



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:16 AM GMT

PDB ID : 2ZXW
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (1-s X-ray exposure dataset)
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Hirata, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.
Deposited on : 2009-01-08
Resolution : 2.50 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

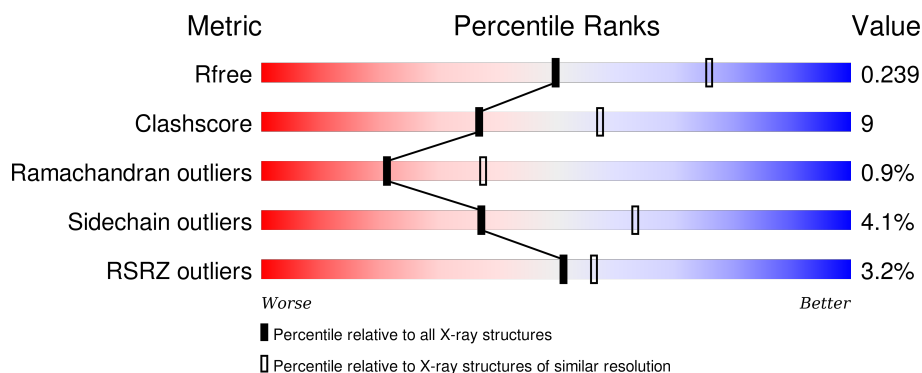
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.













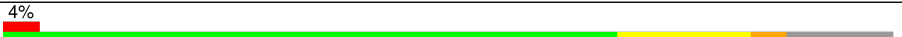

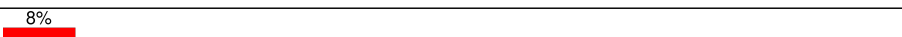
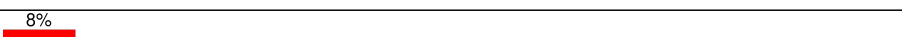
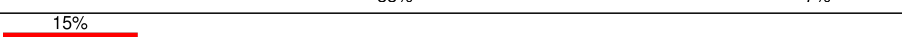
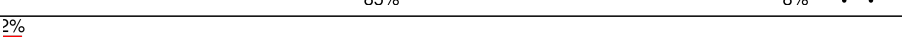

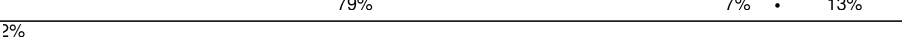

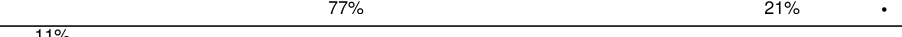
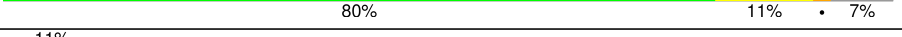
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>82%</div> <div>17%</div> <div>.</div> </div>
1	N	514	<div> <div>82%</div> <div>17%</div> </div>
2	B	227	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
2	O	227	<div> <div>2%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
3	C	261	<div> <div>84%</div> <div>15%</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
15	PER	A	520	-	-	-	X
15	PER	N	520	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	PGV	A	521	-	-	-	X
19	PGV	A	524	-	-	-	X
19	PGV	C	267	-	-	-	X
19	PGV	N	1266	-	-	-	X
19	PGV	N	1268	-	-	-	X
19	PGV	N	1524	-	-	-	X
19	PGV	P	1267	-	-	-	X
21	TGL	B	521	-	-	-	X
21	TGL	D	523	-	-	-	X
21	TGL	L	522	-	-	-	X
21	TGL	N	1521	-	-	-	X
21	TGL	N	1522	-	-	-	X
21	TGL	O	1523	-	-	-	X
22	PSC	B	230	-	-	-	X
22	PSC	O	1230	-	-	-	X
23	CHD	B	1086	X	-	-	-
23	CHD	C	271	X	-	-	X
23	CHD	C	525	X	-	-	-
23	CHD	G	86	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	X	-	-	-
23	CHD	W	1060	X	-	-	X
24	DMU	C	272	X	-	-	X
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	X
24	DMU	Z	1526	X	-	-	-
26	PEK	G	264	-	-	-	X
26	PEK	P	1264	-	-	-	X
27	CDL	C	270	-	-	-	X
27	CDL	G	269	-	-	-	X
27	CDL	P	1270	-	-	-	X
27	CDL	T	1269	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 31827 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	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 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 VIb isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 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			

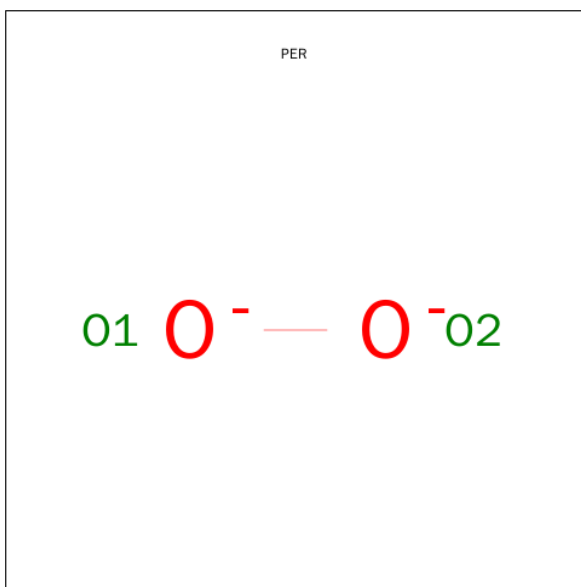
- Molecule 13 is a protein called Cytochrome c oxidase polypeptide 8H.

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

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

- Molecule 15 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

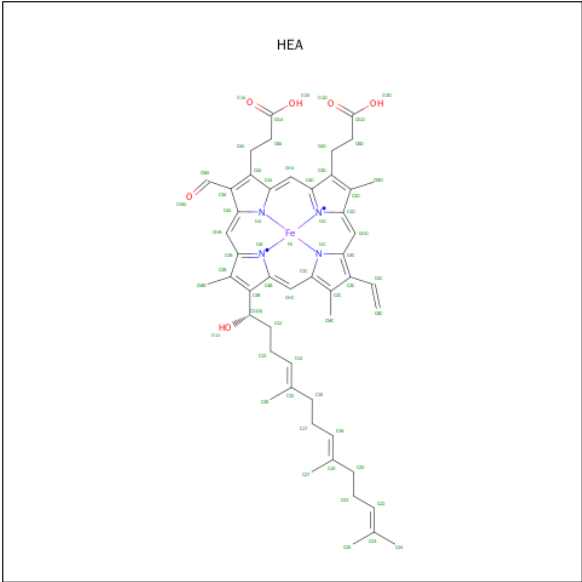
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

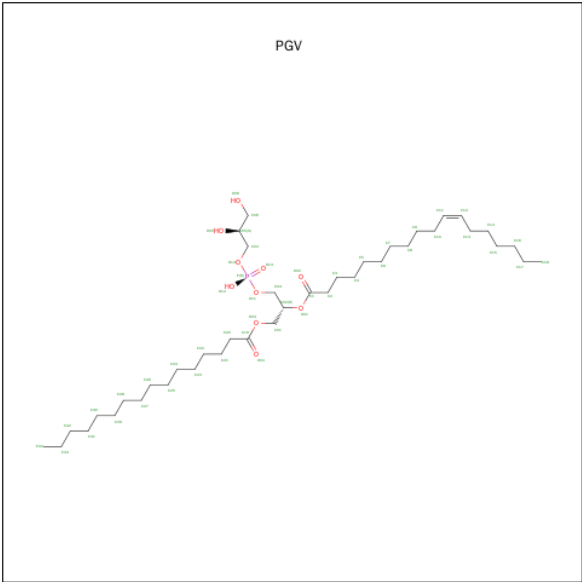
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



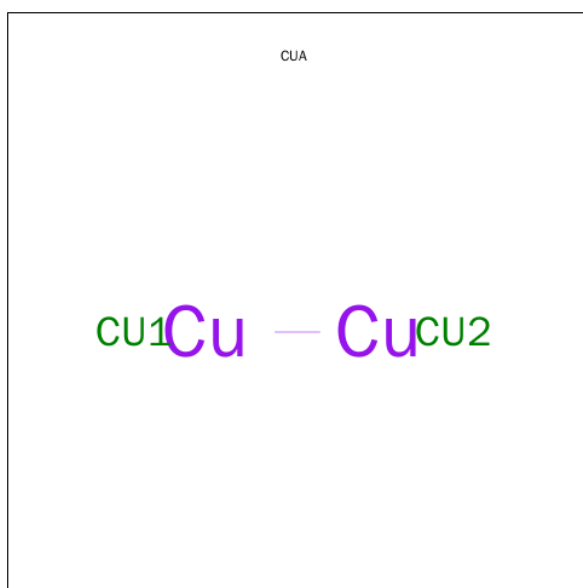
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY} (HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



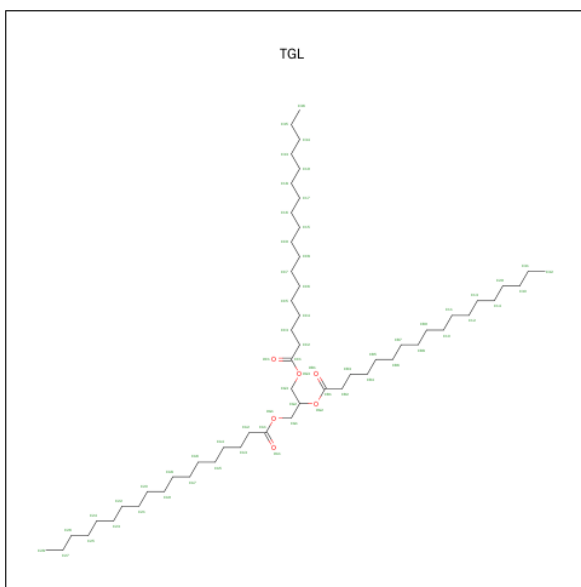
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0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

