



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

PDB ID : 3ASO
Title : Bovine heart cytochrome C oxidase in the fully oxidized state measured at 0.9 angstrom wavelength
Authors : Suga, M.; Yano, N.; Muramoto, K.; Shinzawa-Itoh, K.; Maeda, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-12-17
Resolution : 2.30 Å(reported)

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

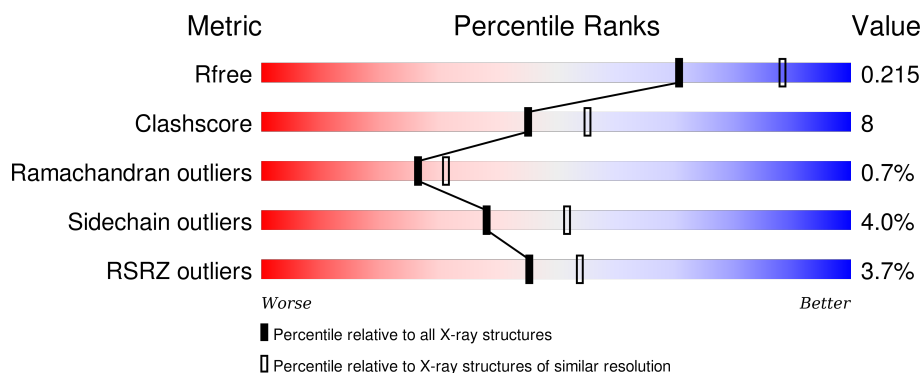
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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

















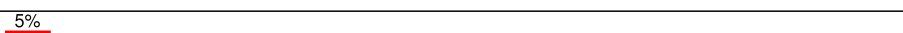
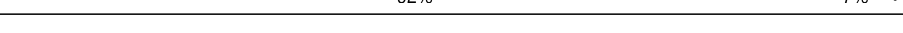





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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>87%</div> <div>12%</div> <div>.</div> </div>
1	N	514	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	B	227	<div> <div>%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	O	227	<div> <div>4%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
3	C	261	<div> <div>87%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	515	X	-	-	-
14	HEA	A	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	515	X	-	-	X
14	HEA	N	516	X	-	-	-
18	TGL	A	521	-	-	-	X
18	TGL	D	523	-	-	-	X
18	TGL	L	522	-	-	-	X
18	TGL	N	1521	-	-	-	X
18	TGL	N	1522	-	-	-	X
18	TGL	Q	1523	-	-	-	X
19	PGV	A	524	-	-	-	X
19	PGV	C	267	-	-	-	X
19	PGV	C	268	-	-	-	X
19	PGV	N	1266	-	-	-	X
19	PGV	N	1524	-	-	-	X
19	PGV	P	1267	-	-	-	X
19	PGV	P	1268	-	-	-	X
21	PSC	B	229	-	-	-	X
21	PSC	O	1229	-	-	-	X
22	CHD	J	60	-	-	-	X
22	CHD	P	1271	-	-	-	X
22	CHD	W	1059	-	-	-	X
24	PEK	G	264	-	-	-	X
24	PEK	T	263	-	-	-	X
25	CDL	C	270	-	-	-	X
25	CDL	G	269	-	-	-	X
25	CDL	P	1270	-	-	-	X
25	CDL	T	1269	-	-	X	X
27	DMU	M	526	X	-	-	-
27	DMU	Z	1526	X	-	-	X

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 32377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 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			

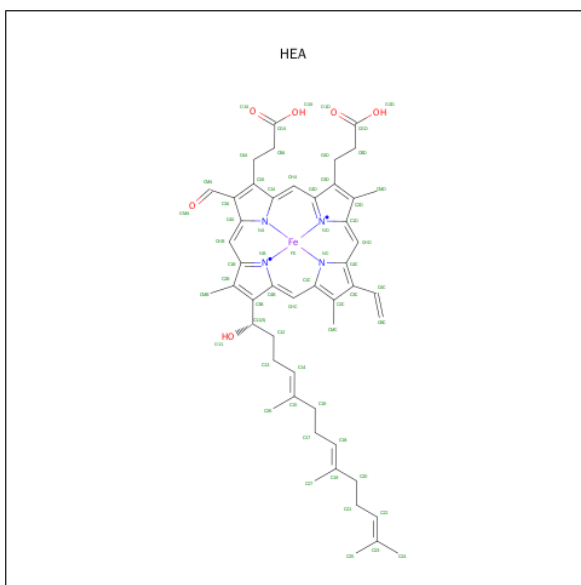
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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		

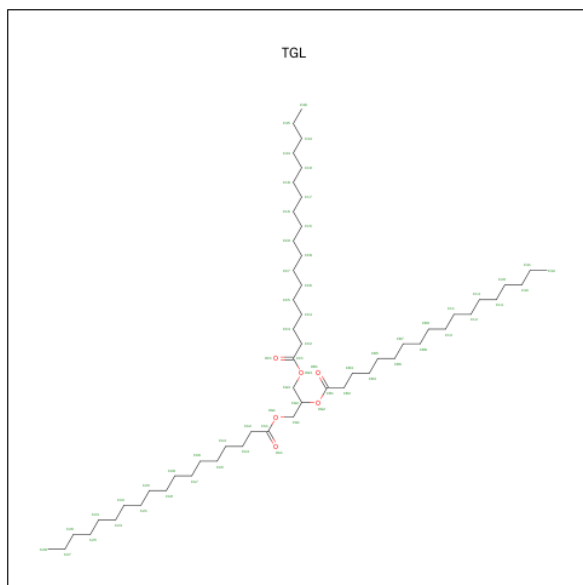
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

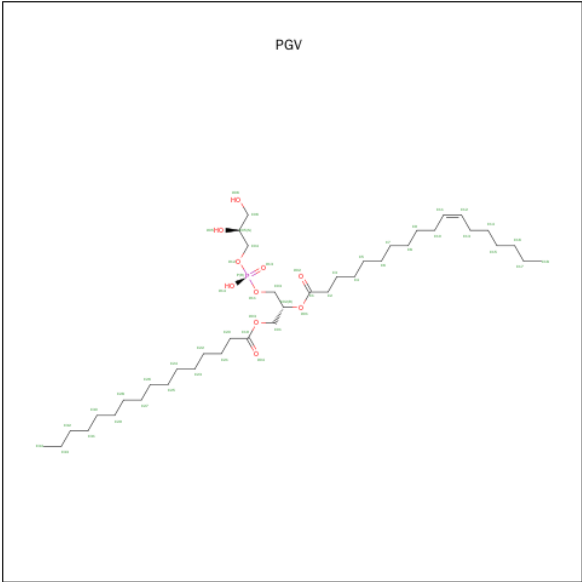
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



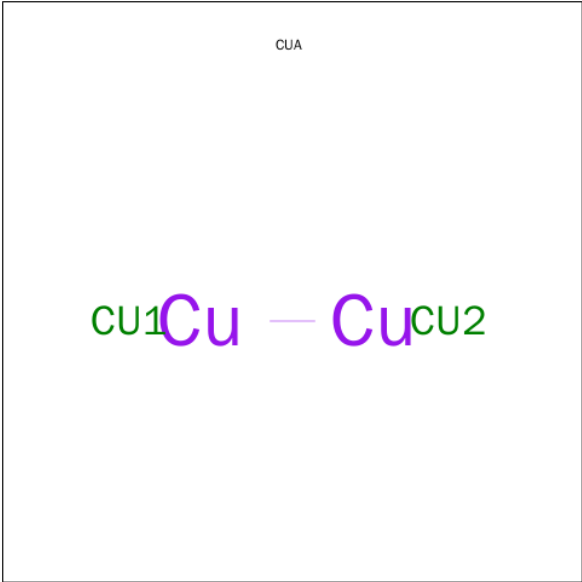
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



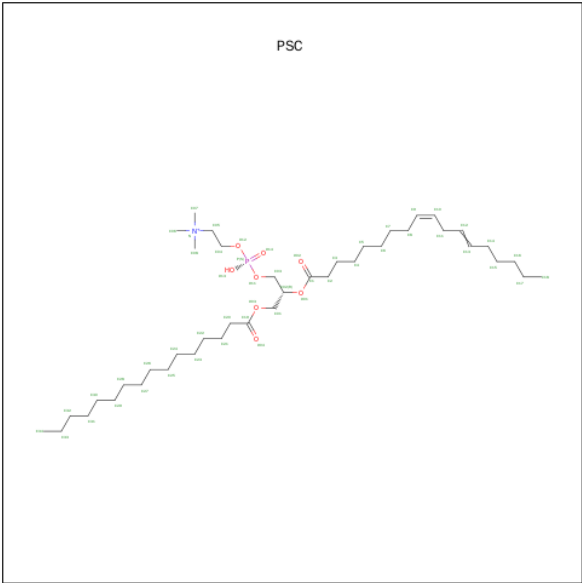
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- 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 (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



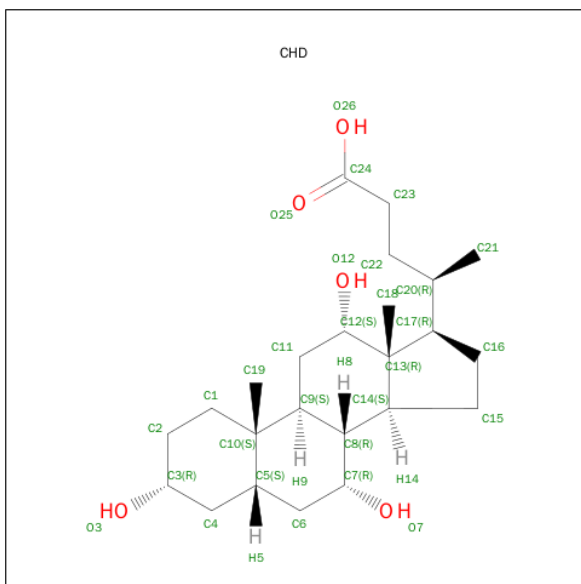
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).

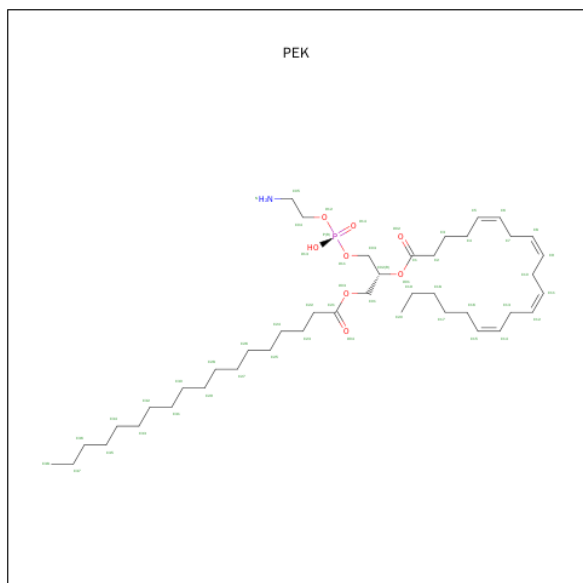


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total 29	C 24	O 5	0	0
22	C	1	Total 29	C 24	O 5	0	0
22	C	1	Total 29	C 24	O 5	0	0
22	G	1	Total 29	C 24	O 5	0	0
22	J	1	Total 29	C 24	O 5	0	0
22	P	1	Total 29	C 24	O 5	0	0
22	P	1	Total 29	C 24	O 5	0	0
22	W	1	Total 29	C 24	O 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

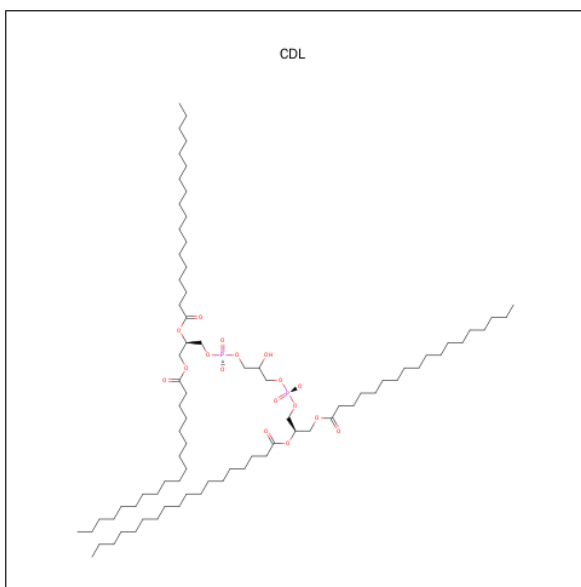
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- Molecule 24 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
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	G	1	Total C N O P 53 43 1 8 1	0	0
24	G	1	Total C N O P 53 43 1 8 1	0	0
24	T	1	Total C N O P 53 43 1 8 1	0	0
24	T	1	Total C N O P 53 43 1 8 1	0	0
24	T	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

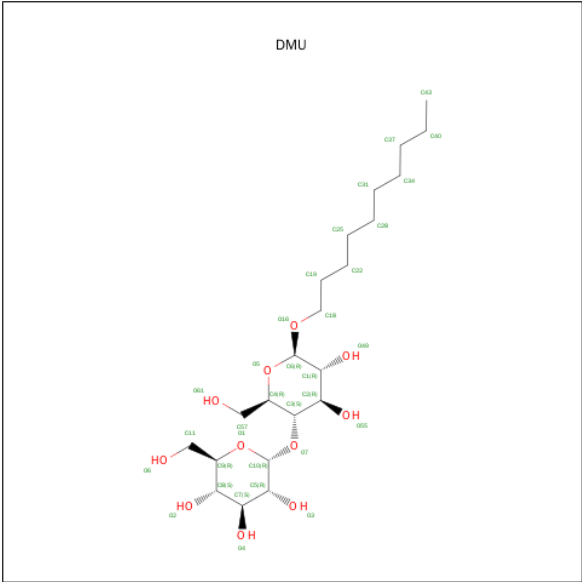


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	215	Total	O	0	0
			215	215		
28	B	124	Total	O	0	0
			124	124		
28	C	109	Total	O	0	0
			109	109		
28	D	102	Total	O	0	0
			102	102		
28	E	67	Total	O	0	0
			67	67		
28	F	81	Total	O	0	0
			81	81		
28	G	48	Total	O	0	0
			48	48		
28	H	48	Total	O	0	0
			48	48		
28	I	31	Total	O	0	0
			31	31		
28	J	16	Total	O	0	0
			16	16		

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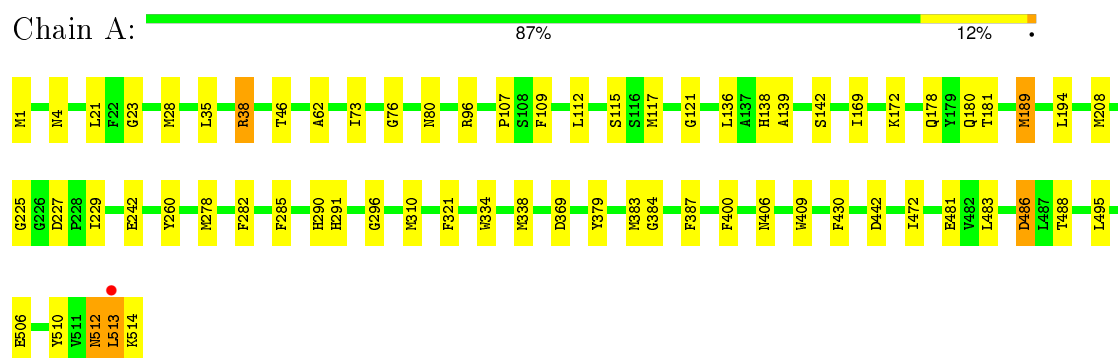
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	26	Total 26	O 26	0	0
28	L	28	Total 28	O 28	0	0
28	M	20	Total 20	O 20	0	0
28	N	220	Total 220	O 220	0	0
28	O	114	Total 114	O 114	0	0
28	P	109	Total 109	O 109	0	0
28	Q	60	Total 60	O 60	0	0
28	R	45	Total 45	O 45	0	0
28	S	77	Total 77	O 77	0	0
28	T	39	Total 39	O 39	0	0
28	U	45	Total 45	O 45	0	0
28	V	21	Total 21	O 21	0	0
28	W	16	Total 16	O 16	0	0
28	X	17	Total 17	O 17	0	0
28	Y	19	Total 19	O 19	0	0
28	Z	14	Total 14	O 14	0	0

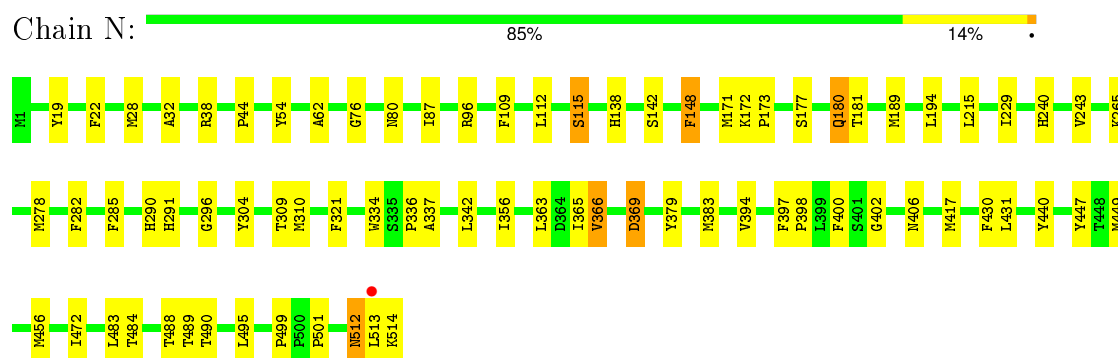
3 Residue-property plots

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

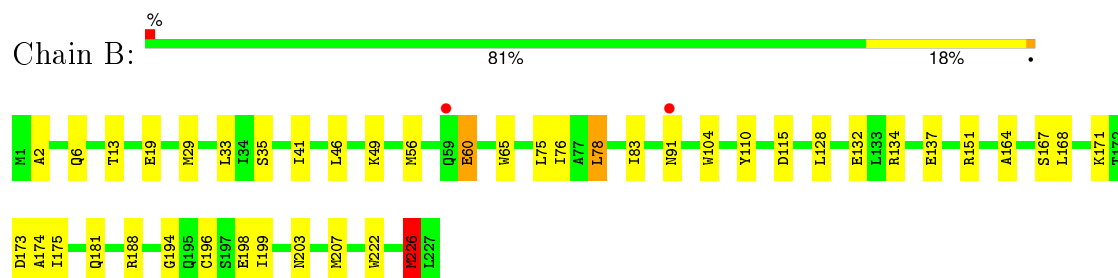
• Molecule 1: Cytochrome c oxidase subunit 1



