96	49,96,124,125	0
28	ZN	F	99	1/1	0.99	0.09	1.89	32,32,32,32	0
17	MG	N	518	1/1	0.95	0.13	1.84	30,30,30,30	0
25	PEK	G	1263	53/53	0.59	0.43	1.66	53,99,127,128	0
25	PEK	P	1265	53/53	0.56	0.31	1.43	46,87,117,120	0
17	MG	A	518	1/1	0.98	0.11	1.34	24,24,24,24	0
27	DMU	M	526	33/33	0.87	0.13	1.24	34,46,66,68	0
21	CHD	A	525	29/29	0.96	0.15	0.95	23,31,37,39	0
21	CHD	P	1525	29/29	0.95	0.14	0.71	28,33,38,42	0
20	PGV	P	1267	51/51	0.97	0.12	0.66	27,39,76,78	0
14	HEA	N	516	60/60	0.98	0.13	0.62	21,29,40,42	0
20	PGV	N	1266	51/51	0.97	0.15	0.61	23,39,64,65	0
20	PGV	C	267	51/51	0.96	0.11	0.55	26,35,69,73	0
25	PEK	G	265	53/53	0.49	0.23	0.55	57,87,115,119	0
28	ZN	S	99	1/1	0.99	0.08	0.45	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	PEK	P	1264	53/53	0.95	0.13	0.45	30,48,75,77	0
25	PEK	C	264	53/53	0.96	0.11	0.37	24,42,72,74	0
20	PGV	A	521	51/51	0.97	0.12	0.34	23,32,57,60	0
18	NA	N	519	1/1	0.97	0.10	0.17	36,36,36,36	0
22	CUA	B	228	2/2	0.99	0.11	0.14	23,23,23,24	0
22	CUA	O	228	2/2	0.97	0.09	0.08	31,31,31,31	0
14	HEA	N	515	60/60	0.98	0.11	0.01	23,30,47,55	0
21	CHD	G	86	29/29	0.95	0.10	-0.36	22,28,34,35	0
14	HEA	A	516	60/60	0.98	0.12	-0.38	14,23,34,36	0
21	CHD	B	1085	29/29	0.95	0.08	-0.43	22,28,33,38	0
14	HEA	A	515	60/60	0.98	0.12	-0.52	17,24,43,60	0
16	CMO	N	520	2/2	0.94	0.12	-1.51	30,30,30,30	0
18	NA	A	519	1/1	0.97	0.05	-2.09	30,30,30,30	0
15	CU	N	517	1/1	0.99	0.14	-	29,29,29,29	0
15	CU	A	517	1/1	0.99	0.13	-	22,22,22,22	0
16	CMO	A	520	2/2	0.92	0.12	-	25,25,25,25	0
24	UNX	C	262	1/1	0.55	0.60	-	69,69,69,69	0
24	UNX	P	262	1/1	0.70	0.62	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.