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



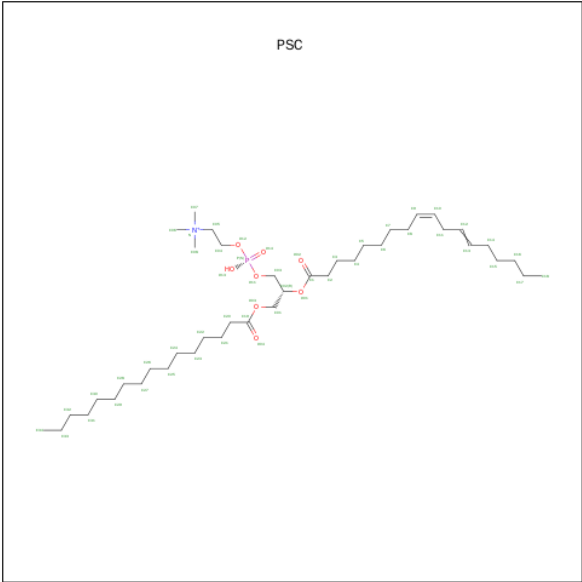
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Cu	0	0
			2	2		
20	O	1	Total	Cu	0	0
			2	2		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



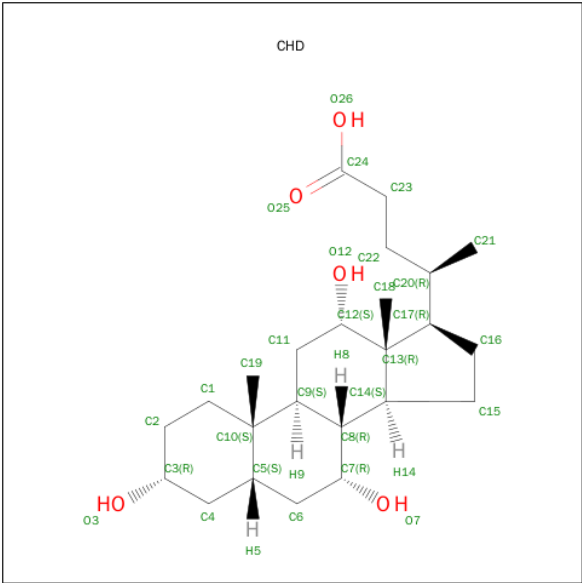
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



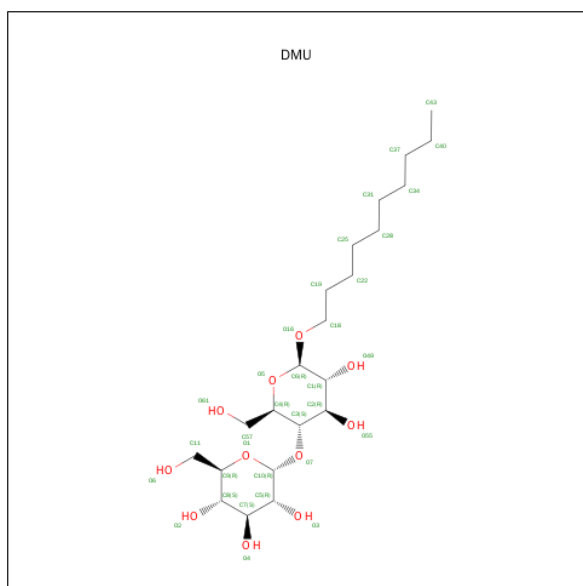
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 24 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).

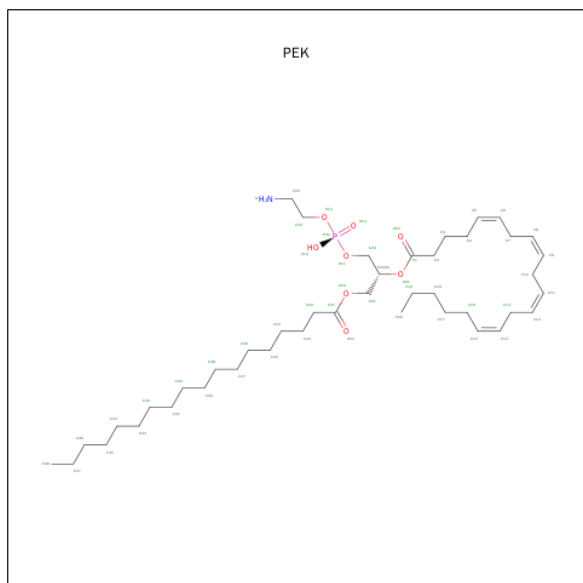


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

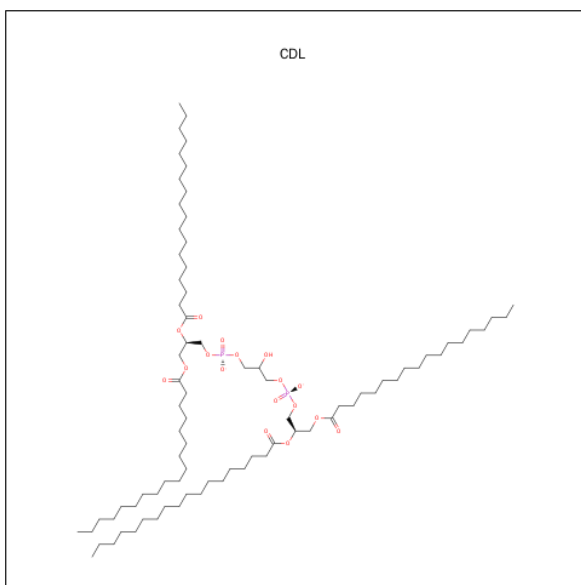
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	P	1	Total X 1 1	0	0
25	C	1	Total X 1 1	0	0

- Molecule 26 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
26	C	1	Total C N O P 53 43 1 8 1	0	0
26	G	1	Total C N O P 53 43 1 8 1	0	0
26	G	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0
26	T	1	Total C N O P 53 43 1 8 1	0	0

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	186	Total	O	0	0
			186	186		
29	B	97	Total	O	0	0
			97	97		
29	C	86	Total	O	0	0
			86	86		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	D	66	Total 66	O 66	0	0
29	E	43	Total 43	O 43	0	0
29	F	61	Total 61	O 61	0	0
29	G	42	Total 42	O 42	0	0
29	H	27	Total 27	O 27	0	0
29	I	23	Total 23	O 23	0	0
29	J	12	Total 12	O 12	0	0
29	K	14	Total 14	O 14	0	0
29	L	17	Total 17	O 17	0	0
29	M	13	Total 13	O 13	0	0
29	N	171	Total 171	O 171	0	0
29	O	90	Total 90	O 90	0	0
29	P	80	Total 80	O 80	0	0
29	Q	43	Total 43	O 43	0	0
29	R	37	Total 37	O 37	0	0
29	S	50	Total 50	O 50	0	0
29	T	37	Total 37	O 37	0	0
29	U	31	Total 31	O 31	0	0
29	V	20	Total 20	O 20	0	0
29	W	9	Total 9	O 9	0	0
29	X	11	Total 11	O 11	0	0

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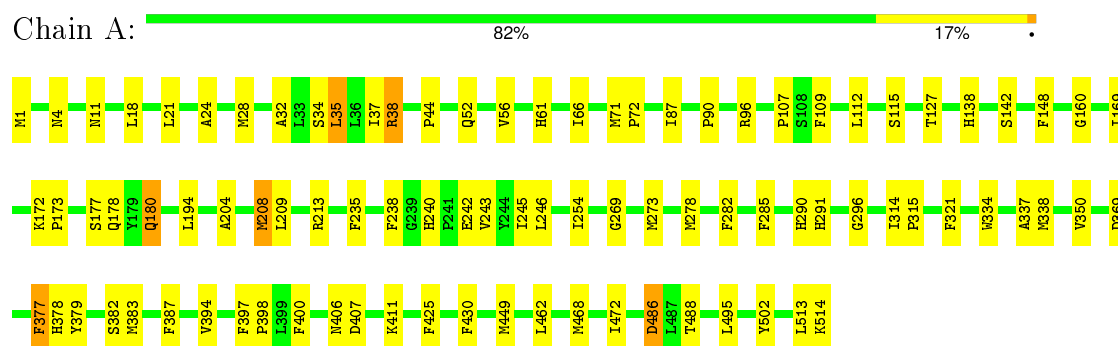
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	17	Total 17	O 17	0	0
29	Z	8	Total 8	O 8	0	0

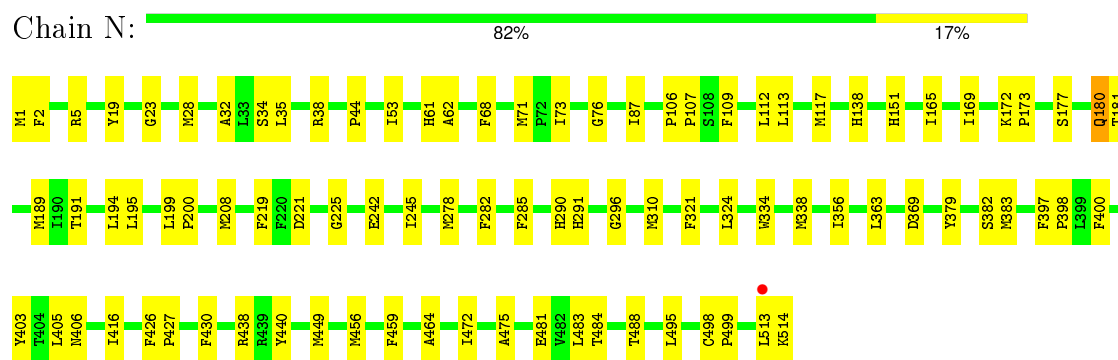
3 Residue-property plots

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.