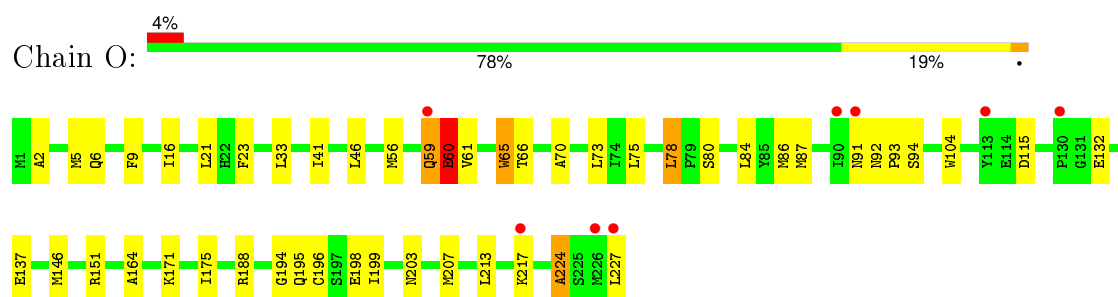
• Molecule 1: Cytochrome c oxidase subunit 1



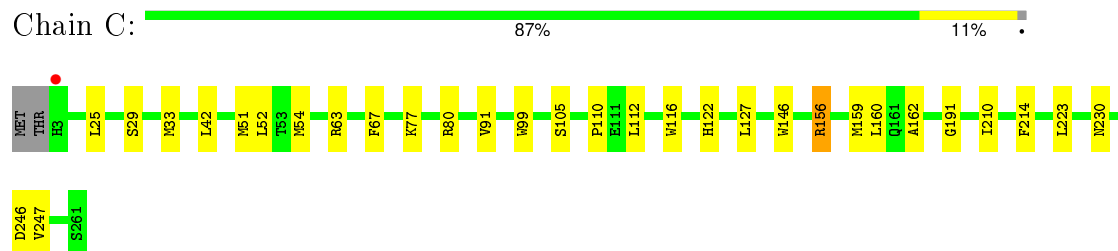
• Molecule 2: Cytochrome c oxidase subunit 2



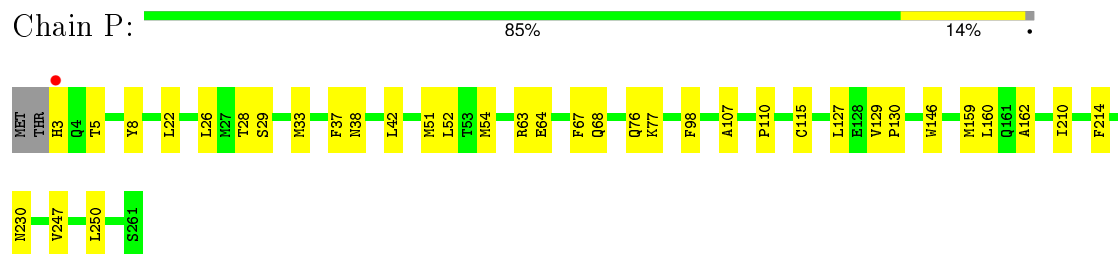
• Molecule 2: Cytochrome c oxidase subunit 2



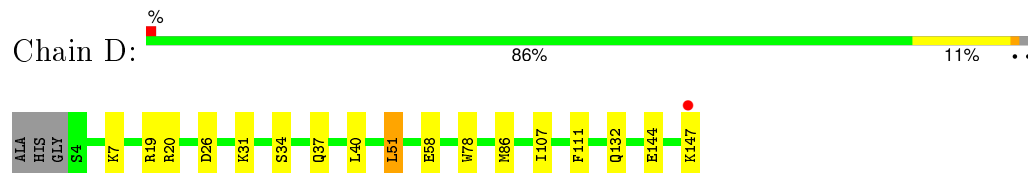
- Molecule 3: Cytochrome c oxidase subunit 3



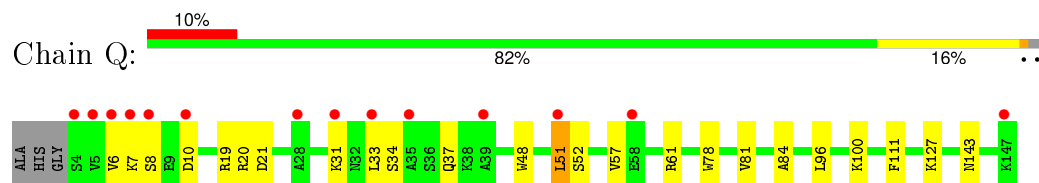
- Molecule 3: Cytochrome c oxidase subunit 3



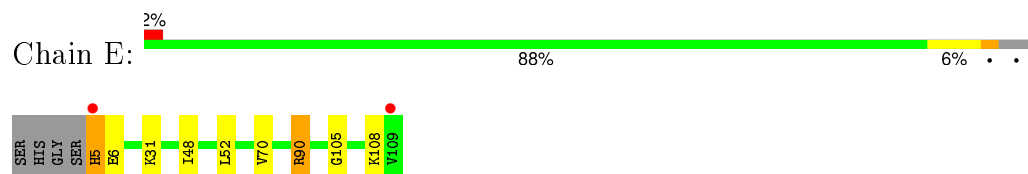
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



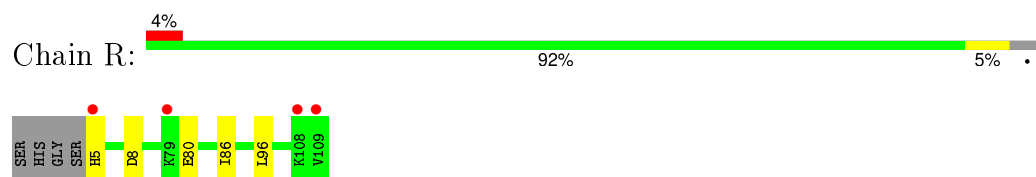
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



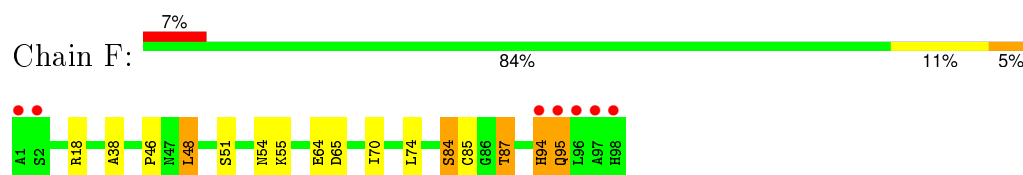
- Molecule 5: Cytochrome c oxidase subunit 5A



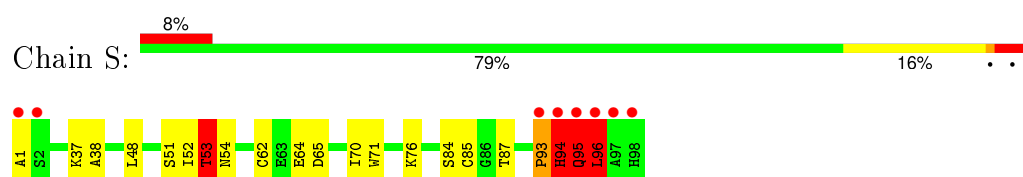
- Molecule 5: Cytochrome c oxidase subunit 5A



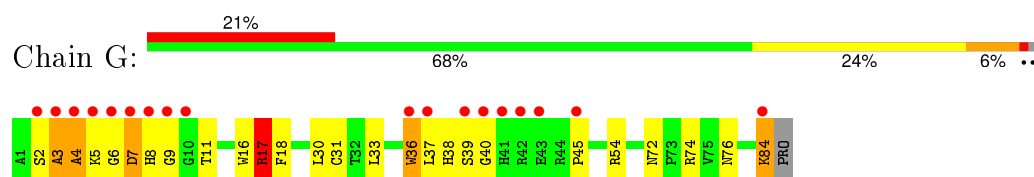
- Molecule 6: Cytochrome c oxidase subunit 5B



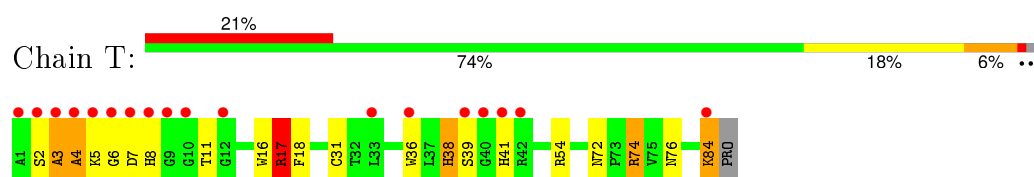
- Molecule 6: Cytochrome c oxidase subunit 5B



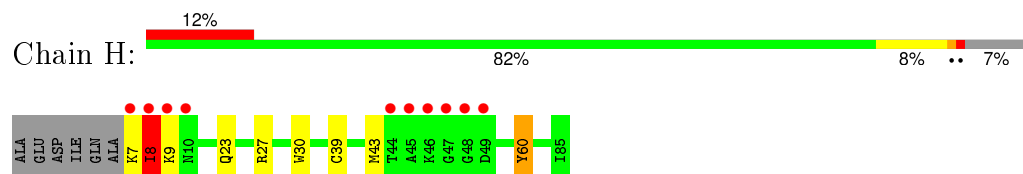
- Molecule 7: Cytochrome c oxidase subunit 6A2



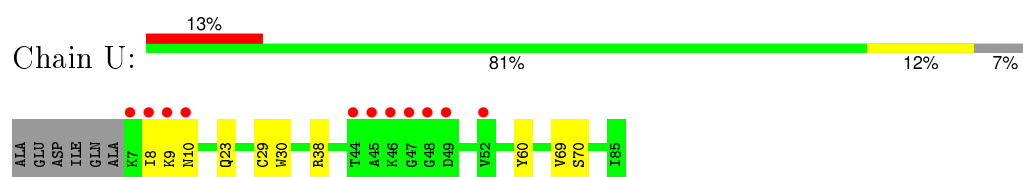
- Molecule 7: Cytochrome c oxidase subunit 6A2



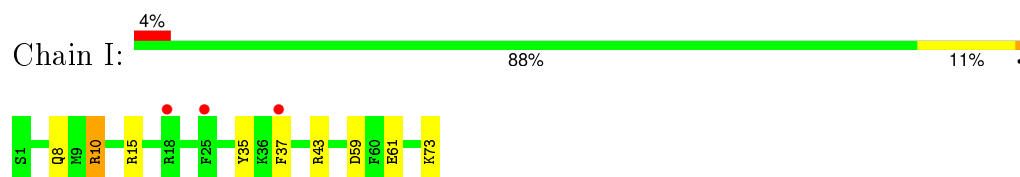
- Molecule 8: Cytochrome c oxidase subunit 6B1



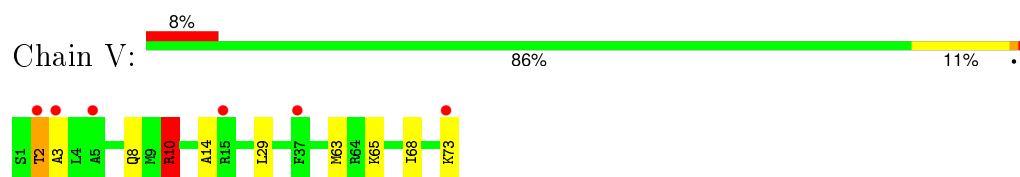
- Molecule 8: Cytochrome c oxidase subunit 6B1



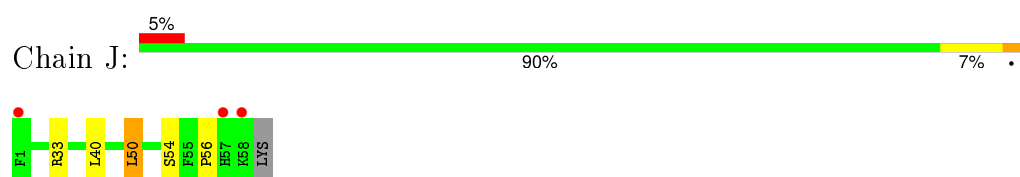
- Molecule 9: Cytochrome c oxidase subunit 6C



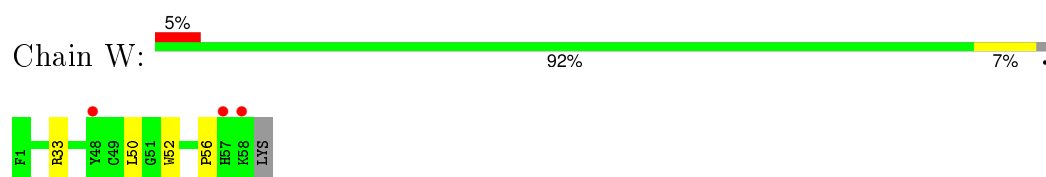
- Molecule 9: Cytochrome c oxidase subunit 6C



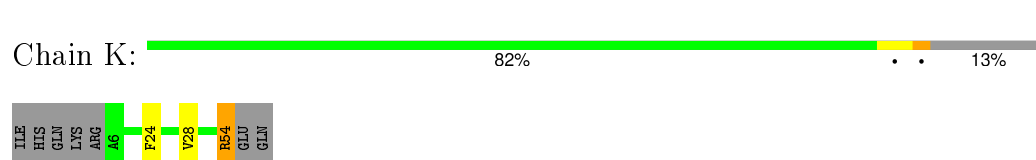
- Molecule 10: Cytochrome c oxidase subunit 7A1



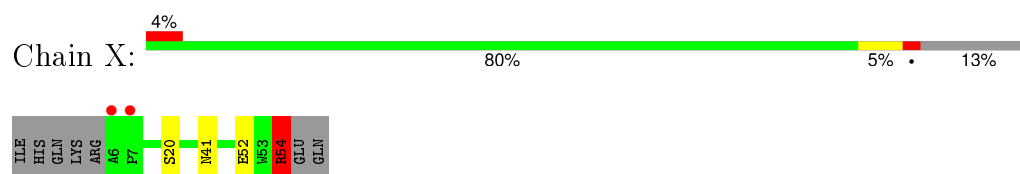
- Molecule 10: Cytochrome c oxidase subunit 7A1



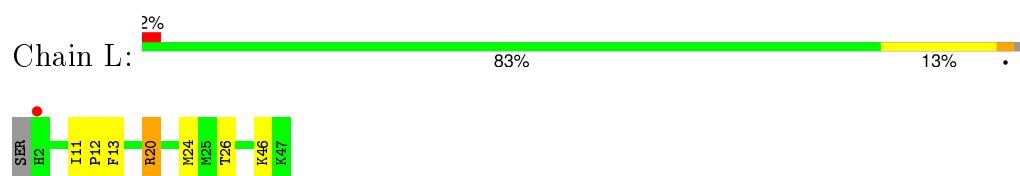
- Molecule 11: Cytochrome c oxidase subunit 7B



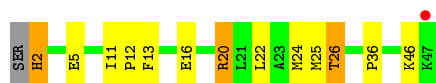
- Molecule 11: Cytochrome c oxidase subunit 7B



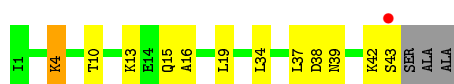
- Molecule 12: Cytochrome c oxidase subunit 7C