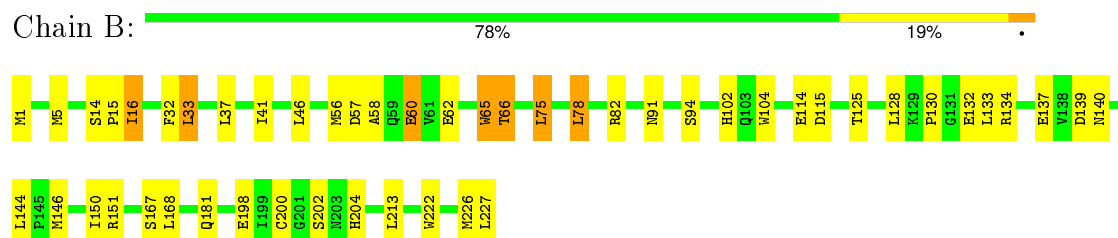
• Molecule 1: Cytochrome c oxidase subunit 1



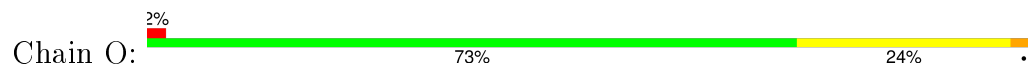
• Molecule 1: Cytochrome c oxidase subunit 1

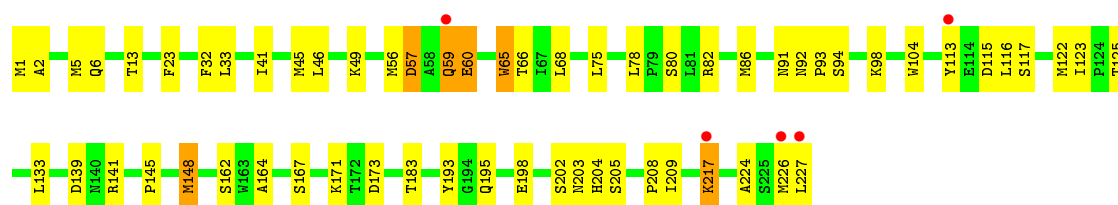


• Molecule 2: Cytochrome c oxidase subunit 2



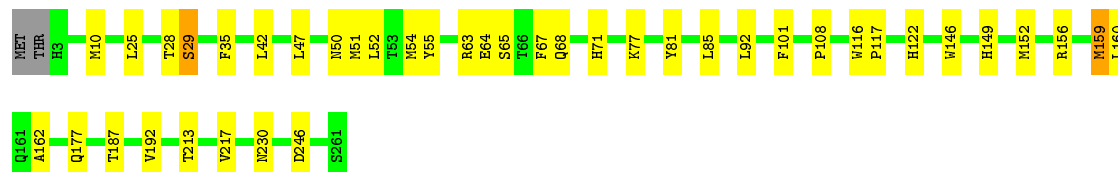
• Molecule 2: Cytochrome c oxidase subunit 2





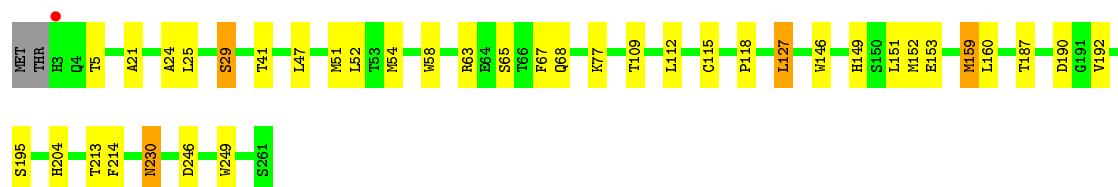
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 84% 15% ..



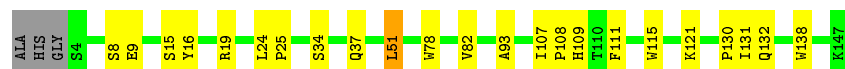
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 85% 13% ..



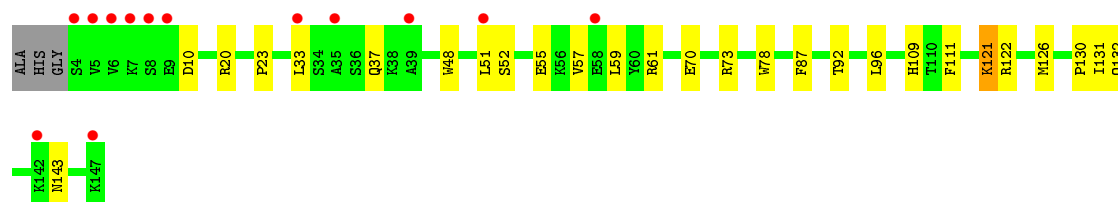
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 82% 15% ..



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 9% 80% 18% ..

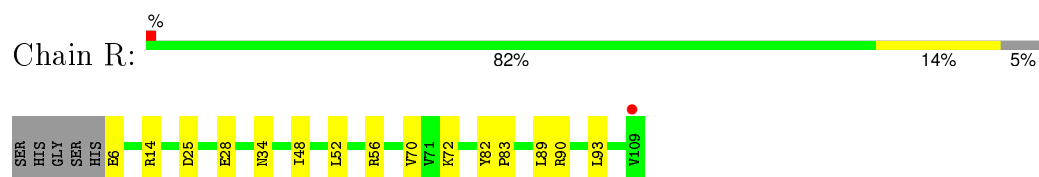


• Molecule 5: Cytochrome c oxidase subunit 5A

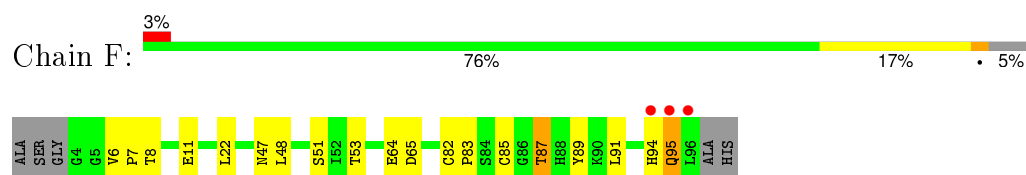
Chain E: 3% 81% 15% 5%



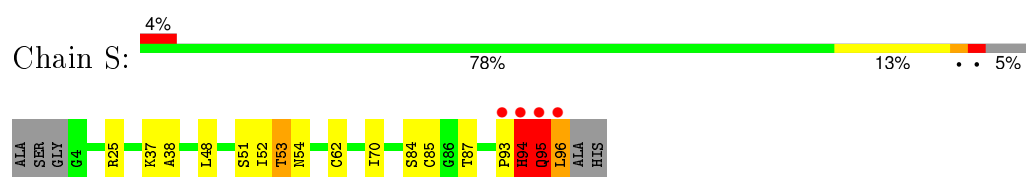
- Molecule 5: Cytochrome c oxidase subunit 5A



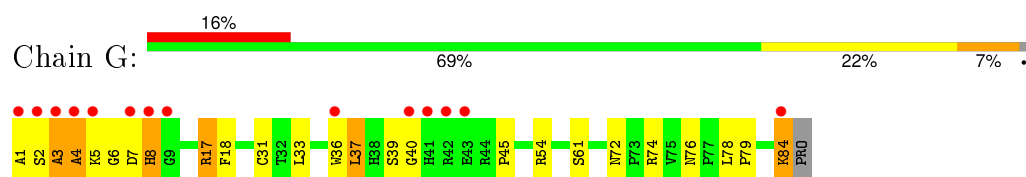
- Molecule 6: Cytochrome c oxidase subunit 5B



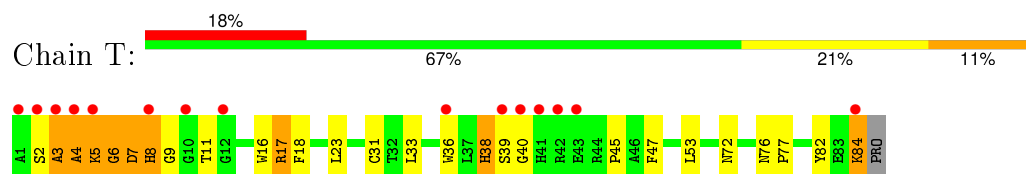
- Molecule 6: Cytochrome c oxidase subunit 5B



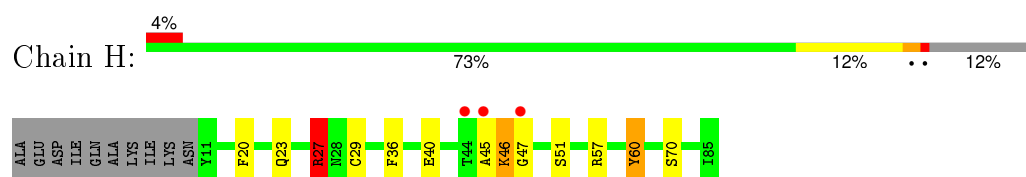
- Molecule 7: Cytochrome c oxidase polypeptide 6A2



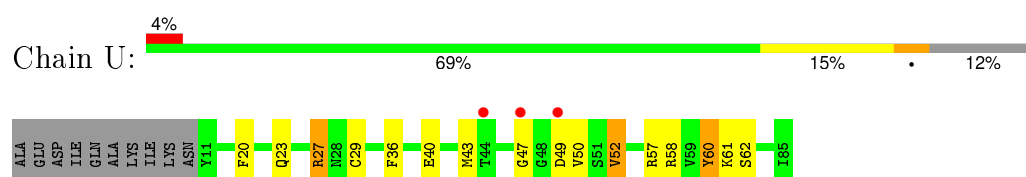
- Molecule 7: Cytochrome c oxidase polypeptide 6A2



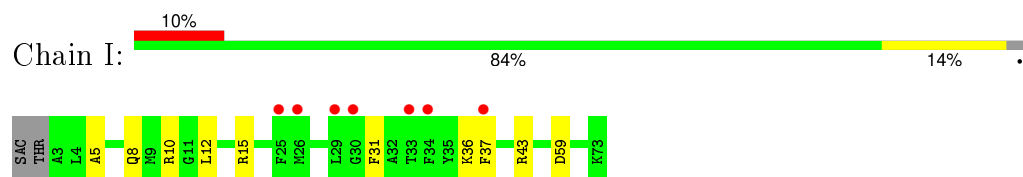
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



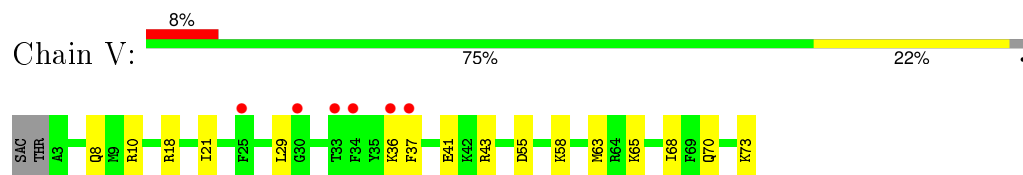
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