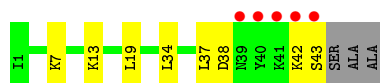
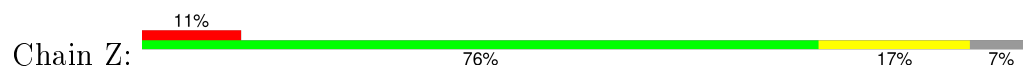
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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	181.87Å 204.11Å 177.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 107.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 99.7 (107.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.169 , 0.205 0.183 , 0.215	Depositor DCC
R_{free} test set	14475 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.8	EDS
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 290988 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.14	4/4156 (0.1%)	0.90	15/5678 (0.3%)
1	N	1.07	2/4156 (0.0%)	0.83	3/5678 (0.1%)
2	B	1.12	2/1860 (0.1%)	0.93	3/2534 (0.1%)
2	O	0.98	2/1860 (0.1%)	0.92	1/2534 (0.0%)
3	C	1.04	0/2197	0.79	2/3005 (0.1%)
3	P	1.04	1/2197 (0.0%)	0.79	0/3005
4	D	1.07	0/1229	0.92	3/1658 (0.2%)
4	Q	0.91	0/1229	0.79	2/1658 (0.1%)
5	E	1.04	0/871	0.92	2/1182 (0.2%)
5	R	0.94	0/871	0.84	0/1182
6	F	1.03	0/765	0.95	2/1038 (0.2%)
6	S	1.08	1/765 (0.1%)	1.03	3/1038 (0.3%)
7	G	1.10	1/690 (0.1%)	0.93	1/937 (0.1%)
7	T	1.02	1/690 (0.1%)	0.89	1/937 (0.1%)
8	H	1.00	0/682	0.80	0/921
8	U	0.91	1/682 (0.1%)	0.83	1/921 (0.1%)
9	I	0.99	0/605	0.83	2/802 (0.2%)
9	V	0.94	0/605	0.90	1/802 (0.1%)
10	J	0.91	0/471	0.78	0/636
10	W	0.91	0/471	0.80	0/636
11	K	1.02	0/398	0.86	1/546 (0.2%)
11	X	0.92	0/398	0.76	1/546 (0.2%)
12	L	1.02	0/393	0.84	1/526 (0.2%)
12	Y	1.10	1/393 (0.3%)	0.74	0/526
13	M	1.03	0/345	0.85	0/470
13	Z	0.87	0/345	0.79	0/470
All	All	1.04	16/29324 (0.1%)	0.86	45/39866 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ALA	CA-CB	8.23	1.69	1.52
7	T	36	TRP	CB-CG	7.35	1.63	1.50
7	G	36	TRP	CB-CG	7.22	1.63	1.50
6	S	54	ASN	CB-CG	-7.02	1.34	1.51
1	A	260	TYR	CD1-CE1	6.95	1.49	1.39
1	A	242	GLU	CG-CD	6.85	1.62	1.51
2	O	198	GLU	C-O	6.31	1.35	1.23
12	Y	16	GLU	CG-CD	6.18	1.61	1.51
2	B	198	GLU	C-O	6.16	1.35	1.23
1	A	260	TYR	CD2-CE2	6.02	1.48	1.39
2	B	174	ALA	CA-CB	5.66	1.64	1.52
8	U	69	VAL	CB-CG1	5.44	1.64	1.52
1	N	148	PHE	CE1-CZ	5.19	1.47	1.37
3	P	115	CYS	CB-SG	5.10	1.91	1.82
1	N	366	VAL	CB-CG1	-5.08	1.42	1.52
2	O	60	GLU	CB-CG	5.02	1.61	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH1	10.61	125.61	120.30
4	D	20	ARG	NE-CZ-NH2	-10.49	115.06	120.30
7	G	17	ARG	NE-CZ-NH2	-9.43	115.58	120.30
2	B	188	ARG	NE-CZ-NH2	-8.84	115.88	120.30
7	T	17	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	96	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	117	MET	CG-SD-CE	-7.65	87.96	100.20
9	V	10	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	136	LEU	CA-CB-CG	7.19	131.84	115.30
5	E	90	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	136	LEU	CB-CG-CD1	7.03	122.96	111.00
1	A	136	LEU	CB-CG-CD2	-6.89	99.28	111.00
4	D	26	ASP	CB-CG-OD1	6.64	124.28	118.30
11	K	54	ARG	NE-CZ-NH1	-6.63	116.99	120.30
4	Q	20	ARG	NE-CZ-NH2	-6.58	117.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	N	369	ASP	CB-CG-OD2	6.35	124.01	118.30
1	N	96	ARG	NE-CZ-NH2	-6.32	117.14	120.30
3	C	80	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	208	MET	CG-SD-CE	6.17	110.06	100.20
2	B	173	ASP	CB-CG-OD1	6.12	123.80	118.30
2	O	188	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	227	ASP	CB-CG-OD2	6.05	123.75	118.30
6	S	54	ASN	CB-CA-C	-5.92	98.57	110.40
1	A	189	MET	CG-SD-CE	-5.87	90.81	100.20
3	C	156	ARG	NE-CZ-NH2	-5.86	117.37	120.30
6	S	94	HIS	N-CA-C	5.68	126.32	111.00
9	I	10	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	486	ASP	CB-CG-OD1	5.62	123.35	118.30
12	L	20	ARG	NE-CZ-NH2	-5.54	117.53	120.30
4	D	51	LEU	CA-CB-CG	5.40	127.73	115.30
8	U	38	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	38	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	35	LEU	CA-CB-CG	-5.28	103.16	115.30
1	N	512	ASN	CB-CA-C	-5.24	99.92	110.40
11	X	54	ARG	NE-CZ-NH2	5.23	122.91	120.30
6	F	18	ARG	NE-CZ-NH2	-5.21	117.70	120.30
9	I	59	ASP	CB-CG-OD2	5.14	122.92	118.30
4	Q	20	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	B	226	MET	CB-CG-SD	5.08	127.63	112.40
1	A	442	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	512	ASN	CB-CA-C	-5.07	100.25	110.40
6	F	94	HIS	N-CA-C	5.06	124.67	111.00
1	A	169	ILE	CB-CA-C	-5.05	101.49	111.60
6	S	53	THR	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

5.2 Too-close contacts

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	48	0
1	N	4027	0	4001	70	0
2	B	1824	0	1833	27	0
2	O	1824	0	1833	32	0
3	C	2110	0	2027	25	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	3	0
5	R	852	0	845	5	0
6	F	748	0	728	9	0
6	S	748	0	728	27	0
7	G	675	0	644	27	0
7	T	675	0	644	28	0
8	H	662	0	623	7	0
8	U	662	0	623	2	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	460	0	459	7	0
10	W	460	0	459	4	0
11	K	384	0	366	1	0
11	X	384	0	366	6	0
12	L	380	0	380	10	0
12	Y	380	0	380	11	0
13	M	335	0	352	7	0
13	Z	335	0	352	3	0
14	A	120	0	108	6	0
14	N	120	0	108	9	0
15	A	1	0	0	0	0
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	63	0	110	6	0
18	D	63	0	110	6	0
18	L	63	0	110	15	0
18	N	126	0	220	21	0
18	Q	63	0	110	4	0
19	A	102	0	152	10	0
19	C	102	0	152	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	102	0	152	10	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	52	0	80	13	0
21	O	52	0	80	17	0
22	B	29	0	39	1	0
22	C	58	0	78	3	0
22	G	29	0	39	0	0
22	J	29	0	38	3	0
22	P	58	0	78	1	0
22	W	29	0	38	3	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	5	0
24	G	106	0	154	12	0
24	T	159	0	231	21	0
25	C	100	0	156	17	0
25	G	100	0	156	18	0
25	P	100	0	156	14	0
25	T	100	0	156	22	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	41	0	0
27	Z	33	0	40	0	0
28	A	215	0	0	7	0
28	B	124	0	0	2	0
28	C	109	0	0	2	0
28	D	102	0	0	3	0
28	E	67	0	0	1	0
28	F	81	0	0	1	0
28	G	48	0	0	5	0
28	H	48	0	0	2	0
28	I	31	0	0	1	0
28	J	16	0	0	0	0
28	K	26	0	0	2	0
28	L	28	0	0	1	0
28	M	20	0	0	0	0
28	N	220	0	0	6	0
28	O	114	0	0	0	0
28	P	109	0	0	4	0
28	Q	60	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	R	45	0	0	0	0
28	S	77	0	0	4	0
28	T	39	0	0	2	0
28	U	45	0	0	0	0
28	V	21	0	0	2	0
28	W	16	0	0	0	0
28	X	17	0	0	2	0
28	Y	19	0	0	1	0
28	Z	14	0	0	1	0
All	All	32377	0	31229	485	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 8.

All (485) 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)
6:S:52:ILE:O	6:S:94:HIS:CE1	1.76	1.38
6:S:52:ILE:O	6:S:94:HIS:NE2	1.66	1.26
7:T:84:LYS:H	7:T:84:LYS:HD2	0.95	1.12
1:N:513:LEU:O	1:N:514:LYS:HB2	1.47	1.11
24:T:1265:PEK:H383	25:T:1269:CDL:C27	1.81	1.10
24:C:265:PEK:H383	25:G:269:CDL:H273	1.28	1.10
24:T:1265:PEK:H383	25:T:1269:CDL:H273	1.10	1.09
7:G:84:LYS:HD2	7:G:84:LYS:H	1.05	1.09
24:C:265:PEK:H383	25:G:269:CDL:C27	1.83	1.08
25:G:269:CDL:H541	25:G:269:CDL:H231	1.37	1.05
21:O:1229:PSC:H142	21:O:1229:PSC:H343	1.40	1.02
2:B:41:ILE:HD13	21:B:229:PSC:H342	1.42	1.02
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.22	1.01
6:S:85:CYS:SG	6:S:87:THR:HG23	2.01	1.00
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.40	0.99
18:D:523:TGL:H361	28:I:4610:HOH:O	1.62	0.99
24:T:1265:PEK:C38	25:T:1269:CDL:H273	1.95	0.96
6:F:85:CYS:SG	6:F:87:THR:HG23	2.05	0.96
2:O:224:ALA:O	2:O:227:LEU:HG	1.63	0.95
7:T:72:ASN:H	7:T:76:ASN:HD22	1.14	0.94
7:T:84:LYS:N	7:T:84:LYS:HD2	1.80	0.94
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.47	0.94
6:S:52:ILE:O	6:S:94:HIS:CD2	2.22	0.93
7:T:84:LYS:H	7:T:84:LYS:CD	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.51	0.92
6:S:53:THR:HA	6:S:94:HIS:CE1	2.03	0.92
24:C:265:PEK:C38	25:G:269:CDL:H273	1.99	0.92
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.32	0.91
28:N:4772:HOH:O	24:T:1264:PEK:H381	1.72	0.89
3:P:3:HIS:HB3	28:P:4285:HOH:O	1.72	0.89
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.55	0.89
4:D:31:LYS:HD2	28:D:4414:HOH:O	1.73	0.88
18:D:523:TGL:HC21	18:D:523:TGL:HG11	1.56	0.88
21:B:229:PSC:H072	9:I:10:ARG:HH21	1.39	0.87
21:O:1229:PSC:C34	21:O:1229:PSC:H142	2.04	0.87
7:G:84:LYS:HD2	7:G:84:LYS:N	1.90	0.86
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.56	0.86
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.12	0.84
19:C:268:PGV:H42	28:P:4823:HOH:O	1.75	0.84
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.84
1:N:513:LEU:O	1:N:514:LYS:CB	2.21	0.84
25:T:1269:CDL:H541	25:T:1269:CDL:H231	1.59	0.84
21:B:229:PSC:C07	9:I:10:ARG:HH21	1.89	0.84
6:S:53:THR:HA	6:S:94:HIS:HE1	1.42	0.83
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.44	0.83
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.43	0.83
1:A:1:FME:HG3	28:L:4907:HOH:O	1.78	0.82
18:N:1521:TGL:H241	18:N:1521:TGL:H201	1.62	0.81
6:S:52:ILE:C	6:S:94:HIS:CE1	2.56	0.79
21:O:1229:PSC:H343	21:O:1229:PSC:C14	2.14	0.77
7:G:76:ASN:HD21	24:G:264:PEK:HN2	1.28	0.77
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.67	0.77
2:O:59:GLN:O	2:O:59:GLN:HG3	1.83	0.77
24:G:264:PEK:H101	24:G:264:PEK:H161	1.68	0.76
19:P:1268:PGV:H062	28:P:4397:HOH:O	1.84	0.76
25:G:269:CDL:C54	25:G:269:CDL:H231	2.15	0.76
7:G:84:LYS:H	7:G:84:LYS:CD	1.89	0.76
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.26	0.75
1:A:112:LEU:HG	28:A:2701:HOH:O	1.87	0.74
7:T:76:ASN:HD21	24:T:1264:PEK:HN2	1.34	0.74
2:B:49:LYS:HE2	28:E:4606:HOH:O	1.87	0.74
7:T:3:ALA:HB1	24:T:263:PEK:H382	1.68	0.73
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.71	0.73
18:Q:1523:TGL:HC21	18:Q:1523:TGL:HG11	1.71	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.72	0.72
19:C:267:PGV:H12	19:C:267:PGV:H161	1.72	0.72
4:D:34:SER:H	4:D:37:GLN:HE21	1.36	0.72
3:C:246:ASP:HB2	28:C:4249:HOH:O	1.89	0.71
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.30	0.71
7:T:72:ASN:H	7:T:76:ASN:ND2	1.87	0.71
18:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.72	0.70
1:A:513:LEU:O	1:A:514:LYS:HB2	1.91	0.70
6:F:54:ASN:HB2	28:F:4662:HOH:O	1.90	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.75	0.69
7:T:5:LYS:HD2	24:T:263:PEK:H371	1.74	0.69
12:L:11:ILE:CG2	18:L:522:TGL:H271	2.23	0.69
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.75	0.69
4:Q:31:LYS:HB3	28:Q:4834:HOH:O	1.92	0.68
10:W:33:ARG:HG2	22:W:1059:CHD:H151	1.75	0.68
1:A:406:ASN:HD21	19:A:524:PGV:H22	1.59	0.68
4:Q:100:LYS:HE2	28:Q:4478:HOH:O	1.94	0.68
9:V:65:LYS:O	11:X:54:ARG:NH1	2.27	0.67
6:S:95:GLN:HB2	28:S:4523:HOH:O	1.93	0.67
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.67
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.75	0.67
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.75	0.67
28:G:4789:HOH:O	19:P:1268:PGV:H341	1.93	0.67
18:N:1521:TGL:C28	18:N:1521:TGL:H101	2.25	0.67
2:O:59:GLN:O	2:O:59:GLN:CG	2.42	0.66
1:A:406:ASN:HD21	19:A:524:PGV:C2	2.08	0.66
18:N:1521:TGL:HC22	28:V:3606:HOH:O	1.95	0.66
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.60	0.66
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.78	0.66
1:A:278:MET:SD	7:T:5:LYS:HB3	2.36	0.66
7:G:17:ARG:HD2	28:G:2446:HOH:O	1.95	0.65
1:A:486:ASP:OD2	4:D:19:ARG:HD3	1.96	0.65
21:O:1229:PSC:H21	21:O:1229:PSC:H222	1.78	0.65
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.60	0.65
2:B:56:MET:HG2	21:B:229:PSC:H211	1.78	0.65
7:G:2:SER:O	24:G:1263:PEK:H322	1.97	0.64
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.79	0.64
2:B:41:ILE:CD1	21:B:229:PSC:H342	2.25	0.63
8:H:27:ARG:HD3	28:H:4760:HOH:O	1.98	0.63
21:O:1229:PSC:C07	9:V:10:ARG:HH21	2.12	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:ILE:HG12	19:C:267:PGV:H132	1.81	0.62
7:T:3:ALA:O	7:T:4:ALA:HB2	2.00	0.62
6:S:1:ALA:N	24:T:1265:PEK:H041	2.14	0.61
7:G:3:ALA:O	7:G:4:ALA:HB2	2.00	0.61
5:R:80:GLU:N	5:R:80:GLU:OE1	2.33	0.61
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.66	0.61
2:O:41:ILE:HD13	21:O:1229:PSC:H342	1.82	0.61
7:T:3:ALA:CB	24:T:263:PEK:H382	2.30	0.61
25:C:270:CDL:H642	25:C:270:CDL:H191	1.82	0.60
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.01	0.60
19:A:524:PGV:H062	28:A:2126:HOH:O	2.00	0.60
6:S:52:ILE:O	6:S:94:HIS:CG	2.54	0.60
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.16	0.60
18:A:521:TGL:H111	2:B:35:SER:OG	2.02	0.60
10:W:33:ARG:HG2	22:W:1059:CHD:C15	2.32	0.60
7:G:45:PRO:HD2	28:G:2099:HOH:O	2.01	0.60
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	2.01	0.60
18:D:523:TGL:HB62	18:D:523:TGL:HA52	1.83	0.60
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.01	0.60
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.84	0.60
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.83	0.60
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.85	0.59
19:A:524:PGV:H82	19:A:524:PGV:H262	1.84	0.59
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.59
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.14	0.59
1:N:28:MET:CE	14:N:515:HEA:C27	2.80	0.59
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.84	0.59
2:O:56:MET:HG2	21:O:1229:PSC:H211	1.84	0.59
1:N:28:MET:CE	14:N:515:HEA:H271	2.32	0.58
24:C:265:PEK:H383	25:G:269:CDL:H272	1.80	0.58
7:G:31:CYS:SG	25:G:269:CDL:H552	2.44	0.58
18:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.85	0.58
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.85	0.58
4:D:34:SER:H	4:D:37:GLN:NE2	2.01	0.58
6:F:64:GLU:O	6:F:65:ASP:HB2	2.04	0.58
6:S:52:ILE:O	6:S:94:HIS:ND1	2.30	0.58
21:O:1229:PSC:O01	21:O:1229:PSC:H212	2.04	0.58
12:L:11:ILE:HG22	18:L:522:TGL:H271	1.85	0.57
28:B:3446:HOH:O	7:T:17:ARG:HD2	2.03	0.57
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.86	0.57
4:Q:7:LYS:HA	28:Q:4706:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:CB	24:T:263:PEK:H362	2.27	0.57
6:S:87:THR:HG22	28:S:4582:HOH:O	2.04	0.57
21:B:229:PSC:H142	21:B:229:PSC:H343	1.86	0.57
1:N:400:PHE:HB3	18:N:1522:TGL:H282	1.87	0.57
12:L:20:ARG:HH22	18:L:522:TGL:HC62	1.70	0.57
18:N:1521:TGL:H252	18:N:1521:TGL:HA91	1.86	0.57
4:Q:127:LYS:HD2	28:V:3618:HOH:O	2.05	0.57
19:A:522:PGV:H183	24:G:264:PEK:H332	1.87	0.56
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.40	0.56
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.05	0.56
24:G:1263:PEK:H132	3:P:247:VAL:CG1	2.36	0.56
1:A:488:THR:HB	1:A:495:LEU:HD13	1.87	0.56
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.34	0.56
1:N:472:ILE:HG21	18:N:1522:TGL:HA91	1.88	0.55
6:S:1:ALA:H2	24:T:1265:PEK:H041	1.71	0.55
1:A:21:LEU:HD23	18:L:522:TGL:H211	1.88	0.55
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.89	0.55
6:S:53:THR:CA	6:S:94:HIS:CE1	2.86	0.55
3:C:210:ILE:HD13	19:C:267:PGV:H301	1.88	0.55
10:J:50:LEU:HD22	10:J:54:SER:HG	1.71	0.55
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.19	0.54
18:A:521:TGL:HC22	28:D:2606:HOH:O	2.06	0.54
21:B:229:PSC:H322	21:B:229:PSC:H12	1.89	0.54
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.88	0.54
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.89	0.54
1:N:430:PHE:HE1	18:N:1521:TGL:HB21	1.72	0.54
7:G:37:LEU:CD2	25:G:269:CDL:H361	2.38	0.54
2:B:19:GLU:HG3	2:B:83:ILE:HG12	1.88	0.54
9:V:2:THR:HG22	9:V:3:ALA:H	1.72	0.54
4:Q:78:TRP:HA	18:Q:1523:TGL:HB22	1.89	0.53
18:N:1521:TGL:H281	18:N:1521:TGL:H101	1.90	0.53
2:B:13:THR:HB	2:B:168:LEU:HD23	1.90	0.53
2:O:84:LEU:HA	2:O:87:MET:HE2	1.89	0.53
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.90	0.53
21:O:1229:PSC:H071	9:V:10:ARG:HE	1.73	0.53
1:N:417:MET:CE	28:N:3166:HOH:O	2.56	0.53
7:G:30:LEU:CD2	25:G:269:CDL:H462	2.39	0.53
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.25	0.53
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.53
1:N:321:PHE:CD2	21:O:1229:PSC:H341	2.44	0.52
7:T:5:LYS:HD2	24:T:263:PEK:C37	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:HD21	25:C:270:CDL:H412	1.91	0.52
11:X:52:GLU:HG2	28:X:4813:HOH:O	2.09	0.52
12:Y:2:HIS:N	28:Y:4664:HOH:O	2.43	0.52
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.39	0.52
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.10	0.52
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.90	0.52
7:T:3:ALA:O	7:T:4:ALA:CB	2.56	0.52
12:L:12:PRO:HB2	18:L:522:TGL:HG2	1.92	0.52
1:N:28:MET:HE2	14:N:515:HEA:C27	2.40	0.52
19:A:524:PGV:H02	19:A:524:PGV:O14	2.10	0.52
3:C:54:MET:HE3	25:C:270:CDL:H612	1.92	0.52
7:G:72:ASN:H	7:G:76:ASN:ND2	1.99	0.52
18:L:522:TGL:CC6	18:L:522:TGL:HC22	2.40	0.52
12:L:20:ARG:HH12	18:L:522:TGL:HC62	1.75	0.52
18:N:1521:TGL:C10	18:N:1521:TGL:H281	2.40	0.51
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.91	0.51
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.92	0.51
19:N:1524:PGV:H011	19:N:1524:PGV:H22	1.91	0.51
1:N:449:MET:SD	2:O:5:MET:HG2	2.50	0.51
12:L:20:ARG:HH12	18:L:522:TGL:CC6	2.23	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.45	0.51
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.40	0.51
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.91	0.51
18:D:523:TGL:HA91	18:D:523:TGL:H242	1.91	0.51
1:N:400:PHE:O	18:N:1522:TGL:H283	2.11	0.51
1:N:112:LEU:HG	28:N:3701:HOH:O	2.09	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
7:G:4:ALA:CB	1:N:282:PHE:HA	2.41	0.51
1:A:112:LEU:CG	28:A:2701:HOH:O	2.54	0.51
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.24	0.51
14:A:516:HEA:HBC1	14:A:516:HEA:HMC1	1.92	0.51
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.26	0.51
12:L:24:MET:SD	18:L:522:TGL:H161	2.51	0.51
7:G:30:LEU:HD21	25:G:269:CDL:H462	1.92	0.50
1:N:366:VAL:HG11	2:O:9:PHE:CE2	2.46	0.50
1:N:488:THR:HB	1:N:495:LEU:HD13	1.93	0.50
3:P:76:GLN:NE2	28:P:3284:HOH:O	2.37	0.50
3:P:54:MET:HE3	25:P:1270:CDL:H612	1.92	0.50
1:N:400:PHE:HB3	18:N:1522:TGL:C28	2.40	0.50
1:N:472:ILE:HD13	18:N:1522:TGL:HA91	1.94	0.50
3:P:5:THR:HG22	6:S:96:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:164:ALA:O	2:O:194:GLY:HA3	2.12	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.94	0.50
7:T:2:SER:O	24:T:263:PEK:H322	2.12	0.50
3:P:210:ILE:HD13	19:P:1267:PGV:H301	1.93	0.50
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.50
2:O:146:MET:HA	2:O:213:LEU:HD12	1.94	0.50
21:O:1229:PSC:H071	9:V:10:ARG:HH21	1.77	0.50
1:A:430:PHE:CE1	18:A:521:TGL:HB21	2.47	0.50
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.93	0.50
1:N:177:SER:H	1:N:180:GLN:HE21	1.59	0.50
8:H:7:LYS:O	8:H:8:ILE:HB	2.11	0.50
21:B:229:PSC:H222	21:B:229:PSC:H21	1.94	0.49
4:D:78:TRP:HA	18:D:523:TGL:HB22	1.94	0.49
1:N:172:LYS:HD2	1:N:181:THR:HG22	1.93	0.49
18:L:522:TGL:OA1	18:L:522:TGL:OG3	2.30	0.49
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.47	0.49
18:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.95	0.49
7:G:3:ALA:O	7:G:4:ALA:CB	2.60	0.49
25:T:1269:CDL:H172	25:T:1269:CDL:H511	1.94	0.49
24:G:1263:PEK:H182	3:P:98:PHE:CD2	2.48	0.49
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.95	0.49
18:N:1522:TGL:H271	12:Y:11:ILE:CG2	2.43	0.49
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.11	0.48
10:J:50:LEU:HD22	10:J:54:SER:OG	2.14	0.48
1:A:506:GLU:HG3	28:A:4882:HOH:O	2.12	0.48
4:D:86:MET:CE	28:K:4688:HOH:O	2.61	0.48
24:G:1263:PEK:H132	3:P:247:VAL:HG12	1.94	0.48
25:T:1269:CDL:C57	25:T:1269:CDL:H782	2.32	0.48
2:O:41:ILE:CD1	21:O:1229:PSC:H342	2.43	0.48
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
7:T:38:HIS:NE2	25:T:1269:CDL:H111	2.29	0.48
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.53	0.48
21:O:1229:PSC:H081	5:R:8:ASP:OD1	2.14	0.48
1:N:112:LEU:HD23	1:N:112:LEU:C	2.34	0.48
11:K:24:PHE:O	11:K:28:VAL:HG12	2.14	0.48
3:C:91:VAL:HG22	24:T:263:PEK:H14	1.95	0.48
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.48
11:X:41:ASN:OD1	28:X:4655:HOH:O	2.20	0.48
5:E:105:GLY:O	5:E:108:LYS:HG2	2.14	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
1:A:28:MET:CE	14:A:515:HEA:H271	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.15	0.47
3:C:122:HIS:HD2	28:C:4770:HOH:O	1.97	0.47
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.14	0.47
2:B:78:LEU:CD1	25:T:1269:CDL:H352	2.44	0.47
2:B:29:MET:HG3	9:I:35:TYR:CD2	2.49	0.47
18:N:1521:TGL:C24	18:N:1521:TGL:H201	2.41	0.47
28:B:3446:HOH:O	7:T:17:ARG:CD	2.63	0.47
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.96	0.47
1:N:243:VAL:HB	14:N:516:HEA:CAC	2.45	0.47
25:C:270:CDL:CB3	25:C:270:CDL:HB21	2.45	0.47
28:G:4541:HOH:O	19:P:1268:PGV:H301	2.14	0.47
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.97	0.47
18:N:1522:TGL:H302	28:N:4751:HOH:O	2.15	0.47
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.96	0.47
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.45	0.47
3:C:191:GLY:HA3	28:G:2132:HOH:O	2.14	0.47
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.14	0.47
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.14	0.47
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.80	0.47
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.97	0.47
3:P:51:MET:HB3	25:P:1270:CDL:H622	1.96	0.47
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.47
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.80	0.46
1:A:46:THR:HG23	28:A:2466:HOH:O	2.15	0.46
1:A:379:TYR:O	1:A:383:MET:HB2	2.16	0.46
18:A:521:TGL:HC82	28:A:4504:HOH:O	2.14	0.46
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.79	0.46
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.97	0.46
21:B:229:PSC:C07	9:I:10:ARG:NH2	2.68	0.46
1:N:148:PHE:HB3	3:P:28:THR:HB	1.97	0.46
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.15	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.97	0.46
2:O:56:MET:HA	21:O:1229:PSC:H202	1.98	0.46
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.16	0.46
25:G:269:CDL:H1	25:G:269:CDL:OB4	2.16	0.46
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.46
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.97	0.46
24:T:1264:PEK:C10	24:T:1264:PEK:H161	2.46	0.45
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.51	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.50	0.45
25:C:270:CDL:OA5	25:C:270:CDL:HB22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.97	0.45
2:B:222:TRP:O	2:B:226:MET:HB2	2.16	0.45
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.99	0.45
1:N:87:ILE:O	1:N:173:PRO:HD3	2.15	0.45
6:S:51:SER:O	6:S:94:HIS:HA	2.16	0.45
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.56	0.45
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.52	0.45
1:A:321:PHE:CD2	21:B:229:PSC:H341	2.51	0.45
14:N:515:HEA:H273	14:N:515:HEA:H172	1.41	0.45
4:D:86:MET:HE3	28:K:4688:HOH:O	2.17	0.45
25:T:1269:CDL:H171	28:T:4708:HOH:O	2.17	0.45
25:C:270:CDL:H172	25:C:270:CDL:H741	1.98	0.45
6:F:70:ILE:HG13	6:F:84:SER:HB3	1.98	0.45
6:F:55:LYS:HA	6:F:74:LEU:O	2.16	0.45
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.45
24:T:1264:PEK:H161	24:T:1264:PEK:H102	1.98	0.45
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.71	0.45
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.98	0.45
10:W:56:PRO:HD3	12:Y:46:LYS:HG2	1.98	0.45
12:Y:22:LEU:O	12:Y:26:THR:HB	2.17	0.45
3:P:250:LEU:HD22	25:T:1269:CDL:H662	1.98	0.45
8:H:60:TYR:C	8:H:60:TYR:CD1	2.89	0.45
3:C:105:SER:HA	3:C:116:TRP:CE3	2.52	0.45
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.52	0.44
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.52	0.44
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.82	0.44
25:C:270:CDL:H611	25:C:270:CDL:H652	2.00	0.44
1:N:309:THR:HG22	14:N:516:HEA:HMB2	1.97	0.44
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.05	0.44
18:A:521:TGL:H281	18:A:521:TGL:H101	1.99	0.44
2:O:16:ILE:HD11	2:O:86:MET:HG2	2.00	0.44
1:A:1:FME:HCN	1:A:4:ASN:H	1.82	0.44
21:B:229:PSC:H062	21:B:229:PSC:H042	1.80	0.44
18:L:522:TGL:H231	18:L:522:TGL:H202	1.41	0.44
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.48	0.44
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.44
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.83	0.44
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.82	0.44
2:B:78:LEU:HD12	25:T:1269:CDL:C35	2.48	0.44
25:P:1270:CDL:H242	25:P:1270:CDL:H661	1.98	0.44
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:1085:CHD:H212	22:B:1085:CHD:H12	1.99	0.44
10:J:40:LEU:HD12	22:J:60:CHD:H183	2.00	0.44
1:N:501:PRO:HB3	12:Y:5:GLU:OE2	2.17	0.44
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.44
5:R:80:GLU:CD	5:R:80:GLU:H	2.20	0.44
1:A:481:GLU:HB2	13:M:4:LYS:HE2	2.00	0.44
25:C:270:CDL:C19	25:C:270:CDL:H642	2.47	0.44
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.75	0.43
19:A:524:PGV:H312	13:M:16:ALA:HA	1.99	0.43
1:N:334:TRP:CZ3	18:Q:1523:TGL:HA51	2.53	0.43
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.18	0.43
13:Z:37:LEU:HA	13:Z:37:LEU:HD23	1.79	0.43
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.32	0.43
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.87	0.43
24:T:1265:PEK:H383	25:T:1269:CDL:H272	1.90	0.43
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.53	0.43
3:P:64:GLU:HA	3:P:68:GLN:HE21	1.83	0.43
6:S:87:THR:HG21	28:S:3514:HOH:O	2.18	0.43
25:G:269:CDL:H352	2:O:78:LEU:HD12	2.00	0.43
2:O:65:TRP:CZ3	21:O:1229:PSC:H331	2.54	0.43
3:P:63:ARG:NE	25:P:1270:CDL:HA22	2.07	0.43
1:A:282:PHE:HA	7:T:4:ALA:CB	2.45	0.43
1:N:215:LEU:HD11	24:T:1264:PEK:H271	2.00	0.43
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.80	0.43
19:C:267:PGV:H182	25:C:270:CDL:C67	2.49	0.43
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.53	0.43
1:N:472:ILE:HG21	18:N:1522:TGL:CA9	2.49	0.43
19:N:1524:PGV:H132	19:N:1524:PGV:H301	2.01	0.43
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.54	0.43
25:G:269:CDL:H451	2:O:70:ALA:HB1	2.01	0.43
21:O:1229:PSC:C07	9:V:10:ARG:HE	2.32	0.43
22:W:1059:CHD:H193	22:W:1059:CHD:H111	1.73	0.43
10:J:33:ARG:HG2	22:J:60:CHD:C15	2.48	0.43
1:A:383:MET:O	1:A:387:PHE:HB2	2.18	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.96	0.43
4:D:132:GLN:OE1	9:I:43:ARG:HD3	2.19	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.01	0.43
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.76	0.43
3:C:156:ARG:HE	22:C:271:CHD:C24	2.32	0.43
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.43
1:N:365:ILE:HD11	28:N:4859:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:1269:CDL:H182	25:T:1269:CDL:H152	1.85	0.43
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.01	0.43
3:P:107:ALA:HB2	19:P:1268:PGV:H031	2.01	0.43
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.36	0.43
1:N:310:MET:HB3	2:O:73:LEU:HD22	2.00	0.43
25:P:1270:CDL:H642	25:P:1270:CDL:C19	2.49	0.42
12:L:20:ARG:NH2	18:L:522:TGL:HC42	2.34	0.42
13:M:4:LYS:HG2	13:M:4:LYS:H	1.64	0.42
1:N:54:TYR:HB2	28:N:4621:HOH:O	2.19	0.42
4:D:7:LYS:HE3	28:D:4308:HOH:O	2.18	0.42
3:P:29:SER:CB	3:P:42:LEU:HD13	2.48	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
2:B:199:ILE:HG23	2:B:199:ILE:O	2.19	0.42
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.50	0.42
1:N:489:THR:HA	6:S:71:TRP:O	2.19	0.42
21:B:229:PSC:H241	21:B:229:PSC:H62	2.02	0.42
1:N:115:SER:HB2	1:N:142:SER:O	2.20	0.42
2:O:199:ILE:O	2:O:199:ILE:HG23	2.19	0.42
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.18	0.42
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.01	0.42
7:G:31:CYS:SG	25:G:269:CDL:H532	2.59	0.42
3:C:247:VAL:CG1	24:T:263:PEK:H132	2.50	0.42
2:O:9:PHE:HB2	2:O:21:LEU:HD21	2.01	0.42
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.55	0.42
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.01	0.42
10:J:56:PRO:HD3	12:L:46:LYS:HG2	2.01	0.42
5:E:5:HIS:HB3	5:E:6:GLU:H	1.62	0.42
7:T:31:CYS:SG	25:T:1269:CDL:C55	3.07	0.42
3:C:51:MET:HB3	25:C:270:CDL:H622	2.01	0.42
7:G:5:LYS:HD2	24:G:1263:PEK:H371	2.00	0.42
19:C:268:PGV:H341	28:T:4364:HOH:O	2.19	0.42
4:D:78:TRP:CA	18:D:523:TGL:HB22	2.50	0.42
1:N:342:LEU:HD13	2:O:46:LEU:HD11	2.01	0.42
6:S:95:GLN:CB	28:S:4523:HOH:O	2.61	0.42
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.02	0.42
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.20	0.41
1:A:115:SER:HB2	1:A:142:SER:O	2.20	0.41
9:V:73:LYS:HE3	9:V:73:LYS:HB3	1.96	0.41
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.55	0.41
1:N:22:PHE:HA	18:N:1522:TGL:HB72	2.02	0.41
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:TYR:O	1:N:383:MET:HB2	2.20	0.41
2:B:29:MET:HG3	9:I:35:TYR:CG	2.55	0.41
1:N:456:MET:HG2	4:Q:96:LEU:HD13	2.01	0.41
1:N:243:VAL:HB	14:N:516:HEA:HAC	2.01	0.41
1:N:431:LEU:HD22	1:N:447:TYR:HB3	2.03	0.41
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.56	0.41
19:N:1266:PGV:H183	24:T:1264:PEK:H332	2.03	0.41
1:A:400:PHE:HB3	18:L:522:TGL:H282	2.03	0.41
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.35	0.41
6:F:46:PRO:O	6:F:48:LEU:HD13	2.21	0.41
21:B:229:PSC:H251	21:B:229:PSC:H221	1.79	0.41
1:A:28:MET:HE1	14:A:515:HEA:C27	2.51	0.41
1:N:76:GLY:O	1:N:80:ASN:HB2	2.20	0.41
7:G:7:ASP:O	7:G:9:GLY:N	2.49	0.41
6:S:70:ILE:HG13	6:S:84:SER:HB3	2.01	0.41
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.41
5:E:48:ILE:O	5:E:52:LEU:HG	2.20	0.41
13:M:10:THR:HG22	13:M:15:GLN:HG3	2.02	0.41
1:N:430:PHE:CE1	18:N:1521:TGL:HB21	2.55	0.41
8:H:39:CYS:O	8:H:43:MET:HG2	2.21	0.41
1:N:310:MET:HE2	1:N:356:ILE:HG23	2.02	0.41
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.56	0.41
3:P:129:VAL:N	3:P:130:PRO:CD	2.82	0.41
25:P:1270:CDL:H792	25:P:1270:CDL:H821	1.86	0.41
25:C:270:CDL:H202	25:C:270:CDL:H171	1.87	0.41
24:G:264:PEK:H352	24:G:264:PEK:H382	1.72	0.41
3:C:223:LEU:HD21	22:C:271:CHD:H183	2.01	0.41
7:T:11:TPO:O	7:T:11:TPO:CG2	2.68	0.41
14:A:515:HEA:H172	14:A:515:HEA:H273	1.30	0.41
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.51	0.41
21:O:1229:PSC:H22	9:V:14:ALA:CB	2.51	0.41
24:G:1263:PEK:H132	3:P:247:VAL:HG11	2.03	0.41
6:F:51:SER:O	6:F:94:HIS:N	2.47	0.41
13:Z:7:LYS:NZ	28:Z:4640:HOH:O	2.36	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.90	0.41
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.63	0.40
25:T:1269:CDL:HA62	25:T:1269:CDL:H322	2.02	0.40
24:C:265:PEK:C38	25:G:269:CDL:C27	2.70	0.40
19:N:1524:PGV:H92	4:Q:84:ALA:HB2	2.02	0.40
8:H:27:ARG:NH1	28:H:2431:HOH:O	2.53	0.40
10:J:50:LEU:HD22	10:J:50:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1270:CDL:H652	25:P:1270:CDL:H611	2.03	0.40
1:A:409:TRP:CH2	19:A:524:PGV:H81	2.57	0.40
2:B:196:CYS:CB	2:B:207:MET:HG3	2.52	0.40
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.03	0.40
1:A:194:LEU:HD13	28:A:4206:HOH:O	2.21	0.40
19:C:267:PGV:H172	25:C:270:CDL:H662	2.02	0.40
4:Q:81:VAL:HG11	18:Q:1523:TGL:HB51	2.04	0.40
3:P:22:LEU:O	3:P:26:LEU:HG	2.21	0.40
1:N:402:GLY:HA3	1:N:499:PRO:HD3	2.03	0.40
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.47	0.40