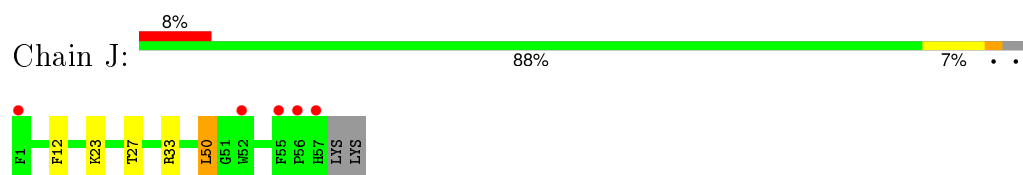
• Molecule 9: Cytochrome c oxidase polypeptide VIc



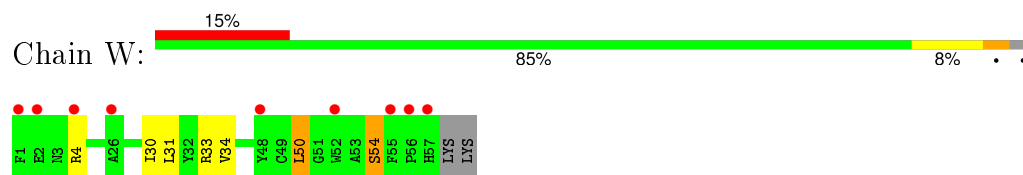
• Molecule 9: Cytochrome c oxidase polypeptide VIc



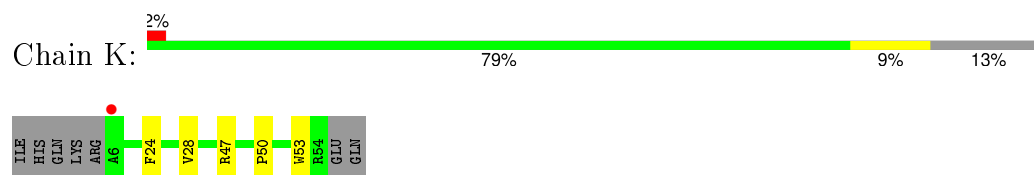
• Molecule 10: Cytochrome c oxidase polypeptide 7A1



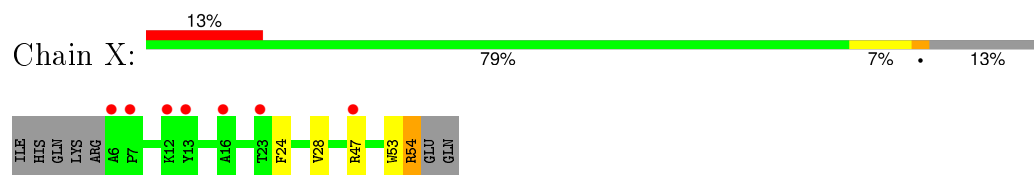
• Molecule 10: Cytochrome c oxidase polypeptide 7A1



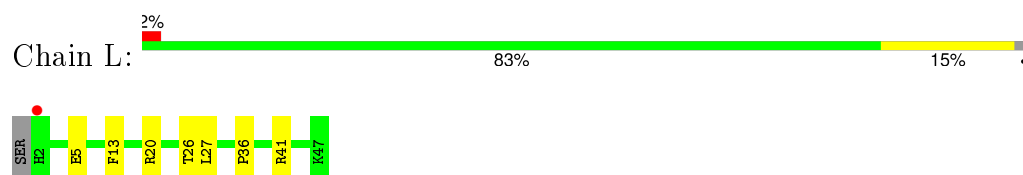
• Molecule 11: Cytochrome c oxidase polypeptide 7B



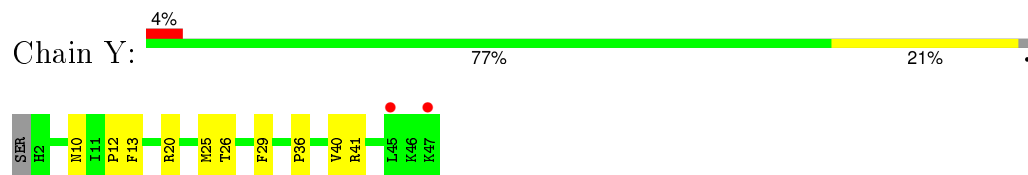
• Molecule 11: Cytochrome c oxidase polypeptide 7B



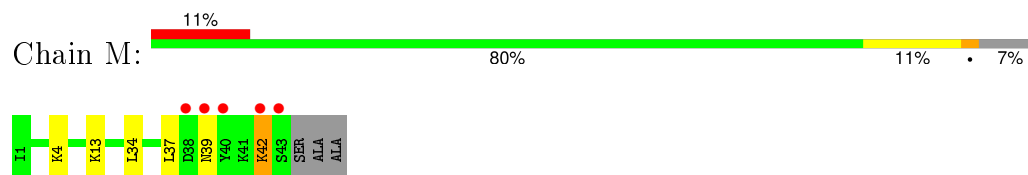
• Molecule 12: Cytochrome c oxidase subunit 7C



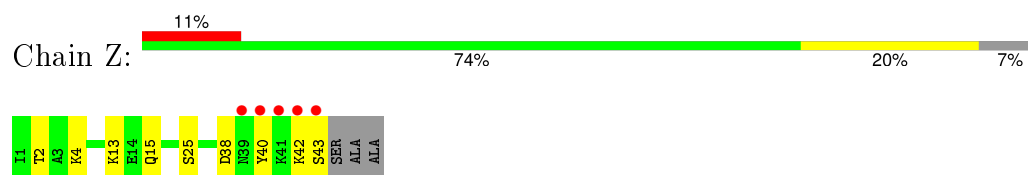
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase polypeptide 8H



- Molecule 13: Cytochrome c oxidase polypeptide 8H



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.16Å 207.62Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 38.33 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.50) 91.1 (38.33-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.185 , 0.233 0.192 , 0.239	Depositor DCC
R_{free} test set	9990 reflections (4.88%)	DCC
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.3	EDS
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 215713 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31827	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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, TPO, CHD, TGL, CDL, PSC, PEK, MG, PER, PGV, UNX, DMU, CUA, NA, FME, CU, HEA