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%)	496 (97%)	15 (3%)	1 (0%)	52	64
1	N	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	39	48
2	O	225/227 (99%)	214 (95%)	8 (4%)	3 (1%)	15	15
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	6 (2%)	1 (0%)	39	48
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	19	21
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	5	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	66 (82%)	9 (11%)	6 (7%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15	15
8	U	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	7	4
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3371 (96%)	107 (3%)	26 (1%)	26	31

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
8	H	8	ILE
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
1	A	384	GLY
2	B	60	GLU
8	U	8	ILE
7	G	6	GLY
2	O	224	ALA
7	T	6	GLY

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Mol	Chain	Res	Type
7	G	3	ALA
7	G	40	GLY
2	O	60	GLU
3	P	38	ASN
7	T	39	SER
8	U	10	ASN
6	S	96	LEU
2	O	92	ASN

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%)	65	81
1	N	426/426 (100%)	415 (97%)	11 (3%)	54	71
2	B	210/210 (100%)	199 (95%)	11 (5%)	29	38
2	O	210/210 (100%)	197 (94%)	13 (6%)	23	30
3	C	224/226 (99%)	218 (97%)	6 (3%)	52	70
3	P	224/226 (99%)	218 (97%)	6 (3%)	52	70
4	D	128/129 (99%)	127 (99%)	1 (1%)	86	94
4	Q	128/129 (99%)	124 (97%)	4 (3%)	47	64
5	E	92/95 (97%)	88 (96%)	4 (4%)	35	47
5	R	92/95 (97%)	91 (99%)	1 (1%)	80	90
6	F	81/81 (100%)	78 (96%)	3 (4%)	41	55
6	S	81/81 (100%)	76 (94%)	5 (6%)	23	30
7	G	67/68 (98%)	60 (90%)	7 (10%)	9	10
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	14
8	H	71/75 (95%)	68 (96%)	3 (4%)	36	49
8	U	71/75 (95%)	67 (94%)	4 (6%)	26	35
9	I	57/57 (100%)	53 (93%)	4 (7%)	19	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	53 (93%)	4 (7%)	19	23
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	79
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	79
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	71
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	39
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	71
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16	20
13	M	37/38 (97%)	30 (81%)	7 (19%)	2	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	5	4
All	All	3040/3082 (99%)	2918 (96%)	122 (4%)	38	52

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	189	MET
1	A	338	MET
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
2	B	226	MET
3	C	33	MET
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN

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Mol	Chain	Res	Type
4	D	51	LEU
5	E	5	HIS
5	E	31	LYS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	84	SER
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	8	ILE
8	H	9	LYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	189	MET
1	N	336	PRO
1	N	363	LEU
1	N	369	ASP
1	N	484	THR

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Mol	Chain	Res	Type
1	N	512	ASN
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	65	TRP
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	171	LYS
2	O	217	LYS
3	P	33	MET
3	P	77	LYS
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	51	LEU
4	Q	52	SER
4	Q	143	ASN
5	R	5	HIS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	95	GLN
6	S	96	LEU
7	T	17	ARG
7	T	18	PHE
7	T	38	HIS
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
8	U	70	SER
9	V	2	THR
9	V	8	GLN

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Mol	Chain	Res	Type
9	V	10	ARG
9	V	29	LEU
10	W	50	LEU
11	X	20	SER
11	X	54	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	178	GLN
1	A	180	GLN
1	A	360	ASN
1	A	512	ASN
2	B	52	HIS
2	B	181	GLN
2	B	195	GLN
3	C	68	GLN
4	D	37	GLN
4	D	143	ASN
5	E	94	ASN
7	G	8	HIS
7	G	71	HIS
7	G	76	ASN
10	J	29	ASN
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS

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Mol	Chain	Res	Type
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	94	ASN
7	T	76	ASN
10	W	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	8,9,10	0.86	0	6,9,11	5.40	3 (50%)
2	FME	B	1	2	8,9,10	1.46	1 (12%)	6,9,11	8.07	5 (83%)
7	TPO	G	11	7	8,10,11	1.89	2 (25%)	7,14,16	1.16	1 (14%)
9	SAC	I	1	9	7,8,9	2.55	2 (28%)	7,9,11	1.84	2 (28%)
1	FME	N	1	1	8,9,10	0.86	0	6,9,11	6.21	2 (33%)
2	FME	O	1	2	8,9,10	0.86	0	6,9,11	6.43	3 (50%)
7	TPO	T	11	7	8,10,11	1.78	2 (25%)	7,14,16	1.26	1 (14%)
9	SAC	V	1	9	7,8,9	2.45	2 (28%)	7,9,11	3.49	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O2P	2.16	1.62	1.54
7	G	11	TPO	P-OG1	2.16	1.66	1.60
2	B	1	FME	CA-N	3.01	1.50	1.46
7	G	11	TPO	P-O1P	3.02	1.61	1.51
7	T	11	TPO	P-O1P	3.10	1.61	1.51
9	I	1	SAC	CA-N	3.68	1.51	1.46
9	V	1	SAC	OAC-C1A	4.41	1.33	1.23
9	V	1	SAC	CA-N	4.55	1.52	1.46
9	I	1	SAC	OAC-C1A	5.35	1.35	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-17.00	96.68	122.82
2	O	1	FME	CA-N-CN	-14.97	99.80	122.82
1	N	1	FME	CA-N-CN	-14.72	100.18	122.82
1	A	1	FME	CA-N-CN	-12.61	103.43	122.82
9	V	1	SAC	CB-CA-N	-7.71	93.72	110.60
2	B	1	FME	CG-CB-CA	-4.36	100.25	113.06
2	O	1	FME	CG-CB-CA	-3.55	102.64	113.06
9	I	1	SAC	C2A-C1A-N	-3.04	110.29	116.11
2	B	1	FME	O-C-CA	-2.78	118.09	125.44
1	A	1	FME	CG-CB-CA	-2.54	105.62	113.06
7	T	11	TPO	O-C-CA	-2.42	119.05	125.44
7	G	11	TPO	O-C-CA	-2.29	119.39	125.44
2	O	1	FME	O-C-CA	-2.24	119.52	125.44
1	N	1	FME	O-C-CA	-2.15	119.77	125.44
9	V	1	SAC	O-C-CA	-2.15	119.77	125.44
2	B	1	FME	CE-SD-CG	2.01	107.23	100.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CE-SD-CG	2.32	108.29	100.37
9	I	1	SAC	OAC-C1A-N	2.33	126.62	121.86
9	V	1	SAC	CA-N-C1A	3.74	134.07	121.37
2	B	1	FME	O1-CN-N	8.38	136.83	124.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
7	G	11	TPO	1	0
7	T	11	TPO	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 42 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	515	1	40,67,67	1.02	4 (10%)	41,103,103	3.04	14 (34%)
14	HEA	A	516	1	40,67,67	1.21	6 (15%)	41,103,103	2.05	13 (31%)
18	TGL	A	521	-	62,62,62	1.23	6 (9%)	65,65,65	1.79	14 (21%)
19	PGV	A	522	-	50,50,50	0.80	2 (4%)	51,56,56	1.17	2 (3%)
19	PGV	A	524	-	50,50,50	1.14	2 (4%)	51,56,56	1.08	6 (11%)
22	CHD	B	1085	-	29,32,32	1.07	3 (10%)	48,51,51	1.40	8 (16%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	PSC	B	229	-	51,51,51	1.16	3 (5%)	55,59,59	1.08	2 (3%)
24	PEK	C	265	-	51,52,52	1.18	2 (3%)	52,57,57	1.17	5 (9%)
19	PGV	C	267	-	50,50,50	0.80	2 (4%)	51,56,56	1.16	5 (9%)
19	PGV	C	268	-	50,50,50	1.16	2 (4%)	51,56,56	1.32	5 (9%)
25	CDL	C	270	-	99,99,99	1.32	13 (13%)	101,111,111	1.32	12 (11%)
22	CHD	C	271	-	29,32,32	0.52	0	48,51,51	2.03	19 (39%)
22	CHD	C	525	-	29,32,32	0.75	0	48,51,51	0.95	1 (2%)
18	TGL	D	523	-	62,62,62	1.25	6 (9%)	65,65,65	1.59	10 (15%)
24	PEK	G	1263	-	51,52,52	1.17	2 (3%)	52,57,57	1.26	6 (11%)
22	CHD	G	229	-	29,32,32	0.78	0	48,51,51	1.52	11 (22%)
24	PEK	G	264	-	51,52,52	0.98	4 (7%)	52,57,57	1.54	10 (19%)
25	CDL	G	269	-	99,99,99	1.33	12 (12%)	101,111,111	1.33	11 (10%)
22	CHD	J	60	-	29,32,32	0.72	0	48,51,51	2.84	22 (45%)
18	TGL	L	522	-	62,62,62	1.32	7 (11%)	65,65,65	1.53	13 (20%)
27	DMU	M	526	-	34,34,34	0.83	1 (2%)	45,45,45	2.49	17 (37%)
19	PGV	N	1266	-	50,50,50	0.83	2 (4%)	51,56,56	1.26	6 (11%)
18	TGL	N	1521	-	62,62,62	1.19	6 (9%)	65,65,65	1.57	9 (13%)
18	TGL	N	1522	-	62,62,62	1.46	7 (11%)	65,65,65	1.63	15 (23%)
19	PGV	N	1524	-	50,50,50	0.99	2 (4%)	51,56,56	1.19	5 (9%)
14	HEA	N	515	1	40,67,67	1.44	5 (12%)	41,103,103	3.41	20 (48%)
14	HEA	N	516	1	40,67,67	1.09	5 (12%)	41,103,103	1.83	13 (31%)
21	PSC	O	1229	-	51,51,51	1.14	3 (5%)	55,59,59	1.01	2 (3%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	P	1267	-	50,50,50	0.75	1 (2%)	51,56,56	1.15	5 (9%)
19	PGV	P	1268	-	50,50,50	1.13	2 (4%)	51,56,56	1.34	5 (9%)
25	CDL	P	1270	-	99,99,99	1.32	12 (12%)	101,111,111	1.38	15 (14%)
22	CHD	P	1271	-	29,32,32	0.55	0	48,51,51	2.02	17 (35%)
22	CHD	P	1525	-	29,32,32	0.87	1 (3%)	48,51,51	1.39	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	TGL	Q	1523	-	62,62,62	1.27	6 (9%)	65,65,65	1.42	11 (16%)
24	PEK	T	1264	-	51,52,52	0.96	4 (7%)	52,57,57	1.45	9 (17%)
24	PEK	T	1265	-	51,52,52	1.24	3 (5%)	52,57,57	1.18	5 (9%)
25	CDL	T	1269	-	99,99,99	1.31	12 (12%)	101,111,111	1.28	9 (8%)
24	PEK	T	263	-	51,52,52	1.20	3 (5%)	52,57,57	1.20	5 (9%)
22	CHD	W	1059	-	29,32,32	0.76	0	48,51,51	3.16	22 (45%)
27	DMU	Z	1526	-	34,34,34	0.83	1 (2%)	45,45,45	2.53	17 (37%)

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	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1	2/2/7/16	0/24/76/76	0/0/8/8
18	TGL	A	521	-	-	0/65/65/65	0/0/0/0
19	PGV	A	522	-	-	0/55/55/55	0/0/0/0
19	PGV	A	524	-	-	1/55/55/55	0/0/0/0
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	PSC	B	229	-	-	0/55/55/55	0/0/0/0
24	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	-	0/7/74/74	0/4/4/4
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
18	TGL	D	523	-	-	0/65/65/65	0/0/0/0
24	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
22	CHD	G	229	-	-	0/7/74/74	0/4/4/4
24	PEK	G	264	-	-	0/56/56/56	0/0/0/0
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
22	CHD	J	60	-	-	0/7/74/74	0/4/4/4
18	TGL	L	522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	526	-	2/2/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	1/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1	2/2/7/16	0/24/76/76	0/0/8/8
21	PSC	O	1229	-	-	0/55/55/55	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
19	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	-	0/7/74/74	0/4/4/4
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
18	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
24	PEK	T	1264	-	-	0/56/56/56	0/0/0/0
24	PEK	T	1265	-	-	0/56/56/56	0/0/0/0
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
24	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1059	-	-	0/7/74/74	0/4/4/4
27	DMU	Z	1526	-	4/4/10/10	0/19/59/59	0/2/2/2

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	515	HEA	C1A-NA	-3.81	1.31	1.36
25	C	270	CDL	C59-C58	-3.46	1.31	1.51
18	L	522	TGL	C20-CA9	-3.45	1.31	1.51
18	N	1521	TGL	C10-CB9	-3.43	1.31	1.51
18	N	1522	TGL	C20-CA9	-3.36	1.32	1.51
25	P	1270	CDL	C59-C58	-3.31	1.32	1.51
25	P	1270	CDL	C79-C78	-3.26	1.32	1.51
25	T	1269	CDL	C59-C58	-3.26	1.32	1.51
25	C	270	CDL	C62-C61	-3.22	1.32	1.51
25	C	270	CDL	C79-C78	-3.20	1.33	1.51
25	G	269	CDL	C59-C58	-3.16	1.33	1.51
25	T	1269	CDL	C42-C41	-3.15	1.33	1.51
24	T	1264	PEK	O01-C02	-3.13	1.38	1.46
25	P	1270	CDL	C62-C61	-3.13	1.33	1.51
18	A	521	TGL	C10-CB9	-3.12	1.33	1.51
27	M	526	DMU	C3-C4	-3.11	1.44	1.52
25	T	1269	CDL	C62-C61	-3.10	1.33	1.51
18	L	522	TGL	C10-CB9	-3.09	1.33	1.51
25	G	269	CDL	C42-C41	-3.08	1.33	1.51
25	C	270	CDL	C82-C81	-3.03	1.34	1.51
25	P	1270	CDL	C82-C81	-3.02	1.34	1.51
25	C	270	CDL	C19-C18	-3.00	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1270	CDL	C19-C18	-2.99	1.34	1.51
18	Q	1523	TGL	C20-CA9	-2.97	1.34	1.51
18	N	1522	TGL	C10-CB9	-2.96	1.34	1.51
18	Q	1523	TGL	C15-CC9	-2.95	1.34	1.51
25	G	269	CDL	C62-C61	-2.94	1.34	1.51
18	D	523	TGL	C20-CA9	-2.94	1.34	1.51
25	G	269	CDL	C22-C21	-2.93	1.34	1.51
25	C	270	CDL	C22-C21	-2.92	1.34	1.51
24	G	264	PEK	O03-C01	-2.90	1.38	1.45
25	P	1270	CDL	C22-C21	-2.89	1.34	1.51
18	D	523	TGL	C15-CC9	-2.87	1.34	1.51
25	G	269	CDL	C39-C38	-2.87	1.35	1.51
25	G	269	CDL	C19-C18	-2.87	1.35	1.51
25	T	1269	CDL	C19-C18	-2.86	1.35	1.51
18	Q	1523	TGL	C10-CB9	-2.84	1.35	1.51
18	A	521	TGL	C20-CA9	-2.83	1.35	1.51
18	D	523	TGL	C10-CB9	-2.81	1.35	1.51
25	T	1269	CDL	C82-C81	-2.81	1.35	1.51
25	T	1269	CDL	C39-C38	-2.79	1.35	1.51
18	N	1521	TGL	C20-CA9	-2.78	1.35	1.51
25	T	1269	CDL	C79-C78	-2.76	1.35	1.51
25	G	269	CDL	C82-C81	-2.73	1.35	1.51
25	T	1269	CDL	C22-C21	-2.71	1.35	1.51
25	G	269	CDL	C79-C78	-2.67	1.36	1.51
25	P	1270	CDL	C39-C38	-2.66	1.36	1.51
25	C	270	CDL	C42-C41	-2.66	1.36	1.51
18	L	522	TGL	C15-CC9	-2.65	1.36	1.51
25	P	1270	CDL	C42-C41	-2.64	1.36	1.51
18	N	1521	TGL	C15-CC9	-2.62	1.36	1.51
25	C	270	CDL	C39-C38	-2.61	1.36	1.51
18	N	1522	TGL	C15-CC9	-2.60	1.36	1.51
14	N	516	HEA	C1A-NA	-2.53	1.33	1.36
27	Z	1526	DMU	C3-C4	-2.49	1.46	1.52
18	A	521	TGL	C15-CC9	-2.49	1.37	1.51
14	N	515	HEA	C4A-NA	-2.36	1.33	1.36
24	T	1264	PEK	O03-C01	-2.31	1.39	1.45
14	A	516	HEA	C4B-NB	-2.29	1.33	1.36
14	A	516	HEA	C1A-NA	-2.21	1.33	1.36
25	C	270	CDL	OB6-CB4	-2.19	1.41	1.46
24	G	264	PEK	O01-C02	-2.08	1.41	1.46
14	A	516	HEA	C4A-NA	-2.04	1.33	1.36
14	A	516	HEA	C1C-CHC	2.02	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	263	PEK	C03-C02	2.04	1.56	1.50
24	T	1265	PEK	C03-C02	2.10	1.56	1.50
14	N	516	HEA	C18-C19	2.11	1.37	1.33
24	G	264	PEK	O03-C21	2.13	1.39	1.33
14	N	516	HEA	C1C-CHC	2.15	1.45	1.39
22	B	1085	CHD	C4-C3	2.17	1.56	1.51
14	A	516	HEA	C14-C15	2.18	1.37	1.33
14	A	515	HEA	C4D-CHA	2.21	1.45	1.39
22	P	1525	CHD	C11-C9	2.21	1.57	1.53
19	C	267	PGV	O01-C1	2.24	1.41	1.34
14	N	516	HEA	C1B-CHB	2.25	1.46	1.39
14	A	516	HEA	C18-C19	2.26	1.37	1.33
18	L	522	TGL	CG1-CG2	2.26	1.57	1.50
22	B	1085	CHD	C6-C7	2.27	1.56	1.52
14	N	516	HEA	C14-C15	2.29	1.37	1.33
14	A	515	HEA	C4C-CHD	2.30	1.46	1.39
18	N	1522	TGL	CG1-CG2	2.34	1.57	1.50
14	A	515	HEA	C12-C13	2.36	1.61	1.53
14	A	515	HEA	C1B-CHB	2.39	1.46	1.39
22	B	1085	CHD	C11-C12	2.46	1.57	1.53
19	N	1266	PGV	O01-C1	2.47	1.41	1.34
14	N	515	HEA	CAD-C3D	2.58	1.56	1.52
24	T	1264	PEK	O03-C21	2.79	1.41	1.33
19	C	267	PGV	O03-C19	2.83	1.41	1.33
19	A	522	PGV	O01-C1	2.84	1.42	1.34
14	N	515	HEA	C4C-CHD	3.03	1.48	1.39
19	A	522	PGV	O03-C19	3.08	1.42	1.33
18	L	522	TGL	OG3-CC1	3.39	1.43	1.33
24	T	1264	PEK	O01-C1	3.45	1.44	1.34
14	N	515	HEA	O11-C11	3.48	1.50	1.42
25	C	270	CDL	OB6-CB5	3.49	1.44	1.34
19	P	1267	PGV	O03-C19	3.52	1.43	1.33
24	G	264	PEK	O01-C1	3.56	1.44	1.34
18	A	521	TGL	OG3-CC1	3.71	1.44	1.33
18	N	1521	TGL	OG1-CA1	3.74	1.44	1.33
25	P	1270	CDL	OB6-CB5	3.82	1.45	1.34
19	N	1524	PGV	O01-C1	3.82	1.45	1.34
21	B	229	PSC	C13-C12	3.83	1.53	1.31
25	P	1270	CDL	OB8-CB7	3.83	1.44	1.33
19	N	1266	PGV	O03-C19	3.89	1.45	1.33
21	O	1229	PSC	C13-C12	3.91	1.54	1.31
19	A	524	PGV	O01-C1	4.04	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	1522	TGL	OG3-CC1	4.13	1.45	1.33
25	T	1269	CDL	OA8-CA7	4.15	1.45	1.33
21	O	1229	PSC	O01-C1	4.17	1.46	1.34
18	N	1521	TGL	OG2-CB1	4.19	1.46	1.34
21	O	1229	PSC	O03-C19	4.22	1.46	1.33
18	N	1521	TGL	OG3-CC1	4.24	1.46	1.33
25	T	1269	CDL	OB6-CB5	4.25	1.47	1.34
25	G	269	CDL	OA8-CA7	4.28	1.46	1.33
18	A	521	TGL	OG2-CB1	4.28	1.47	1.34
18	D	523	TGL	OG2-CB1	4.29	1.47	1.34
21	B	229	PSC	O01-C1	4.33	1.47	1.34
25	T	1269	CDL	OB8-CB7	4.33	1.46	1.33
25	C	270	CDL	OA6-CA5	4.33	1.47	1.34
25	C	270	CDL	OB8-CB7	4.34	1.46	1.33
21	B	229	PSC	O03-C19	4.39	1.46	1.33
18	D	523	TGL	OG1-CA1	4.42	1.46	1.33
25	G	269	CDL	OB8-CB7	4.46	1.46	1.33
18	Q	1523	TGL	OG3-CC1	4.46	1.46	1.33
25	T	1269	CDL	OA6-CA5	4.47	1.47	1.34
24	G	1263	PEK	O01-C1	4.50	1.47	1.34
25	G	269	CDL	OB6-CB5	4.53	1.47	1.34
24	T	263	PEK	O01-C1	4.55	1.47	1.34
18	D	523	TGL	OG3-CC1	4.55	1.47	1.33
18	Q	1523	TGL	OG1-CA1	4.58	1.47	1.33
19	N	1524	PGV	O03-C19	4.59	1.47	1.33
25	P	1270	CDL	OA6-CA5	4.60	1.48	1.34
24	C	265	PEK	O01-C1	4.65	1.48	1.34
19	P	1268	PGV	O03-C19	4.67	1.47	1.33
19	C	268	PGV	O03-C19	4.68	1.47	1.33
18	L	522	TGL	OG1-CA1	4.72	1.47	1.33
18	A	521	TGL	OG1-CA1	4.77	1.47	1.33
25	C	270	CDL	OA8-CA7	4.86	1.48	1.33
25	G	269	CDL	OA6-CA5	4.88	1.48	1.34
18	Q	1523	TGL	OG2-CB1	4.89	1.48	1.34
25	P	1270	CDL	OA8-CA7	4.90	1.48	1.33
24	T	1265	PEK	O03-C21	5.10	1.48	1.33
24	T	1265	PEK	O01-C1	5.10	1.49	1.34
19	C	268	PGV	O01-C1	5.18	1.49	1.34
19	P	1268	PGV	O01-C1	5.24	1.50	1.34
24	C	265	PEK	O03-C21	5.27	1.49	1.33
24	G	1263	PEK	O03-C21	5.44	1.49	1.33
19	A	524	PGV	O03-C19	5.46	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	522	TGL	OG2-CB1	5.47	1.50	1.34
24	T	263	PEK	O03-C21	5.60	1.50	1.33
18	N	1522	TGL	OG2-CB1	5.86	1.51	1.34
18	N	1522	TGL	OG1-CA1	5.97	1.51	1.33