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	1.01	0/4156	0.85	5/5678 (0.1%)
1	N	0.96	0/4156	0.81	3/5678 (0.1%)
2	B	0.97	1/1860 (0.1%)	0.91	2/2534 (0.1%)
2	O	0.91	1/1860 (0.1%)	0.90	0/2534
3	C	0.98	1/2197 (0.0%)	0.77	0/3005
3	P	0.93	1/2197 (0.0%)	0.81	1/3005 (0.0%)
4	D	0.99	0/1229	0.82	1/1658 (0.1%)
4	Q	0.84	0/1229	0.76	0/1658
5	E	0.94	0/860	0.87	1/1167 (0.1%)
5	R	0.85	0/860	0.78	0/1167
6	F	0.89	0/733	0.94	0/996
6	S	0.83	0/733	0.93	1/996 (0.1%)
7	G	0.98	1/690 (0.1%)	0.88	0/937
7	T	0.94	2/690 (0.3%)	0.88	2/937 (0.2%)
8	H	0.96	0/648	0.82	1/877 (0.1%)
8	U	0.82	0/648	0.73	0/877
9	I	1.00	0/598	0.89	1/792 (0.1%)
9	V	0.93	0/598	0.79	0/792
10	J	0.87	0/462	0.76	0/625
10	W	0.80	0/462	0.82	0/625
11	K	0.97	0/398	0.85	0/546
11	X	0.81	0/398	0.76	0/546
12	L	0.96	0/393	0.85	1/526 (0.2%)
12	Y	0.81	0/393	0.78	0/526
13	M	0.96	0/345	0.80	0/470
13	Z	0.75	0/345	0.69	0/470
All	All	0.94	7/29138 (0.0%)	0.83	19/39622 (0.0%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	7.94	1.64	1.50
2	B	198	GLU	C-O	6.96	1.36	1.23
7	T	36	TRP	CB-CG	6.95	1.62	1.50
2	O	198	GLU	C-O	6.42	1.35	1.23
7	T	5	LYS	CB-CG	5.51	1.67	1.52
3	P	115	CYS	CB-SG	5.49	1.91	1.82
3	C	101	PHE	CE1-CZ	5.24	1.47	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	MET	CG-SD-CE	7.33	111.93	100.20
1	A	35	LEU	CB-CG-CD1	-6.52	99.91	111.00
3	P	152	MET	CG-SD-CE	6.22	110.15	100.20
6	S	94	HIS	N-CA-C	6.16	127.62	111.00
1	A	96	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	96	ARG	NE-CZ-NH1	6.13	123.37	120.30
9	I	59	ASP	CB-CG-OD1	-5.34	113.49	118.30
7	T	33	LEU	CA-CB-CG	5.33	127.55	115.30
1	N	221	ASP	CB-CG-OD1	5.31	123.08	118.30
1	N	221	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	B	75	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	486	ASP	CB-CG-OD1	5.22	123.00	118.30
8	H	27	ARG	NE-CZ-NH1	5.17	122.88	120.30
4	D	51	LEU	CA-CB-CG	5.16	127.17	115.30
1	N	438	ARG	NE-CZ-NH2	-5.16	117.72	120.30
12	L	41	ARG	NE-CZ-NH1	5.10	122.85	120.30
7	T	6	GLY	N-CA-C	5.10	125.85	113.10
2	B	82	ARG	NE-CZ-NH2	-5.04	117.78	120.30
5	E	14	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	69	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	35	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	34	0
3	P	2110	0	2027	31	0
4	D	1195	0	1183	23	0
4	Q	1195	0	1183	22	0
5	E	842	0	838	9	0
5	R	842	0	838	8	0
6	F	717	0	700	11	0
6	S	717	0	700	12	0
7	G	675	0	644	24	0
7	T	675	0	644	37	0
8	H	628	0	580	7	0
8	U	628	0	580	12	0
9	I	585	0	597	9	0
9	V	585	0	597	9	0
10	J	451	0	446	3	0
10	W	451	0	446	5	0
11	K	384	0	366	5	0
11	X	384	0	366	7	0
12	L	380	0	380	11	0
12	Y	380	0	380	9	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	N	1	0	0	0	0
18	A	120	0	108	12	0
18	N	120	0	108	8	0
19	A	102	0	152	5	0
19	C	102	0	152	5	0
19	N	153	0	228	12	0
19	P	51	0	76	5	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	63	0	110	10	0
21	D	63	0	110	5	0
21	L	63	0	110	13	0
21	N	126	0	220	26	0
21	O	63	0	110	6	0
22	B	52	0	80	13	0
22	O	52	0	80	12	0
23	B	29	0	37	0	0
23	C	58	0	73	4	0
23	G	29	0	36	2	0
23	J	29	0	35	2	0
23	P	58	0	73	5	0
23	W	29	0	35	1	0
24	C	33	0	37	2	0
24	M	33	0	38	0	0
24	P	33	0	37	3	0
24	Z	33	0	38	2	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	53	0	77	4	0
26	G	106	0	154	16	0
26	P	106	0	154	13	0
26	T	53	0	77	14	0
27	C	100	0	156	13	0
27	G	100	0	156	17	0
27	P	100	0	156	9	0
27	T	100	0	156	17	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	186	0	0	2	0
29	B	97	0	0	2	0
29	C	86	0	0	5	0
29	D	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	E	43	0	0	1	0
29	F	61	0	0	2	0
29	G	42	0	0	4	0
29	H	27	0	0	1	0
29	I	23	0	0	6	0
29	J	12	0	0	0	0
29	K	14	0	0	0	0
29	L	17	0	0	2	0
29	M	13	0	0	1	0
29	N	171	0	0	2	0
29	O	90	0	0	2	0
29	P	80	0	0	2	0
29	Q	43	0	0	1	0
29	R	37	0	0	0	0
29	S	50	0	0	4	0
29	T	37	0	0	2	0
29	U	31	0	0	0	0
29	V	20	0	0	0	0
29	W	9	0	0	0	0
29	X	11	0	0	0	0
29	Y	17	0	0	0	0
29	Z	8	0	0	1	0
All	All	31827	0	31063	578	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (578) 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)
26:P:1265:PEK:C7	26:P:1265:PEK:C6	1.88	1.48
26:P:1265:PEK:H383	27:T:1269:CDL:H272	1.33	1.08
15:A:520:PER:O1	15:A:520:PER:O2	1.70	1.08
15:N:520:PER:O2	15:N:520:PER:O1	1.70	1.08
6:S:52:ILE:O	6:S:94:HIS:CE1	2.09	1.05
3:C:63:ARG:HE	27:C:270:CDL:HA22	1.23	1.03
21:O:1523:TGL:HC21	21:O:1523:TGL:HG11	1.42	1.01
21:N:1522:TGL:HC62	21:N:1522:TGL:HC22	1.45	0.99
21:D:523:TGL:HC21	21:D:523:TGL:HG11	1.44	0.98
21:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.44	0.98
3:P:63:ARG:HE	27:P:1270:CDL:HA22	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:1521:TGL:H281	21:N:1521:TGL:H101	1.44	0.96
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.47	0.96
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.50	0.94
7:G:72:ASN:H	7:G:76:ASN:HD22	1.04	0.92
7:G:5:LYS:HG3	26:G:1263:PEK:H383	1.52	0.92
7:T:5:LYS:HG3	26:T:263:PEK:H383	1.54	0.90
24:C:272:DMU:H30	24:C:272:DMU:O1	1.72	0.89
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.55	0.89
27:T:1269:CDL:H571	27:T:1269:CDL:H782	1.54	0.89
19:C:267:PGV:H182	27:C:270:CDL:H671	1.56	0.87
26:G:264:PEK:H161	26:G:264:PEK:H102	1.56	0.87
2:O:56:MET:HA	22:O:1230:PSC:H202	1.54	0.87
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.38	0.86
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.57	0.85
1:A:514:LYS:HE2	29:F:2322:HOH:O	1.74	0.85
26:P:1265:PEK:C7	26:P:1265:PEK:C5	2.56	0.84
2:B:56:MET:HG2	22:B:230:PSC:H211	1.59	0.84
2:O:224:ALA:O	2:O:227:LEU:HG	1.78	0.84
4:D:34:SER:H	4:D:37:GLN:HE21	1.23	0.84
12:L:13:PHE:HA	21:L:522:TGL:HC31	1.61	0.83
7:T:72:ASN:H	7:T:76:ASN:HD22	1.23	0.82
1:A:400:PHE:HB3	21:L:522:TGL:H283	1.62	0.81
7:T:2:SER:OG	26:T:263:PEK:H301	1.81	0.81
7:G:45:PRO:HD2	29:G:2141:HOH:O	1.79	0.81
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.64	0.80
19:P:1267:PGV:H182	27:P:1270:CDL:C67	2.12	0.80
27:G:269:CDL:H541	27:G:269:CDL:H231	1.64	0.80
8:U:40:GLU:HG3	8:U:50:VAL:HG13	1.63	0.80
3:P:25:LEU:O	3:P:29:SER:HB2	1.82	0.80
19:P:1267:PGV:H182	27:P:1270:CDL:H671	1.63	0.79
7:T:45:PRO:HD2	29:T:3141:HOH:O	1.83	0.79
26:P:1265:PEK:H383	27:T:1269:CDL:C27	2.14	0.78
3:C:25:LEU:O	3:C:29:SER:HB2	1.83	0.78
27:G:269:CDL:H522	27:G:269:CDL:H202	1.65	0.77
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.66	0.76
7:G:5:LYS:HB3	1:N:278:MET:SD	2.26	0.76
7:G:84:LYS:HD2	7:G:84:LYS:H	1.52	0.75
1:N:112:LEU:HG	29:N:3070:HOH:O	1.87	0.74
1:A:278:MET:SD	7:T:5:LYS:HB3	2.27	0.74
9:I:5:ALA:CB	29:I:4239:HOH:O	2.35	0.74
1:N:177:SER:H	1:N:180:GLN:NE2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:265:PEK:H383	27:G:269:CDL:H272	1.70	0.72
7:T:5:LYS:CG	26:T:263:PEK:H383	2.18	0.72
8:U:40:GLU:HG3	8:U:50:VAL:CG1	2.19	0.72
19:C:267:PGV:H12	19:C:267:PGV:H161	1.70	0.72
3:P:214:PHE:CD1	19:P:1267:PGV:H62	2.25	0.71
7:G:76:ASN:HD21	26:G:264:PEK:HN2	1.36	0.71
7:T:5:LYS:HB2	26:T:263:PEK:H362	1.71	0.71
1:N:400:PHE:HB3	21:N:1522:TGL:C28	2.21	0.71
7:T:31:CYS:SG	27:T:1269:CDL:H532	2.31	0.71
3:C:160:LEU:HD13	23:C:271:CHD:C18	2.20	0.71
1:N:400:PHE:HB3	21:N:1522:TGL:H283	1.73	0.71
7:T:3:ALA:HB1	26:T:263:PEK:H382	1.73	0.70
21:N:1522:TGL:CC6	21:N:1522:TGL:HC22	2.19	0.70
26:P:1265:PEK:C8	26:P:1265:PEK:C6	2.70	0.70
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.72	0.70
7:T:8:HIS:CD2	26:T:263:PEK:H232	2.27	0.70
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.57	0.69
2:O:41:ILE:CD1	22:O:1230:PSC:H342	2.22	0.69
21:B:521:TGL:HC22	29:I:2365:HOH:O	1.92	0.69
7:G:72:ASN:H	7:G:76:ASN:ND2	1.84	0.69
3:C:246:ASP:HB2	29:C:4041:HOH:O	1.92	0.69
7:T:2:SER:O	26:T:263:PEK:H322	1.92	0.69
7:T:5:LYS:HD2	26:T:263:PEK:C38	2.23	0.69
7:G:2:SER:OG	26:G:1263:PEK:H301	1.94	0.68
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.27	0.67
27:G:269:CDL:H782	27:G:269:CDL:H571	1.76	0.67
9:I:5:ALA:HB2	29:I:4239:HOH:O	1.92	0.67
19:A:524:PGV:H062	29:M:2148:HOH:O	1.94	0.67
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.07	0.67
19:N:1524:PGV:H012	29:N:4082:HOH:O	1.95	0.67