All (403) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C17-C18-C19	-11.55	102.64	127.76
14	A	515	HEA	C17-C18-C19	-11.36	103.05	127.76
22	W	1059	CHD	C17-C13-C14	-6.47	93.51	100.05
22	W	1059	CHD	C18-C13-C12	-6.09	103.15	109.09
22	J	60	CHD	C17-C13-C14	-6.01	93.98	100.05
14	A	516	HEA	CAD-CBD-CGD	-5.59	102.49	112.75
14	A	516	HEA	C13-C12-C11	-4.99	107.89	114.51
14	A	515	HEA	C27-C19-C18	-4.79	114.09	123.50
14	N	515	HEA	C27-C19-C18	-4.72	114.24	123.50
18	L	522	TGL	OG3-CC1-OC1	-4.71	111.33	123.49
14	N	515	HEA	C12-C13-C14	-4.65	99.38	112.40
22	G	229	CHD	C18-C13-C12	-4.65	104.55	109.09
14	A	515	HEA	C12-C13-C14	-4.50	99.81	112.40
14	N	516	HEA	C1A-C2A-C3A	-4.47	102.60	107.07
22	C	271	CHD	C19-C10-C1	-4.40	100.80	108.20
19	A	522	PGV	O03-C19-O04	-4.40	112.14	123.49
24	T	1264	PEK	O03-C01-C02	-4.20	97.40	108.69
22	J	60	CHD	C6-C5-C4	-4.17	106.39	111.05
24	G	264	PEK	O01-C1-O02	-4.00	112.94	123.67
19	N	1266	PGV	O03-C19-O04	-3.99	113.19	123.49
18	D	523	TGL	CG3-CG2-CG1	-3.93	102.87	112.07
22	P	1271	CHD	C18-C13-C12	-3.92	105.27	109.09
14	A	516	HEA	C1A-C2A-C3A	-3.83	103.23	107.07
22	P	1271	CHD	C19-C10-C1	-3.64	102.08	108.20
18	Q	1523	TGL	CG3-CG2-CG1	-3.54	103.79	112.07
22	C	271	CHD	C18-C13-C12	-3.50	105.68	109.09
22	J	60	CHD	C19-C10-C5	-3.46	104.14	110.25
22	W	1059	CHD	C1-C10-C9	-3.36	106.02	111.45
22	C	271	CHD	C23-C22-C20	-3.26	110.91	114.75
24	T	1264	PEK	O01-C1-O02	-3.24	114.96	123.67
14	N	516	HEA	CAA-CBA-CGA	-3.20	106.88	112.75
14	N	515	HEA	OMA-CMA-C3A	-3.18	118.69	125.11
25	P	1270	CDL	OB8-CB7-OB9	-3.17	115.30	123.49
14	A	515	HEA	OMA-CMA-C3A	-3.14	118.76	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	C21-C20-C19	-3.09	102.66	112.71
14	N	515	HEA	C20-C21-C22	-3.09	103.61	111.69
24	G	264	PEK	C24-C23-C22	-3.07	102.04	113.29
22	W	1059	CHD	C6-C5-C4	-3.04	107.66	111.05
22	G	229	CHD	C4-C3-C2	-2.97	106.73	110.52
14	N	515	HEA	C26-C15-C16	-2.97	110.86	115.41
18	N	1521	TGL	CG1-OG1-CA1	-2.96	108.56	116.85
22	W	1059	CHD	C19-C10-C5	-2.94	105.06	110.25
14	A	515	HEA	C20-C21-C22	-2.94	104.00	111.69
22	G	229	CHD	C1-C2-C3	-2.93	105.68	110.43
18	A	521	TGL	CA3-CA2-CA1	-2.92	102.10	113.59
14	N	515	HEA	C13-C14-C15	-2.90	121.45	127.76
22	J	60	CHD	C18-C13-C12	-2.89	106.28	109.09
22	J	60	CHD	C1-C10-C9	-2.85	106.86	111.45
14	N	516	HEA	C20-C19-C18	-2.83	115.67	121.05
25	T	1269	CDL	OA6-CA5-OA7	-2.80	116.15	123.67
22	B	1085	CHD	C19-C10-C5	-2.79	105.33	110.25
18	D	523	TGL	OG2-CB1-OB1	-2.77	116.23	123.67
24	G	264	PEK	O03-C01-C02	-2.74	101.31	108.69
24	C	265	PEK	O03-C21-O04	-2.74	116.42	123.49
24	G	264	PEK	O01-C02-C01	-2.71	98.80	108.36
25	C	270	CDL	CA6-CA4-CA3	-2.71	105.73	112.07
22	G	229	CHD	C6-C5-C4	-2.71	108.02	111.05
14	N	515	HEA	C21-C20-C19	-2.66	104.04	112.71
18	A	521	TGL	OG3-CC1-OC1	-2.66	116.64	123.49
19	N	1266	PGV	O01-C1-O02	-2.64	116.59	123.67
25	C	270	CDL	C52-C51-CB5	-2.62	103.29	113.59
14	A	516	HEA	C20-C19-C18	-2.62	116.08	121.05
22	P	1525	CHD	C10-C9-C8	-2.61	109.02	111.88
18	N	1522	TGL	OB1-CB1-CB2	-2.60	113.32	123.72
22	W	1059	CHD	C23-C22-C20	-2.58	111.71	114.75
19	N	1524	PGV	O03-C19-O04	-2.58	116.83	123.49
25	P	1270	CDL	CB6-CB4-CB3	-2.57	106.07	112.07
19	P	1267	PGV	C27-C26-C25	-2.56	101.29	114.53
14	N	516	HEA	C13-C12-C11	-2.56	111.11	114.51
22	P	1525	CHD	C21-C20-C22	-2.55	106.10	110.35
22	P	1271	CHD	C23-C22-C20	-2.53	111.77	114.75
18	N	1522	TGL	OG3-CC1-OC1	-2.52	117.00	123.49
24	T	1264	PEK	C24-C23-C22	-2.51	104.08	113.29
19	C	267	PGV	C9-C10-C11	-2.51	99.27	112.45
25	G	269	CDL	OA6-CA5-OA7	-2.51	116.93	123.67
18	D	523	TGL	CC3-CC2-CC1	-2.50	103.75	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	1265	PEK	O03-C21-O04	-2.50	117.03	123.49
19	C	267	PGV	C8-C9-C10	-2.49	104.14	113.86
22	P	1271	CHD	C5-C4-C3	-2.49	109.21	112.91
19	A	524	PGV	C4-C3-C2	-2.48	104.19	113.29
25	T	1269	CDL	OA8-CA7-OA9	-2.45	117.16	123.49
19	P	1267	PGV	O01-C1-O02	-2.45	117.10	123.67
22	J	60	CHD	C19-C10-C1	-2.43	104.11	108.20
14	N	516	HEA	CAD-CBD-CGD	-2.43	108.30	112.75
14	N	515	HEA	CAA-CBA-CGA	-2.41	108.33	112.75
24	T	1264	PEK	C30-C29-C28	-2.40	102.15	114.53
14	N	515	HEA	C1A-C2A-C3A	-2.40	104.67	107.07
25	C	270	CDL	C53-C52-C51	-2.39	104.51	113.29
22	G	229	CHD	O3-C3-C4	-2.39	105.11	109.86
19	C	268	PGV	O03-C19-O04	-2.37	117.38	123.49
18	L	522	TGL	CA8-CA7-CA6	-2.34	102.43	114.53
18	A	521	TGL	OB1-CB1-CB2	-2.34	114.36	123.72
14	N	516	HEA	C12-C13-C14	-2.34	105.86	112.40
25	C	270	CDL	OB8-CB7-OB9	-2.33	117.47	123.49
18	A	521	TGL	CG1-OG1-CA1	-2.33	110.34	116.85
25	P	1270	CDL	OA8-CA7-OA9	-2.30	117.55	123.49
24	G	264	PEK	C25-C24-C23	-2.30	102.64	114.53
14	A	515	HEA	CMB-C2B-C1B	-2.30	124.56	128.36
18	Q	1523	TGL	CC3-CC2-CC1	-2.29	104.58	113.59
19	P	1268	PGV	C03-C02-C01	-2.29	106.72	112.07
25	G	269	CDL	OB8-CB7-OB9	-2.27	117.62	123.49
24	T	1264	PEK	C34-C33-C32	-2.27	102.79	114.53
19	N	1524	PGV	C4-C3-C2	-2.27	104.96	113.29
19	P	1267	PGV	C8-C9-C10	-2.26	105.03	113.86
19	C	267	PGV	C4-C3-C2	-2.26	105.01	113.29
18	L	522	TGL	CB4-CB3-CB2	-2.25	105.03	113.29
18	A	521	TGL	CB7-CB6-CB5	-2.25	102.93	114.53
22	B	1085	CHD	O3-C3-C4	-2.24	105.41	109.86
18	L	522	TGL	OB1-CB1-CB2	-2.24	114.76	123.72
24	G	264	PEK	C27-C26-C25	-2.24	102.96	114.53
18	Q	1523	TGL	OG1-CA1-OA1	-2.23	117.73	123.49
22	P	1271	CHD	C14-C8-C9	-2.23	106.55	109.62
19	P	1268	PGV	O03-C19-O04	-2.22	117.77	123.49
18	N	1522	TGL	OA1-CA1-CA2	-2.20	114.94	123.72
14	A	516	HEA	C21-C22-C23	-2.20	119.28	127.73
22	P	1525	CHD	C6-C5-C4	-2.18	108.61	111.05
19	P	1268	PGV	O02-C1-C2	-2.16	115.08	123.72
18	N	1521	TGL	CB7-CB6-CB5	-2.15	103.41	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C25-C23-C22	-2.14	115.72	122.61
25	C	270	CDL	C57-C56-C55	-2.12	103.61	114.53
19	C	268	PGV	O02-C1-C2	-2.11	115.28	123.72
24	G	264	PEK	C32-C31-C30	-2.11	103.65	114.53
24	G	1263	PEK	O03-C21-O04	-2.11	118.06	123.49
18	N	1522	TGL	C25-C24-C23	-2.10	103.69	114.53
18	D	523	TGL	OG1-CA1-OA1	-2.10	118.08	123.49
27	Z	1526	DMU	C10-O1-C9	-2.09	109.68	113.75
25	G	269	CDL	OA8-CA7-OA9	-2.09	118.09	123.49
24	T	1264	PEK	C28-C27-C26	-2.09	103.75	114.53
25	P	1270	CDL	C53-C52-C51	-2.09	105.63	113.29
22	C	271	CHD	C5-C4-C3	-2.08	109.81	112.91
14	N	515	HEA	CAD-CBD-CGD	-2.07	108.95	112.75
25	P	1270	CDL	CA6-CA4-CA3	-2.06	107.25	112.07
19	N	1266	PGV	C01-O03-C19	-2.05	111.13	116.85
25	P	1270	CDL	OA6-CA5-OA7	-2.05	118.18	123.67
22	P	1525	CHD	C9-C11-C12	-2.04	111.78	114.36
19	P	1267	PGV	C25-C24-C23	-2.04	103.99	114.53
22	B	1085	CHD	C13-C17-C20	-2.04	117.02	119.50
14	A	516	HEA	C3C-CAC-CBC	-2.03	122.16	126.32
22	P	1525	CHD	C16-C15-C14	-2.03	101.04	105.12
22	G	229	CHD	O12-C12-C13	-2.02	107.83	111.11
22	G	229	CHD	C13-C14-C8	-2.02	112.15	114.75
19	P	1267	PGV	C4-C3-C2	-2.01	105.91	113.29
22	C	271	CHD	C22-C23-C24	-2.01	104.83	113.02
25	P	1270	CDL	OA8-CA6-CA4	2.00	114.08	108.69
14	A	516	HEA	C21-C20-C19	2.00	119.23	112.71
18	N	1522	TGL	C15-CC9-CC8	2.00	124.87	114.53
25	P	1270	CDL	C42-C41-C40	2.01	124.93	114.53
18	N	1522	TGL	CC3-CC2-CC1	2.03	121.56	113.59
22	J	60	CHD	O7-C7-C8	2.03	113.74	109.26
19	A	524	PGV	C02-O01-C1	2.03	122.77	117.89
18	A	521	TGL	C21-C20-CA9	2.03	125.04	114.53
18	Q	1523	TGL	C11-C10-CB9	2.04	125.06	114.53
25	P	1270	CDL	C40-C39-C38	2.05	125.10	114.53
25	T	1269	CDL	OB8-CB6-CB4	2.05	114.21	108.69
27	Z	1526	DMU	O55-C2-C3	2.06	114.75	109.87
18	L	522	TGL	CG1-OG1-CA1	2.06	122.62	116.85
22	G	229	CHD	C5-C6-C7	2.07	116.74	114.44
25	C	270	CDL	C42-C41-C40	2.07	125.21	114.53
18	L	522	TGL	C15-CC9-CC8	2.08	125.26	114.53
25	T	1269	CDL	C83-C82-C81	2.08	125.29	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	229	CHD	C18-C13-C14	2.09	114.51	111.22
25	C	270	CDL	C40-C39-C38	2.09	125.34	114.53
22	P	1271	CHD	O7-C7-C8	2.10	113.89	109.26
25	P	1270	CDL	OA4-PA1-OA3	2.10	123.91	112.53
14	N	516	HEA	CBD-CAD-C3D	2.13	116.34	112.53
27	M	526	DMU	C57-C4-C3	2.13	119.44	113.25
18	Q	1523	TGL	OG1-CG1-CG2	2.13	114.43	108.69
27	M	526	DMU	C6-C1-C2	2.13	114.17	109.97
14	A	516	HEA	CMC-C2C-C3C	2.14	129.27	125.09
22	W	1059	CHD	C11-C9-C8	2.16	113.80	110.73
25	G	269	CDL	C83-C82-C81	2.18	125.77	114.53
14	A	516	HEA	C27-C19-C20	2.18	118.74	115.41
25	T	1269	CDL	C82-C81-C80	2.18	125.80	114.53
22	C	271	CHD	C16-C17-C13	2.20	105.79	103.60
22	P	1271	CHD	C6-C5-C10	2.20	115.08	112.66
14	N	515	HEA	C3B-C4B-NB	2.21	115.12	110.94
18	L	522	TGL	OG2-CG2-CG1	2.21	116.16	108.36
22	B	1085	CHD	C14-C8-C7	2.21	114.81	111.74
19	C	267	PGV	C01-O03-C19	2.22	123.06	116.85
18	N	1522	TGL	OG2-CG2-CG1	2.22	116.20	108.36
27	Z	1526	DMU	C11-C9-C8	2.23	118.51	113.02
18	N	1522	TGL	C11-C10-CB9	2.23	126.04	114.53
19	A	524	PGV	O03-C01-C02	2.23	114.70	108.69
19	A	524	PGV	C01-O03-C19	2.24	123.10	116.85
18	L	522	TGL	OG1-CG1-CG2	2.24	114.72	108.69
19	N	1266	PGV	O01-C1-C2	2.24	116.40	111.53
24	T	1265	PEK	O03-C01-C02	2.25	114.73	108.69
25	G	269	CDL	CA6-OA8-CA7	2.25	123.13	116.85
22	G	229	CHD	C11-C9-C8	2.25	113.92	110.73
22	P	1271	CHD	C18-C13-C14	2.29	114.83	111.22
27	M	526	DMU	O3-C5-C7	2.30	115.52	110.34
22	C	271	CHD	C15-C14-C13	2.30	105.89	103.60
22	J	60	CHD	C17-C13-C12	2.32	119.74	117.68
18	N	1521	TGL	C21-C20-CA9	2.33	126.57	114.53
18	A	521	TGL	OG1-CA1-CA2	2.33	119.01	111.90
22	C	271	CHD	C9-C10-C5	2.34	112.13	108.67
24	G	264	PEK	O01-C1-C2	2.35	116.63	111.53
24	T	1264	PEK	O13-P-O14	2.35	125.28	112.53
27	Z	1526	DMU	C10-C5-C7	2.36	114.62	109.97
24	C	265	PEK	C24-C23-C22	2.36	121.95	113.29
22	J	60	CHD	C14-C8-C7	2.36	115.02	111.74
19	C	267	PGV	O01-C1-C2	2.38	116.70	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	1523	TGL	OG2-CG2-CG3	2.40	116.82	108.36
22	C	271	CHD	C11-C12-C13	2.40	113.64	111.20
18	N	1521	TGL	OG1-CG1-CG2	2.42	115.21	108.69
24	G	264	PEK	C01-O03-C21	2.42	123.63	116.85
22	W	1059	CHD	C4-C3-C2	2.43	113.61	110.52
25	P	1270	CDL	C39-C38-C37	2.43	127.07	114.53
22	P	1525	CHD	C14-C8-C9	2.43	112.96	109.62
22	P	1271	CHD	C15-C14-C8	2.45	121.87	118.32
22	C	271	CHD	C6-C5-C10	2.45	115.36	112.66
25	C	270	CDL	C39-C38-C37	2.48	127.31	114.53
24	T	1264	PEK	O01-C1-C2	2.48	116.92	111.53
14	N	516	HEA	C20-C21-C22	2.48	118.19	111.69
19	C	268	PGV	C01-O03-C19	2.49	123.83	116.85
19	N	1524	PGV	C01-O03-C19	2.50	123.84	116.85
14	A	515	HEA	CMC-C2C-C3C	2.51	130.00	125.09
14	A	516	HEA	C4B-C3B-C11	2.55	129.78	127.01
22	C	271	CHD	C14-C13-C12	2.57	109.69	107.39
14	A	516	HEA	C3C-C4C-NC	2.57	112.53	109.21
19	N	1266	PGV	O03-C01-C02	2.57	115.62	108.69
25	T	1269	CDL	CB6-OB8-CB7	2.58	124.05	116.85
27	Z	1526	DMU	O3-C5-C7	2.58	116.14	110.34
22	C	525	CHD	C6-C7-C8	2.59	114.22	111.47
22	J	60	CHD	C18-C13-C17	2.59	115.30	111.22
14	N	516	HEA	C4B-C3B-C11	2.59	129.82	127.01
21	B	229	PSC	O03-C19-C20	2.60	119.81	111.90
25	G	269	CDL	CB6-OB8-CB7	2.62	124.19	116.85
14	A	515	HEA	C3C-C4C-NC	2.64	112.62	109.21
24	T	263	PEK	C02-O01-C1	2.65	124.25	117.89
19	A	524	PGV	O03-C19-C20	2.66	119.99	111.90
18	Q	1523	TGL	CG2-OG2-CB1	2.66	124.26	117.89
24	C	265	PEK	C01-O03-C21	2.66	124.28	116.85
27	Z	1526	DMU	C7-C8-C9	2.66	114.83	110.20
25	G	269	CDL	C80-C79-C78	2.67	128.30	114.53
25	P	1270	CDL	OB6-CB5-C51	2.67	117.33	111.53
14	A	516	HEA	C25-C23-C24	2.69	121.24	114.64
18	N	1522	TGL	OG1-CG1-CG2	2.70	115.94	108.69
24	T	263	PEK	O03-C01-C02	2.70	115.96	108.69
22	C	271	CHD	O7-C7-C8	2.70	115.22	109.26
27	M	526	DMU	C10-C5-C7	2.70	115.30	109.97
22	W	1059	CHD	C4-C5-C10	2.71	115.65	112.66
22	B	1085	CHD	C1-C10-C5	2.72	112.28	107.81
21	O	1229	PSC	O01-C1-C2	2.74	117.49	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	526	DMU	C1-C2-C3	2.74	115.63	109.60
22	B	1085	CHD	C15-C14-C13	2.75	106.33	103.60
18	Q	1523	TGL	OG3-CC1-CC2	2.76	120.31	111.90
18	D	523	TGL	CB3-CB2-CB1	2.76	124.46	113.59
14	N	516	HEA	C27-C19-C20	2.78	119.65	115.41
14	N	515	HEA	C16-C15-C14	2.78	126.32	121.05
22	B	1085	CHD	C22-C20-C17	2.79	116.11	110.24
22	C	271	CHD	C15-C14-C8	2.81	122.40	118.32
24	T	1264	PEK	C01-O03-C21	2.81	124.72	116.85
19	A	524	PGV	O01-C02-C01	2.81	118.28	108.36
27	M	526	DMU	C7-C8-C9	2.83	115.12	110.20
22	P	1271	CHD	C9-C10-C5	2.83	112.86	108.67
25	G	269	CDL	OA8-CA7-C31	2.84	120.54	111.90
18	A	521	TGL	OG3-CC1-CC2	2.85	120.57	111.90
18	N	1521	TGL	OG1-CA1-CA2	2.88	120.66	111.90
22	C	271	CHD	C5-C6-C7	2.88	117.65	114.44
22	J	60	CHD	C5-C6-C7	2.90	117.67	114.44
22	B	1085	CHD	C4-C3-C2	2.91	114.23	110.52
18	D	523	TGL	OG1-CA1-CA2	2.92	120.78	111.90
22	C	271	CHD	C6-C7-C8	2.93	114.57	111.47
25	C	270	CDL	OA8-CA6-CA4	2.93	116.58	108.69
18	A	521	TGL	OG2-CG2-CG1	2.93	118.69	108.36
22	P	1271	CHD	C6-C7-C8	2.93	114.58	111.47
18	L	522	TGL	CC3-CC2-CC1	2.94	125.14	113.59
18	L	522	TGL	OG2-CB1-CB2	2.96	117.97	111.53
18	A	521	TGL	OG2-CG2-CG3	2.97	118.82	108.36
25	C	270	CDL	OA8-CA7-C31	2.97	120.94	111.90
18	L	522	TGL	OG1-CA1-CA2	2.97	120.96	111.90
18	N	1522	TGL	OG3-CC1-CC2	2.99	121.00	111.90
22	P	1271	CHD	C16-C17-C13	3.00	106.58	103.60
22	W	1059	CHD	C10-C9-C8	3.01	115.19	111.88
18	N	1522	TGL	CG3-OG3-CC1	3.03	125.31	116.85
27	M	526	DMU	C11-C9-C8	3.03	120.50	113.02
27	Z	1526	DMU	O7-C3-C4	3.05	117.33	109.32
22	P	1271	CHD	C1-C10-C5	3.06	112.83	107.81
24	T	263	PEK	C01-O03-C21	3.09	125.49	116.85
21	O	1229	PSC	O03-C19-C20	3.09	121.33	111.90
22	W	1059	CHD	C1-C10-C5	3.10	112.90	107.81
25	G	269	CDL	C79-C78-C77	3.12	130.64	114.53
27	Z	1526	DMU	C57-C4-C3	3.13	122.35	113.25
24	G	1263	PEK	C01-O03-C21	3.14	125.63	116.85
18	N	1521	TGL	OG2-CB1-CB2	3.16	118.40	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	1523	TGL	OG1-CA1-CA2	3.17	121.56	111.90
22	G	229	CHD	C10-C9-C8	3.17	115.37	111.88
14	A	515	HEA	C12-C11-C3B	3.18	119.16	112.59
24	C	265	PEK	O01-C1-C2	3.19	118.47	111.53
18	D	523	TGL	OG3-CC1-CC2	3.20	121.66	111.90
22	J	60	CHD	C4-C3-C2	3.21	114.62	110.52
25	P	1270	CDL	OA8-CA7-C31	3.22	121.72	111.90
27	Z	1526	DMU	C2-C3-C4	3.23	118.15	110.84
14	A	515	HEA	C16-C17-C18	3.24	120.18	111.69
22	C	271	CHD	C1-C10-C5	3.24	113.14	107.81
27	M	526	DMU	O16-C6-C1	3.29	112.19	108.04
22	J	60	CHD	C16-C17-C20	3.29	117.92	112.05
25	T	1269	CDL	OA8-CA7-C31	3.30	121.96	111.90
22	W	1059	CHD	C5-C6-C7	3.33	118.15	114.44
24	G	1263	PEK	O01-C1-C2	3.34	118.79	111.53
14	N	516	HEA	C12-C11-C3B	3.34	119.51	112.59
24	T	1265	PEK	C01-O03-C21	3.35	126.20	116.85
24	G	1263	PEK	C02-O01-C1	3.40	126.04	117.89
24	G	1263	PEK	O03-C01-C02	3.40	117.85	108.69
14	N	516	HEA	C17-C18-C19	3.40	135.17	127.76
22	P	1271	CHD	C15-C14-C13	3.44	107.02	103.60
24	T	263	PEK	O01-C1-C2	3.47	119.07	111.53
14	A	516	HEA	C17-C18-C19	3.48	135.32	127.76
25	P	1270	CDL	OB8-CB7-C71	3.53	122.66	111.90
22	J	60	CHD	C4-C5-C10	3.54	116.55	112.66
18	Q	1523	TGL	CG3-OG3-CC1	3.55	126.78	116.85
25	C	270	CDL	OB8-CB7-C71	3.56	122.73	111.90
22	P	1525	CHD	C15-C14-C13	3.56	107.14	103.60
19	N	1524	PGV	O03-C19-C20	3.57	122.78	111.90
22	W	1059	CHD	C5-C4-C3	3.58	118.25	112.91
18	L	522	TGL	CG2-OG2-CB1	3.60	126.52	117.89
22	C	271	CHD	C10-C9-C8	3.60	115.83	111.88
22	W	1059	CHD	C17-C13-C12	3.61	120.88	117.68
22	P	1271	CHD	C10-C9-C8	3.66	115.90	111.88
14	N	516	HEA	C3C-C4C-NC	3.66	113.95	109.21
27	M	526	DMU	O5-C4-C3	3.68	117.52	109.75
19	N	1524	PGV	O01-C1-C2	3.69	119.54	111.53
22	W	1059	CHD	C22-C20-C17	3.70	118.01	110.24
22	W	1059	CHD	C18-C13-C17	3.76	117.14	111.22
24	G	264	PEK	C2-C3-C4	3.76	120.79	113.30
24	T	1265	PEK	O03-C21-C22	3.80	123.47	111.90
18	N	1522	TGL	OG2-CB1-CB2	3.80	119.79	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	526	DMU	C8-C7-C5	3.81	117.90	110.79
18	D	523	TGL	CG3-OG3-CC1	3.82	127.52	116.85
24	T	1265	PEK	O01-C1-C2	3.83	119.85	111.53
27	Z	1526	DMU	O1-C10-C5	3.83	118.14	110.28
18	N	1521	TGL	OG2-CG2-CG3	3.88	122.03	108.36
18	N	1522	TGL	OG1-CA1-CA2	3.90	123.80	111.90
18	L	522	TGL	OG3-CC1-CC2	3.92	123.84	111.90
14	A	515	HEA	C20-C19-C18	3.94	128.52	121.05
22	C	271	CHD	C1-C2-C3	3.94	116.82	110.43
21	B	229	PSC	O01-C1-C2	3.97	120.16	111.53
22	C	271	CHD	C2-C1-C10	3.97	119.93	112.84
24	T	263	PEK	O03-C21-C22	3.98	124.04	111.90
18	A	521	TGL	CG3-OG3-CC1	4.00	128.05	116.85
14	N	515	HEA	CBA-CAA-C2A	4.01	119.71	112.53
22	J	60	CHD	C22-C20-C17	4.04	118.72	110.24
22	J	60	CHD	C14-C13-C12	4.14	111.10	107.39
22	J	60	CHD	C1-C10-C5	4.15	114.62	107.81
24	C	265	PEK	O03-C21-C22	4.16	124.57	111.90
18	D	523	TGL	OG1-CG1-CG2	4.20	119.99	108.69
19	A	522	PGV	O03-C19-C20	4.21	124.72	111.90
27	Z	1526	DMU	O5-C4-C3	4.21	118.65	109.75
19	C	268	PGV	O03-C19-C20	4.26	124.87	111.90
18	A	521	TGL	OG1-CG1-CG2	4.28	120.22	108.69
24	G	1263	PEK	O03-C21-C22	4.34	125.13	111.90
27	Z	1526	DMU	C8-C7-C5	4.37	118.95	110.79
19	P	1268	PGV	O03-C19-C20	4.38	125.25	111.90
14	N	515	HEA	C12-C11-C3B	4.40	121.69	112.59
22	J	60	CHD	C5-C4-C3	4.41	119.48	112.91
18	A	521	TGL	OG2-CB1-CB2	4.42	121.12	111.53
14	N	515	HEA	C20-C19-C18	4.42	129.43	121.05
18	N	1522	TGL	CG2-OG2-CB1	4.44	128.54	117.89
22	P	1271	CHD	C1-C2-C3	4.47	117.68	110.43
19	N	1266	PGV	O03-C19-C20	4.47	125.51	111.90
18	N	1522	TGL	CG1-OG1-CA1	4.48	129.37	116.85
27	Z	1526	DMU	O5-C4-C57	4.62	118.03	106.36
22	P	1271	CHD	C2-C1-C10	4.66	121.16	112.84
25	T	1269	CDL	OB6-CB5-C51	4.72	121.79	111.53
27	M	526	DMU	O5-C6-C1	4.73	119.98	110.28
27	M	526	DMU	O1-C9-C11	4.73	118.31	106.36
27	M	526	DMU	O1-C9-C8	4.75	118.59	109.68
14	N	515	HEA	C4B-C3B-C11	4.77	132.19	127.01
27	M	526	DMU	O1-C10-C5	4.78	120.08	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	270	CDL	OA6-CA5-C11	4.85	122.06	111.53
27	M	526	DMU	O7-C3-C2	4.85	119.68	107.17
25	T	1269	CDL	OA6-CA5-C11	4.88	122.13	111.53
18	N	1521	TGL	CG3-OG3-CC1	4.92	130.60	116.85
25	G	269	CDL	OB6-CB5-C51	4.96	122.31	111.53
14	A	515	HEA	C4B-C3B-C11	4.98	132.42	127.01
18	Q	1523	TGL	OG2-CB1-CB2	5.01	122.41	111.53
27	Z	1526	DMU	O1-C9-C11	5.04	119.09	106.36
22	J	60	CHD	C9-C10-C5	5.11	116.24	108.67
22	J	60	CHD	C10-C9-C8	5.13	117.51	111.88
25	G	269	CDL	OA6-CA5-C11	5.19	122.81	111.53
27	M	526	DMU	C2-C3-C4	5.23	122.67	110.84
25	P	1270	CDL	OA6-CA5-C11	5.27	122.98	111.53
27	M	526	DMU	O5-C4-C57	5.30	119.75	106.36
18	D	523	TGL	OG2-CB1-CB2	5.31	123.06	111.53
27	Z	1526	DMU	O5-C6-C1	5.33	121.22	110.28
27	Z	1526	DMU	O1-C9-C8	5.34	119.70	109.68
22	W	1059	CHD	C9-C11-C12	5.37	121.15	114.36
22	W	1059	CHD	C9-C10-C5	5.48	116.78	108.67
19	C	268	PGV	O01-C1-C2	5.53	123.54	111.53
22	W	1059	CHD	C6-C5-C10	5.87	119.12	112.66
22	W	1059	CHD	C14-C13-C12	6.05	112.81	107.39
19	P	1268	PGV	O01-C1-C2	6.12	124.82	111.53
22	J	60	CHD	C13-C17-C20	6.15	127.00	119.50
18	N	1521	TGL	CG2-OG2-CB1	6.21	132.78	117.89
14	N	515	HEA	CAD-C3D-C4D	6.41	133.96	127.01
27	Z	1526	DMU	O7-C3-C2	6.49	123.93	107.17
22	J	60	CHD	C6-C5-C10	6.80	120.15	112.66
22	W	1059	CHD	C11-C12-C13	6.83	118.14	111.20
18	A	521	TGL	CG2-OG2-CB1	7.23	135.23	117.89
22	W	1059	CHD	C13-C17-C20	7.52	128.65	119.50
14	A	515	HEA	C17-C16-C15	8.16	139.29	112.71
14	N	515	HEA	C17-C16-C15	8.94	141.84	112.71