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.77	0.67
12:L:5:GLU:HB2	29:L:4231:HOH:O	1.94	0.67
12:L:20:ARG:HH22	21:L:522:TGL:HC62	1.58	0.66
21:N:1521:TGL:C10	21:N:1521:TGL:H281	2.21	0.66
19:C:268:PGV:H062	29:C:4330:HOH:O	1.95	0.66
21:N:1522:TGL:H361	21:N:1522:TGL:HB91	1.77	0.66
21:B:521:TGL:HA82	21:B:521:TGL:H222	1.76	0.66
27:C:270:CDL:OA5	27:C:270:CDL:HB22	1.96	0.66
3:P:160:LEU:HD13	23:P:1271:CHD:C18	2.25	0.65
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.77	0.65
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.78	0.65
27:T:1269:CDL:C57	27:T:1269:CDL:H782	2.25	0.65
19:C:267:PGV:H182	27:C:270:CDL:C67	2.26	0.65
1:A:472:ILE:HG21	21:L:522:TGL:HA91	1.79	0.65
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.79	0.65
2:O:116:LEU:HD12	2:O:117:SER:N	2.12	0.65
21:O:1523:TGL:HG11	21:O:1523:TGL:CC2	2.22	0.65
19:N:1524:PGV:H062	29:Z:3148:HOH:O	1.97	0.64
2:B:56:MET:HA	22:B:230:PSC:H202	1.79	0.64
21:N:1522:TGL:H202	21:N:1522:TGL:H242	1.80	0.64
26:C:265:PEK:H383	27:G:269:CDL:C27	2.28	0.64
24:C:272:DMU:H30	24:C:272:DMU:C10	2.27	0.64
21:N:1521:TGL:C28	21:N:1521:TGL:H101	2.22	0.64
11:K:24:PHE:O	11:K:28:VAL:HG12	1.98	0.64
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.78	0.64
12:L:20:ARG:NH2	21:L:522:TGL:HC32	2.14	0.62
1:A:87:ILE:O	1:A:173:PRO:HD3	1.99	0.62
1:N:514:LYS:HE2	29:S:3322:HOH:O	1.97	0.62
21:B:521:TGL:C28	21:B:521:TGL:H101	2.29	0.62
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.81	0.62
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.35	0.62
22:B:230:PSC:H281	22:B:230:PSC:H322	1.82	0.61
3:P:246:ASP:HB2	29:P:4136:HOH:O	1.98	0.61
18:N:516:HEA:HBC1	18:N:516:HEA:HMC1	1.82	0.61
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.00	0.61
3:P:67:PHE:HE1	27:P:1270:CDL:H1	1.64	0.61
4:D:78:TRP:HA	21:D:523:TGL:HB22	1.83	0.61
3:P:213:THR:HG23	27:P:1270:CDL:H762	1.82	0.60
7:G:31:CYS:SG	27:G:269:CDL:H532	2.40	0.60
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.82	0.60
6:F:64:GLU:O	6:F:65:ASP:HB2	2.01	0.60
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.82	0.60
4:D:131:ILE:HD12	4:D:131:ILE:N	2.17	0.60
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.34	0.60
5:E:78:HIS:HD2	9:I:12:LEU:HD13	1.68	0.59
1:A:52:GLN:O	1:A:56:VAL:HG23	2.02	0.59
8:U:43:MET:HE2	8:U:52:VAL:HG21	1.85	0.59
21:N:1522:TGL:H202	21:N:1522:TGL:C24	2.32	0.59
24:P:1272:DMU:O1	24:P:1272:DMU:H30	2.01	0.59
26:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.48	0.59
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:ALA:N	29:I:4239:HOH:O	2.30	0.59
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.38	0.58
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.33	0.58
21:O:1523:TGL:HB22	4:Q:78:TRP:HA	1.84	0.58
7:G:5:LYS:HG3	26:G:1263:PEK:C38	2.28	0.58
27:G:269:CDL:C23	27:G:269:CDL:H541	2.33	0.58
11:X:24:PHE:O	11:X:28:VAL:HG12	2.03	0.58
12:L:20:ARG:HH22	21:L:522:TGL:CC6	2.16	0.58
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.68	0.58
2:B:37:LEU:HB2	29:I:4437:HOH:O	2.02	0.58
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.04	0.58
27:T:1269:CDL:H541	27:T:1269:CDL:H232	1.85	0.57
1:N:87:ILE:O	1:N:173:PRO:HD3	2.03	0.57
7:T:72:ASN:H	7:T:76:ASN:ND2	1.99	0.57
1:A:28:MET:CE	18:A:515:HEA:H271	2.33	0.57
1:N:488:THR:HB	1:N:495:LEU:HD13	1.84	0.57
8:H:36:PHE:CE1	8:H:57:ARG:HB2	2.40	0.57
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.38	0.57
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.86	0.57
26:P:1265:PEK:C38	27:T:1269:CDL:H272	2.22	0.57
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.87	0.57
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.86	0.57
1:N:28:MET:CE	18:N:515:HEA:H271	2.35	0.56
12:L:20:ARG:HH22	21:L:522:TGL:HC32	1.69	0.56
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.86	0.56
21:D:523:TGL:HC21	21:D:523:TGL:CG1	2.27	0.56
2:B:56:MET:HA	22:B:230:PSC:C20	2.34	0.56
7:G:84:LYS:H	7:G:84:LYS:CD	2.18	0.56
22:B:230:PSC:H343	22:B:230:PSC:H142	1.87	0.56
1:A:240:HIS:O	1:A:243:VAL:HG22	2.06	0.56
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.86	0.56
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.05	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
19:N:1524:PGV:H011	19:N:1524:PGV:H22	1.88	0.56
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.86	0.56
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.70	0.56
27:T:1269:CDL:OB4	27:T:1269:CDL:H1	2.06	0.55
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.87	0.55
7:T:84:LYS:H	7:T:84:LYS:HD2	1.71	0.55
26:G:1263:PEK:H042	3:P:77:LYS:NZ	2.22	0.55
21:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.88	0.55
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.41	0.55
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.41	0.55
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.89	0.55
10:J:50:LEU:HD22	10:J:50:LEU:O	2.06	0.55
18:A:516:HEA:OMA	18:A:516:HEA:HHB	2.05	0.55
1:A:1:FME:HCN	1:A:4:ASN:H	1.71	0.55
3:P:47:LEU:O	3:P:51:MET:HG2	2.06	0.55
4:D:9:GLU:N	4:D:9:GLU:OE2	2.35	0.55
27:G:269:CDL:HA21	27:G:269:CDL:H111	1.89	0.55
3:P:230:ASN:HB2	29:P:3271:HOH:O	2.06	0.55
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.41	0.54
8:H:46:LYS:HB2	8:U:52:VAL:HG12	1.89	0.54
1:A:112:LEU:HD12	29:A:2070:HOH:O	2.06	0.54
3:P:149:HIS:O	3:P:153:GLU:HG3	2.08	0.54
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.89	0.54
1:N:35:LEU:HB3	24:Z:1526:DMU:H24	1.90	0.54
26:G:1263:PEK:H12	29:G:4260:HOH:O	2.08	0.54
1:N:151:HIS:CD2	26:P:1264:PEK:H382	2.43	0.54
5:E:78:HIS:CD2	9:I:12:LEU:HD13	2.42	0.54
1:A:379:TYR:O	1:A:383:MET:HB2	2.08	0.54
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.16	0.53
5:E:105:GLY:O	5:E:108:LYS:HG2	2.07	0.53
8:H:60:TYR:C	8:H:60:TYR:CD1	2.81	0.53
27:G:269:CDL:H761	1:N:282:PHE:HZ	1.73	0.53
4:D:34:SER:H	4:D:37:GLN:NE2	1.99	0.53
4:Q:122:ARG:O	4:Q:126:MET:HG2	2.09	0.53
2:B:58:ALA:O	2:B:62:GLU:HG3	2.08	0.53
3:P:127:LEU:HG	27:T:1269:CDL:OB3	2.09	0.53
3:P:187:THR:HG22	26:P:1264:PEK:H052	1.89	0.53
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.90	0.53
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.90	0.53
21:L:522:TGL:HC22	21:L:522:TGL:HC62	1.90	0.53
19:C:268:PGV:H101	29:C:4467:HOH:O	2.08	0.53
26:P:1265:PEK:H6	26:P:1265:PEK:H221	1.89	0.53
9:V:65:LYS:O	11:X:54:ARG:NH1	2.34	0.53
3:C:149:HIS:HA	3:C:152:MET:HE2	1.90	0.53
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.90	0.53
6:S:70:ILE:HG13	6:S:84:SER:HB3	1.91	0.53
21:N:1521:TGL:H301	21:N:1521:TGL:HA92	1.91	0.52
7:G:4:ALA:CB	1:N:282:PHE:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:22:LEU:HD12	29:F:4476:HOH:O	2.09	0.52
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.74	0.52
9:V:55:ASP:OD2	9:V:58:LYS:HB2	2.09	0.52
21:B:521:TGL:H281	21:B:521:TGL:H101	1.91	0.52
21:B:521:TGL:C10	21:B:521:TGL:H281	2.38	0.52
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.45	0.52
3:P:52:LEU:HD21	27:P:1270:CDL:H412	1.91	0.52
7:G:3:ALA:HB1	26:G:1263:PEK:H382	1.90	0.52
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.09	0.52
1:N:177:SER:H	1:N:180:GLN:HE21	1.54	0.52
3:C:67:PHE:HE1	27:C:270:CDL:H1	1.73	0.52
27:P:1270:CDL:H231	27:P:1270:CDL:H642	1.92	0.52
7:T:3:ALA:CB	26:T:263:PEK:H382	2.39	0.52
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.45	0.52
6:S:95:GLN:HG2	29:S:4510:HOH:O	2.10	0.51
7:G:2:SER:O	26:G:1263:PEK:H322	2.10	0.51
6:S:25:ARG:HD3	29:S:4299:HOH:O	2.09	0.51
21:N:1522:TGL:HC62	21:N:1522:TGL:CC2	2.18	0.51
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.44	0.51
3:P:190:ASP:HB3	7:T:53:LEU:HD22	1.92	0.51
1:N:472:ILE:HG21	21:N:1522:TGL:CA9	2.41	0.51
26:C:265:PEK:C38	27:G:269:CDL:H273	2.40	0.51
21:N:1521:TGL:H201	21:N:1521:TGL:H241	1.93	0.51
7:G:72:ASN:N	7:G:76:ASN:HD22	1.89	0.51
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.45	0.51
7:G:5:LYS:HD2	26:G:1263:PEK:H371	1.91	0.51
7:G:3:ALA:O	7:G:4:ALA:HB2	2.10	0.51
1:A:35:LEU:HD11	1:A:462:LEU:HD22	1.93	0.51
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.41	0.51
27:C:270:CDL:H661	27:C:270:CDL:H242	1.93	0.50
26:C:265:PEK:C38	27:G:269:CDL:C27	2.89	0.50
1:N:113:LEU:HD13	21:N:1522:TGL:H292	1.93	0.50
1:N:117:MET:HB3	10:W:54:SER:OG	2.11	0.50
7:T:5:LYS:HD2	26:T:263:PEK:H371	1.93	0.50
24:P:1272:DMU:C10	24:P:1272:DMU:H30	2.41	0.50
19:N:1524:PGV:H061	19:N:1524:PGV:O11	2.11	0.50
2:B:15:PRO:HD2	29:B:2132:HOH:O	2.12	0.50
1:A:160:GLY:HA3	29:A:2061:HOH:O	2.12	0.50
1:N:400:PHE:HB3	21:N:1522:TGL:H282	1.94	0.50
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.29	0.50
19:A:524:PGV:H152	19:A:524:PGV:H321	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:524:PGV:H061	19:A:524:PGV:P	2.51	0.50
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.47	0.50
2:O:125:THR:N	29:O:3143:HOH:O	2.45	0.50
7:T:23:LEU:HD12	27:T:1269:CDL:H273	1.93	0.50
2:O:65:TRP:CZ3	22:O:1230:PSC:H331	2.47	0.50
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.93	0.50
26:G:1263:PEK:H042	3:P:77:LYS:HZ1	1.77	0.50
27:G:269:CDL:H241	27:G:269:CDL:H541	1.92	0.50
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.75	0.50
4:D:93:ALA:HB3	11:K:28:VAL:HG22	1.94	0.50
1:A:449:MET:SD	2:B:5:MET:HG2	2.51	0.50
1:A:488:THR:HB	1:A:495:LEU:HD13	1.93	0.49
1:N:426:PHE:HB3	1:N:427:PRO:HD3	1.94	0.49
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.47	0.49
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.01	0.49
4:Q:109:HIS:HD2	29:Q:3147:HOH:O	1.95	0.49
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.94	0.49
27:P:1270:CDL:H352	27:P:1270:CDL:H162	1.94	0.49
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.95	0.49
1:N:398:PRO:HA	1:N:403:TYR:O	2.12	0.49
3:C:55:TYR:CD1	27:C:270:CDL:H532	2.48	0.49
2:B:1:FME:SD	2:B:133:LEU:CD1	3.00	0.49
1:A:21:LEU:HD23	21:L:522:TGL:H212	1.95	0.49
27:G:269:CDL:H473	29:G:4294:HOH:O	2.13	0.49
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.94	0.49
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.27	0.49
3:C:63:ARG:NE	27:C:270:CDL:HA22	2.07	0.49
21:B:521:TGL:CA8	21:B:521:TGL:H222	2.41	0.49
21:D:523:TGL:HB62	21:D:523:TGL:HA52	1.95	0.48
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.27	0.48
2:O:1:FME:SD	2:O:133:LEU:HD13	2.53	0.48
1:A:169:ILE:HG23	7:T:9:GLY:HA2	1.95	0.48
1:N:1:FME:CN	1:N:2:PHE:N	2.76	0.48
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.96	0.48
2:B:32:PHE:HZ	21:B:521:TGL:HA31	1.78	0.48
7:T:84:LYS:H	7:T:84:LYS:CD	2.25	0.48
6:S:53:THR:HB	6:S:54:ASN:H	1.33	0.48
2:B:102:HIS:O	2:B:104:TRP:HA	2.14	0.48
6:S:52:ILE:C	6:S:94:HIS:CE1	2.84	0.48
7:G:3:ALA:O	29:G:4448:HOH:O	2.20	0.48
3:C:213:THR:O	3:C:217:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:270:CDL:H522	27:C:270:CDL:OB9	2.13	0.48
18:N:515:HEA:H273	18:N:515:HEA:C16	2.43	0.48
2:B:57:ASP:H	22:B:230:PSC:H201	1.78	0.47
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.27	0.47
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.63	0.47
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.95	0.47
7:G:1:ALA:HB2	19:N:1268:PGV:H312	1.97	0.47
12:L:20:ARG:HD2	29:L:4423:HOH:O	2.13	0.47
19:A:524:PGV:C15	19:A:524:PGV:H321	2.45	0.47
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.79	0.47
2:O:226:MET:O	2:O:226:MET:HG3	2.14	0.47
3:C:156:ARG:HE	23:C:271:CHD:C24	2.27	0.47
26:G:1263:PEK:H282	26:G:1263:PEK:H312	1.67	0.47
2:O:1:FME:HCN	2:O:193:TYR:HB2	1.96	0.47
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.79	0.47
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.15	0.47
1:A:278:MET:HB3	7:T:5:LYS:HG2	1.97	0.47
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.61	0.47
18:N:515:HEA:C27	18:N:515:HEA:C16	2.92	0.47
1:A:430:PHE:HE1	21:B:521:TGL:HB21	1.79	0.47
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.30	0.47
9:V:37:PHE:HA	9:V:41:GLU:HB2	1.97	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.47
1:A:115:SER:HB2	1:A:142:SER:O	2.15	0.47
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.45	0.47
2:B:62:GLU:O	2:B:66:THR:HB	2.15	0.47
7:T:17:ARG:HD2	29:T:3293:HOH:O	2.14	0.47
2:O:162:SER:HA	2:O:173:ASP:HA	1.97	0.47
19:N:1266:PGV:H181	26:P:1264:PEK:H321	1.97	0.46
1:A:32:ALA:CB	12:L:36:PRO:HG2	2.42	0.46
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.50	0.46
1:N:199:LEU:N	1:N:200:PRO:CD	2.79	0.46
3:P:204:HIS:CE1	3:P:249:TRP:HB2	2.50	0.46
26:G:264:PEK:H71	26:G:264:PEK:H32	1.98	0.46
1:A:278:MET:HB3	7:T:5:LYS:CG	2.45	0.46
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.97	0.46
3:C:108:PRO:HA	29:C:2192:HOH:O	2.15	0.46
2:O:57:ASP:H	22:O:1230:PSC:C20	2.28	0.46
1:A:172:LYS:NZ	1:A:178:GLN:NE2	2.64	0.46
5:E:63:SER:O	5:E:67:ILE:HG13	2.16	0.46
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:CYS:SG	6:F:87:THR:HG23	2.55	0.46
23:G:86:CHD:H212	23:G:86:CHD:H12	1.96	0.46
23:P:1525:CHD:H12	23:P:1525:CHD:H212	1.97	0.46
22:O:1230:PSC:C02	22:O:1230:PSC:H212	2.46	0.46
2:O:59:GLN:O	2:O:59:GLN:HG3	2.15	0.46
3:P:54:MET:HB3	3:P:58:TRP:CZ3	2.50	0.46
1:A:24:ALA:HA	18:A:515:HEA:H22	1.97	0.46
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.51	0.46
5:R:89:LEU:O	5:R:93:LEU:HG	2.16	0.46
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.97	0.46
21:N:1522:TGL:HA82	12:Y:29:PHE:HZ	1.80	0.46
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.66	0.46
22:O:1230:PSC:H212	22:O:1230:PSC:O01	2.15	0.46
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.51	0.46
4:D:78:TRP:CA	21:D:523:TGL:HB22	2.46	0.46
27:G:269:CDL:H152	27:G:269:CDL:H182	1.70	0.46
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.80	0.46
2:O:141:ARG:HG3	9:V:70:GLN:HE22	1.81	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.85	0.46
3:P:63:ARG:NE	27:P:1270:CDL:HA22	2.11	0.45
2:B:1:FME:SD	2:B:133:LEU:HD11	2.56	0.45
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.16	0.45
2:O:82:ARG:HG2	2:O:86:MET:CE	2.47	0.45
18:A:516:HEA:HHC	18:A:516:HEA:O11	2.16	0.45
1:A:209:LEU:O	1:A:213:ARG:HG3	2.16	0.45
1:N:472:ILE:HG21	21:N:1522:TGL:HA91	1.97	0.45
27:G:269:CDL:H222	27:G:269:CDL:H252	1.73	0.45
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.97	0.45
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.31	0.45
3:P:65:SER:HB2	19:P:1267:PGV:H041	1.98	0.45
7:T:5:LYS:CD	26:T:263:PEK:H383	2.46	0.45
18:A:516:HEA:HMC1	18:A:516:HEA:HBC1	1.98	0.45
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.50	0.45
21:L:522:TGL:H251	21:L:522:TGL:H282	1.64	0.45
1:N:169:ILE:HD11	1:N:189:MET:SD	2.57	0.45
26:P:1265:PEK:C38	27:T:1269:CDL:C27	2.87	0.45
3:C:51:MET:HB3	27:C:270:CDL:H622	1.99	0.45
21:O:1523:TGL:HC21	21:O:1523:TGL:CG1	2.30	0.45
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.99	0.45
7:T:5:LYS:CD	26:T:263:PEK:C38	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:MET:CE	18:A:515:HEA:H212	2.47	0.45
2:O:98:LYS:HE2	8:U:62:SER:O	2.17	0.45
4:D:132:GLN:OE1	9:I:43:ARG:HD3	2.16	0.45
13:Z:42:LYS:HA	13:Z:42:LYS:HD2	1.82	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
27:C:270:CDL:H192	27:C:270:CDL:H642	1.97	0.45
4:D:78:TRP:O	4:D:82:VAL:HG23	2.16	0.45
18:N:515:HEA:C27	18:N:515:HEA:H161	2.47	0.45
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.82	0.45
21:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.99	0.45
7:T:5:LYS:HD2	26:T:263:PEK:C37	2.47	0.45
1:A:1:FME:HA	1:A:1:FME:CE	2.47	0.45
1:A:127:THR:HG22	1:A:235:PHE:CE2	2.52	0.45
3:C:52:LEU:HD23	27:C:270:CDL:H362	1.99	0.44
1:A:377:PHE:HE2	1:A:378:HIS:CE1	2.35	0.44
1:A:1:FME:HE2	1:A:1:FME:HA	2.00	0.44
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.99	0.44
4:Q:70:GLU:O	4:Q:73:ARG:HG2	2.18	0.44
1:A:11:ASN:HB2	1:A:502:TYR:CZ	2.51	0.44
3:C:187:THR:HG22	26:G:264:PEK:H052	2.00	0.44
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.51	0.44
1:A:407:ASP:O	1:A:411:LYS:HG3	2.18	0.44
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.54	0.44
8:U:58:ARG:HD2	8:U:58:ARG:HA	1.84	0.44
1:N:191:THR:HG23	1:N:245:ILE:HG23	2.00	0.44
4:D:109:HIS:HE1	4:D:115:TRP:CZ3	2.35	0.44
1:A:148:PHE:HB3	3:C:28:THR:HB	2.00	0.44
3:C:47:LEU:O	3:C:51:MET:HG2	2.18	0.44