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	Z	1526	DMU	C2
27	Z	1526	DMU	C3
27	Z	1526	DMU	C5
27	Z	1526	DMU	C4
14	A	516	HEA	ND

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Mol	Chain	Res	Type	Atom
14	A	516	HEA	NB
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
27	M	526	DMU	C2
27	M	526	DMU	C5
14	A	515	HEA	ND
14	A	515	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NB

All (2) torsion outliers are listed below:

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

There are no ring outliers.

35 monomers are involved in 238 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	5	0
14	A	516	HEA	1	0
18	A	521	TGL	6	0
19	A	522	PGV	1	0
19	A	524	PGV	9	0
22	B	1085	CHD	1	0
21	B	229	PSC	13	0
24	C	265	PEK	5	0
19	C	267	PGV	5	0
19	C	268	PGV	3	0
25	C	270	CDL	17	0
22	C	271	CHD	3	0
18	D	523	TGL	6	0
24	G	1263	PEK	8	0
24	G	264	PEK	4	0
25	G	269	CDL	18	0
22	J	60	CHD	3	0
18	L	522	TGL	15	0
19	N	1266	PGV	2	0
18	N	1521	TGL	9	0
18	N	1522	TGL	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	1524	PGV	8	0
14	N	515	HEA	6	0
14	N	516	HEA	3	0
21	O	1229	PSC	17	0
19	P	1267	PGV	2	0
19	P	1268	PGV	4	0
25	P	1270	CDL	14	0
22	P	1271	CHD	1	0
18	Q	1523	TGL	4	0
24	T	1264	PEK	6	0
24	T	1265	PEK	6	0
25	T	1269	CDL	22	0
24	T	263	PEK	9	0
22	W	1059	CHD	3	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.05	1 (0%) 95 97	15, 20, 27, 56	0
1	N	513/514 (99%)	-0.04	1 (0%) 95 97	17, 22, 29, 55	0
2	B	226/227 (99%)	-0.03	2 (0%) 85 89	14, 24, 51, 74	0
2	O	226/227 (99%)	0.06	8 (3%) 48 56	19, 27, 54, 72	0
3	C	259/261 (99%)	0.04	1 (0%) 93 95	16, 22, 33, 52	0
3	P	259/261 (99%)	0.01	1 (0%) 93 95	17, 23, 36, 55	0
4	D	144/147 (97%)	-0.27	1 (0%) 89 92	17, 25, 44, 70	0
4	Q	144/147 (97%)	0.80	14 (9%) 10 14	24, 35, 59, 101	0
5	E	105/109 (96%)	-0.28	2 (1%) 70 76	16, 23, 51, 89	0
5	R	105/109 (96%)	0.19	4 (3%) 44 53	20, 27, 60, 91	0
6	F	98/98 (100%)	0.38	7 (7%) 19 26	18, 28, 75, 110	0
6	S	98/98 (100%)	0.61	8 (8%) 14 20	16, 26, 79, 108	0
7	G	83/85 (97%)	0.85	18 (21%) 1 2	16, 28, 95, 99	0
7	T	83/85 (97%)	1.00	18 (21%) 1 2	18, 29, 96, 100	0
8	H	79/85 (92%)	0.49	10 (12%) 5 8	20, 31, 79, 104	0
8	U	79/85 (92%)	0.60	11 (13%) 4 6	22, 32, 80, 105	0
9	I	72/73 (98%)	0.19	3 (4%) 40 49	19, 34, 58, 67	0
9	V	72/73 (98%)	0.33	6 (8%) 14 20	20, 39, 59, 83	0
10	J	58/59 (98%)	0.24	3 (5%) 31 39	22, 31, 60, 94	0
10	W	58/59 (98%)	0.26	3 (5%) 31 39	21, 32, 65, 99	0
11	K	49/56 (87%)	-0.11	0 100 100	23, 30, 40, 54	0
11	X	49/56 (87%)	0.29	2 (4%) 41 50	28, 36, 51, 66	0
12	L	46/47 (97%)	0.03	1 (2%) 65 73	19, 26, 50, 74	0
12	Y	46/47 (97%)	0.09	1 (2%) 65 73	21, 28, 54, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.01	1 (2%) 64 72	18, 24, 67, 94	0
13	Z	43/46 (93%)	0.34	5 (11%) 6 10	25, 31, 77, 98	0
All	All	3550/3614 (98%)	0.15	132 (3%) 45 54	14, 24, 55, 110	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	24.4
4	Q	5	VAL	22.8
4	Q	6	VAL	18.4
4	Q	4	SER	18.3
6	F	97	ALA	10.9
6	S	98	HIS	9.9
13	Z	43	SER	9.6
6	F	96	LEU	9.6
6	F	98	HIS	9.0
4	Q	8	SER	8.7
6	S	94	HIS	8.7
7	T	8	HIS	8.7
6	F	1	ALA	8.5
10	W	58	LYS	8.2
10	J	58	LYS	7.5
7	G	8	HIS	7.3
9	I	37	PHE	7.2
13	Z	42	LYS	7.2
5	R	5	HIS	7.0
4	Q	7	LYS	7.0
5	R	109	VAL	7.0
8	U	7	LYS	6.9
6	S	1	ALA	6.8
3	P	3	HIS	6.7
8	H	7	LYS	6.0
11	X	6	ALA	6.0
2	O	226	MET	6.0
7	T	2	SER	5.9
7	T	42	ARG	5.7
6	S	96	LEU	5.7
8	H	47	GLY	5.7
6	F	95	GLN	5.7
7	T	3	ALA	5.7
7	T	40	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
8	H	46	LYS	5.5
10	J	1	PHE	5.5
7	G	3	ALA	5.4
7	T	7	ASP	5.3
6	S	95	GLN	5.1
8	U	8	ILE	5.0
9	V	2	THR	5.0
7	T	10	GLY	4.9
7	T	36	TRP	4.9
7	T	5	LYS	4.9
5	E	5	HIS	4.8
7	G	42	ARG	4.8
2	O	227	LEU	4.7
7	G	36	TRP	4.6
7	G	6	GLY	4.6
7	G	5	LYS	4.6
7	G	4	ALA	4.5
2	O	90	ILE	4.5
10	W	57	HIS	4.5
12	L	2	HIS	4.4
12	Y	47	LYS	4.3
6	S	2	SER	4.3
7	T	84	LYS	4.3
7	G	2	SER	4.3
7	T	1	ALA	4.2
8	H	45	ALA	4.1
7	G	39	SER	4.1
8	U	45	ALA	4.1
2	O	113	TYR	4.0
4	Q	35	ALA	4.0
8	H	8	ILE	4.0
13	Z	41	LYS	3.9
5	E	109	VAL	3.7
8	U	47	GLY	3.7
8	H	48	GLY	3.7
7	T	4	ALA	3.7
6	F	94	HIS	3.6
7	G	7	ASP	3.5
13	M	43	SER	3.5
2	O	91	ASN	3.5
6	F	2	SER	3.4
9	V	37	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
7	T	39	SER	3.3
7	G	43	GLU	3.2
8	U	46	LYS	3.2
4	Q	39	ALA	3.2
8	U	48	GLY	3.2
4	Q	10	ASP	3.2
6	S	93	PRO	3.1
9	V	3	ALA	2.9
4	Q	58	GLU	2.9
5	R	108	LYS	2.9
7	G	41	HIS	2.9
8	U	44	THR	2.8
4	Q	33	LEU	2.8
8	H	10	ASN	2.8
2	O	59	GLN	2.8
7	G	40	GLY	2.8
8	H	49	ASP	2.8
8	H	44	THR	2.8
7	T	12	GLY	2.7
9	I	25	PHE	2.7
9	V	5	ALA	2.6
11	X	7	PRO	2.6
7	G	9	GLY	2.6
10	J	57	HIS	2.6
13	Z	40	TYR	2.6
7	G	10	GLY	2.6
7	G	84	LYS	2.5
4	Q	31	LYS	2.5
7	T	9	GLY	2.5
7	T	41	HIS	2.5
2	B	59	GLN	2.5
8	U	49	ASP	2.5
4	Q	28	ALA	2.4
7	T	33	LEU	2.4
9	V	15	ARG	2.4
9	V	73	LYS	2.3
8	H	9	LYS	2.3
4	Q	51	LEU	2.3
8	U	52	VAL	2.3
7	G	45	PRO	2.3
3	C	3	HIS	2.3
2	O	217	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	513	LEU	2.3
7	G	37	LEU	2.2
13	Z	39	ASN	2.2
7	T	6	GLY	2.1
2	O	130	PRO	2.1
4	Q	147	LYS	2.1
10	W	48	TYR	2.1
1	A	513	LEU	2.1
5	R	79	LYS	2.1
8	U	9	LYS	2.1
2	B	91	ASN	2.0
8	U	10	ASN	2.0
4	D	147	LYS	2.0
9	I	18	ARG	2.0

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	0.97	0.20	-	25,26,33,38	0
7	TPO	G	11	11/12	0.44	0.36	-	63,71,87,88	0
2	FME	B	1	10/11	0.95	0.17	-	23,24,33,45	0
9	SAC	V	1	9/10	0.48	0.58	-	88,90,91,91	0
1	FME	N	1	10/11	0.94	0.21	-	37,41,58,60	0
7	TPO	T	11	11/12	0.52	0.36	-	66,73,89,89	0
9	SAC	I	1	9/10	0.56	0.44	-	76,79,82,83	0
1	FME	A	1	10/11	0.89	0.17	-	36,39,58,66	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
25	CDL	P	1270	100/100	0.73	0.36	15.67	45,85,107,109	0
25	CDL	C	270	100/100	0.75	0.36	13.76	42,84,106,108	0
19	PGV	A	524	51/51	0.74	0.30	11.73	34,69,94,96	0
22	CHD	J	60	29/29	0.52	0.41	11.47	99,107,110,111	0
22	CHD	W	1059	29/29	0.48	0.42	10.76	95,105,107,107	0
19	PGV	N	1524	51/51	0.70	0.34	10.57	43,69,102,102	0
18	TGL	L	522	63/63	0.74	0.30	8.15	38,62,80,83	0
18	TGL	N	1521	63/63	0.79	0.27	7.73	48,73,88,91	0
19	PGV	P	1268	51/51	0.59	0.34	7.04	77,90,102,103	0
18	TGL	D	523	63/63	0.75	0.26	6.00	50,69,91,91	0
18	TGL	A	521	63/63	0.82	0.25	5.78	50,70,88,92	0
18	TGL	N	1522	63/63	0.64	0.32	5.62	47,71,84,86	0
14	HEA	N	515	60/60	0.95	0.19	4.60	20,33,50,53	0
18	TGL	Q	1523	63/63	0.64	0.28	3.68	49,74,91,92	0
25	CDL	G	269	100/100	0.61	0.36	3.45	65,85,106,111	0
22	CHD	P	1271	29/29	0.74	0.24	3.31	82,90,91,91	0
19	PGV	P	1267	51/51	0.97	0.18	3.25	19,29,65,69	0
24	PEK	G	264	53/53	0.95	0.18	3.12	17,41,71,72	0
25	CDL	T	1269	100/100	0.56	0.36	2.91	56,86,108,109	0
27	DMU	Z	1526	33/33	0.92	0.18	2.90	37,45,57,57	0
19	PGV	C	267	51/51	0.96	0.18	2.89	17,29,64,69	0
21	PSC	B	229	52/52	0.67	0.33	2.87	48,92,113,115	0
19	PGV	C	268	51/51	0.61	0.32	2.66	63,88,101,102	0
21	PSC	O	1229	52/52	0.66	0.35	2.45	40,85,110,113	0
19	PGV	N	1266	51/51	0.97	0.17	2.33	19,38,57,59	0
24	PEK	T	1264	53/53	0.94	0.16	1.77	19,44,71,73	0
19	PGV	A	522	51/51	0.97	0.17	1.54	19,32,54,56	0
24	PEK	T	1265	53/53	0.54	0.34	1.51	42,90,101,102	0
14	HEA	A	515	60/60	0.98	0.16	1.46	14,19,41,50	0
26	ZN	S	99	1/1	0.99	0.14	1.46	23,23,23,23	0
24	PEK	T	263	53/53	0.47	0.42	1.34	51,91,109,111	0
24	PEK	C	265	53/53	0.53	0.32	1.21	43,91,99,100	0
24	PEK	G	1263	53/53	0.58	0.37	1.18	55,94,110,110	0
22	CHD	C	271	29/29	0.76	0.26	1.06	79,89,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	ZN	F	99	1/1	0.99	0.15	0.97	23,23,23,23	0
14	HEA	N	516	60/60	0.98	0.14	0.65	15,19,26,30	0
20	CUA	B	228	2/2	0.99	0.14	0.42	18,18,18,18	0
27	DMU	M	526	33/33	0.92	0.13	0.28	34,40,51,52	0
14	HEA	A	516	60/60	0.98	0.14	-0.02	11,18,24,26	0
22	CHD	C	525	29/29	0.96	0.13	-0.62	24,29,32,33	0
22	CHD	B	1085	29/29	0.97	0.11	-0.62	12,15,23,33	0
22	CHD	G	229	29/29	0.98	0.10	-0.70	10,16,19,25	0
16	MG	N	518	1/1	0.81	0.13	-1.02	23,23,23,23	0
20	CUA	O	228	2/2	0.97	0.12	-1.35	22,22,22,22	0
22	CHD	P	1525	29/29	0.95	0.11	-1.52	24,28,31,33	0
17	NA	N	519	1/1	0.97	0.07	-2.96	24,24,24,24	0
16	MG	A	518	1/1	0.93	0.10	-3.17	21,21,21,21	0
17	NA	A	519	1/1	0.98	0.08	-4.49	22,22,22,22	0
15	CU	N	517	1/1	1.00	0.20	-	23,23,23,23	0
23	UNX	P	262	1/1	0.53	0.28	-	44,44,44,44	0
15	CU	A	517	1/1	0.99	0.19	-	20,20,20,20	0
23	UNX	C	262	1/1	0.64	0.42	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.