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.00	0.44
3:C:116:TRP:HA	3:C:117:PRO:C	2.38	0.44
5:E:81:ILE:O	5:E:85:VAL:HG23	2.17	0.44
2:B:146:MET:HA	2:B:213:LEU:HD12	2.00	0.44
6:S:51:SER:O	6:S:94:HIS:N	2.37	0.44
26:G:1263:PEK:H331	26:G:1263:PEK:H362	1.70	0.44
1:A:350:VAL:HG13	21:B:521:TGL:HB81	2.00	0.44
2:O:1:FME:SD	2:O:133:LEU:CD1	3.06	0.44
1:A:314:ILE:HB	1:A:315:PRO:CD	2.47	0.44
27:T:1269:CDL:H111	27:T:1269:CDL:HA21	2.00	0.43
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.99	0.43
21:N:1521:TGL:H282	21:N:1521:TGL:H252	1.80	0.43
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:HD22	2:B:150:ILE:HD13	2.00	0.43
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.53	0.43
2:O:217:LYS:HA	2:O:217:LYS:HE2	2.00	0.43
7:T:77:PRO:HD3	7:T:82:TYR:CE1	2.52	0.43
3:C:50:ASN:HD21	3:C:54:MET:HE1	1.83	0.43
2:O:13:THR:HG22	2:O:13:THR:O	2.18	0.43
4:Q:132:GLN:OE1	9:V:43:ARG:HD3	2.18	0.43
7:T:3:ALA:O	7:T:4:ALA:CB	2.66	0.43
3:C:50:ASN:ND2	3:C:54:MET:CE	2.81	0.43
1:N:379:TYR:O	1:N:383:MET:HB2	2.17	0.43
27:T:1269:CDL:H541	27:T:1269:CDL:C23	2.48	0.43
22:O:1230:PSC:C14	22:O:1230:PSC:H343	2.48	0.43
24:P:1272:DMU:H25	26:P:1264:PEK:H341	2.00	0.43
6:S:87:THR:HG22	29:S:3333:HOH:O	2.18	0.43
24:Z:1526:DMU:H15	24:Z:1526:DMU:H9	1.79	0.43
8:H:27:ARG:NH1	29:H:2287:HOH:O	2.52	0.43
10:J:12:PHE:O	10:J:23:LYS:HE2	2.19	0.43
1:N:28:MET:HE2	18:N:515:HEA:H271	2.01	0.43
2:B:65:TRP:HZ3	22:B:230:PSC:H331	1.84	0.43
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.07	0.43
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.62	0.43
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.34	0.43
5:E:31:LYS:HE3	6:F:83:PRO:O	2.18	0.43
3:P:214:PHE:CE1	19:P:1267:PGV:H62	2.54	0.43
7:G:8:HIS:ND1	26:G:1263:PEK:H312	2.34	0.43
22:B:230:PSC:C07	9:I:10:ARG:HE	2.32	0.43
19:N:1524:PGV:H222	13:Z:15:GLN:HE22	1.83	0.43
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.17	0.43
2:O:59:GLN:O	2:O:59:GLN:CG	2.67	0.43
21:L:522:TGL:HC22	21:L:522:TGL:CC6	2.48	0.43
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.19	0.43
1:A:90:PRO:HB2	3:C:10:MET:CE	2.48	0.43
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.53	0.43
7:T:38:HIS:NE2	27:T:1269:CDL:H111	2.34	0.42
6:S:94:HIS:O	6:S:95:GLN:HB2	2.19	0.42
1:N:397:PHE:N	1:N:398:PRO:CD	2.81	0.42
2:O:49:LYS:NZ	21:O:1523:TGL:HC71	2.34	0.42
1:A:28:MET:HE3	18:A:515:HEA:H271	2.01	0.42
1:A:378:HIS:CG	1:A:425:PHE:CE2	3.07	0.42
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.18	0.42
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:PHE:HB3	1:A:398:PRO:HD3	2.01	0.42
22:B:230:PSC:C34	22:B:230:PSC:H142	2.49	0.42
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.54	0.42
19:N:1524:PGV:H151	4:Q:87:PHE:CZ	2.54	0.42
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.19	0.42
1:N:449:MET:SD	2:O:5:MET:CG	3.07	0.42
1:N:459:PHE:HB3	4:Q:92:THR:HG23	2.01	0.42
1:N:5:ARG:NH2	12:Y:10:ASN:HA	2.34	0.42
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.54	0.42
2:B:222:TRP:O	2:B:226:MET:HB2	2.19	0.42
1:N:400:PHE:O	21:N:1522:TGL:H283	2.19	0.42
4:Q:33:LEU:HB3	4:Q:37:GLN:HB3	2.01	0.42
1:A:269:GLY:O	1:A:273:MET:HG2	2.20	0.42
27:T:1269:CDL:H552	27:T:1269:CDL:H521	1.75	0.42
27:G:269:CDL:C24	27:G:269:CDL:H541	2.49	0.42
18:A:516:HEA:HHD	18:A:516:HEA:HAC	1.72	0.42
2:B:1:FME:SD	2:B:133:LEU:HD13	2.59	0.42
6:F:47:ASN:HB2	6:F:89:TYR:CD1	2.54	0.42
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.82	0.42
9:V:18:ARG:HH11	9:V:18:ARG:HG2	1.84	0.42
21:N:1522:TGL:H251	21:N:1522:TGL:H282	1.71	0.42
22:B:230:PSC:H212	22:B:230:PSC:C02	2.50	0.42
7:T:47:PHE:CE2	7:T:77:PRO:HB2	2.54	0.42
1:A:66:ILE:HG23	1:A:246:LEU:HD21	2.02	0.42
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.20	0.42
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.82	0.42
1:N:405:LEU:HD23	1:N:475:ALA:HB2	2.00	0.42
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.19	0.42
27:T:1269:CDL:H561	27:T:1269:CDL:H592	1.85	0.42
21:O:1523:TGL:HB81	21:O:1523:TGL:H122	2.02	0.42
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42
4:D:131:ILE:HD12	4:D:131:ILE:H	1.83	0.42
4:D:107:ILE:HB	4:D:108:PRO:HD2	2.02	0.42
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.54	0.42
3:P:192:VAL:HA	3:P:195:SER:HB2	2.02	0.42
3:P:63:ARG:O	3:P:68:GLN:HG3	2.20	0.41
1:N:169:ILE:N	1:N:169:ILE:HD13	2.34	0.41
1:A:254:ILE:HD13	1:A:254:ILE:HA	1.95	0.41
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.84	0.41
1:N:165:ILE:O	1:N:169:ILE:HG12	2.20	0.41
7:G:78:LEU:HB3	7:G:79:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:48:TRP:CE2	5:R:56:ARG:NH1	2.88	0.41
27:C:270:CDL:H652	27:C:270:CDL:H621	1.79	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.41
1:N:225:GLY:HA2	3:P:109:THR:OG1	2.19	0.41
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.55	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.01	0.41
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.03	0.41
27:G:269:CDL:H761	1:N:282:PHE:CZ	2.55	0.41
21:B:521:TGL:H241	21:B:521:TGL:H201	2.03	0.41
8:U:49:ASP:O	8:U:52:VAL:HG22	2.20	0.41
19:N:1268:PGV:H51	19:N:1268:PGV:H21	1.84	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:HD1	1.86	0.41
4:Q:51:LEU:HD21	4:Q:59:LEU:CD1	2.51	0.41
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.74	0.41
26:T:263:PEK:H312	26:T:263:PEK:H282	1.82	0.41
22:O:1230:PSC:H322	22:O:1230:PSC:H281	2.01	0.41
1:N:191:THR:CG2	1:N:245:ILE:HG23	2.50	0.41
1:A:486:ASP:OD2	4:D:19:ARG:HD3	2.20	0.41
3:C:159:MET:C	3:C:159:MET:SD	2.99	0.41
1:N:35:LEU:HD23	1:N:35:LEU:HA	1.94	0.41
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.84	0.41
2:B:128:LEU:HD11	2:B:134:ARG:HA	2.02	0.41
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.02	0.41
4:D:8:SER:OG	13:M:4:LYS:NZ	2.53	0.41
1:N:113:LEU:O	1:N:117:MET:HG2	2.20	0.41
1:N:472:ILE:HG21	21:N:1522:TGL:HA92	2.03	0.41
3:C:29:SER:HB3	3:C:42:LEU:HD13	2.03	0.41
1:N:208:MET:HB3	1:N:219:PHE:CD1	2.56	0.41
10:W:50:LEU:HD22	10:W:50:LEU:O	2.21	0.41
12:L:20:ARG:HH12	21:L:522:TGL:HC61	1.86	0.41
8:U:40:GLU:HG3	8:U:50:VAL:HG11	2.00	0.41
4:D:9:GLU:H	4:D:9:GLU:CD	2.22	0.41
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.56	0.41
4:D:121:LYS:HG2	11:K:53:TRP:HD1	1.86	0.41
6:F:6:VAL:HA	6:F:7:PRO:HD2	1.92	0.41
3:C:35:PHE:HA	7:G:61:SER:OG	2.21	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
2:O:123:ILE:HD11	2:O:139:ASP:HA	2.03	0.41
3:P:21:ALA:O	3:P:24:ALA:HB3	2.20	0.41
9:V:73:LYS:HB3	9:V:73:LYS:HE3	1.88	0.41
2:B:200:CYS:SG	2:B:204:HIS:HA	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:209:ILE:HA	29:O:3146:HOH:O	2.19	0.41
5:E:46:LYS:HG2	29:E:4386:HOH:O	2.20	0.41
1:N:430:PHE:HE1	21:N:1521:TGL:HB21	1.86	0.41
23:J:60:CHD:H183	23:J:60:CHD:H222	2.03	0.41
2:B:37:LEU:HD13	29:I:4437:HOH:O	2.20	0.41
5:R:72:LYS:HB2	5:R:82:TYR:CD2	2.56	0.41
2:O:122:MET:HB2	2:O:208:PRO:HD2	2.03	0.41
1:N:195:LEU:HD23	1:N:245:ILE:HD13	2.02	0.40
4:D:121:LYS:HG2	11:K:53:TRP:CD1	2.56	0.40
12:L:27:LEU:HA	12:L:27:LEU:HD23	1.92	0.40
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.21	0.40
1:N:498:CYS:HA	1:N:499:PRO:HA	1.77	0.40
7:T:31:CYS:SG	27:T:1269:CDL:H551	2.61	0.40
1:A:472:ILE:HG21	21:L:522:TGL:CA9	2.48	0.40
1:N:180:GLN:HB2	1:N:180:GLN:HE21	1.63	0.40
8:H:20:PHE:HE2	8:H:27:ARG:HG2	1.86	0.40
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.57	0.40
3:C:122:HIS:HB3	29:C:4383:HOH:O	2.20	0.40
3:C:50:ASN:HD21	3:C:54:MET:CE	2.33	0.40
5:R:48:ILE:O	5:R:52:LEU:HG	2.21	0.40
2:O:164:ALA:HB2	2:O:171:LYS:HG3	2.04	0.40
4:D:24:LEU:HD12	5:E:30:ARG:HA	2.04	0.40
3:C:81:TYR:O	3:C:85:LEU:HG	2.20	0.40
1:A:169:ILE:HD12	7:T:7:ASP:O	2.22	0.40
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.40
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.22	0.40
1:A:383:MET:HA	1:A:387:PHE:CD2	2.56	0.40
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.56	0.40
23:G:86:CHD:H12A	23:G:86:CHD:H112	1.56	0.40
6:F:82:CYS:HA	6:F:83:PRO:HD3	1.97	0.40
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.51	0.40
1:A:204:ALA:O	1:A:208:MET:HG3	2.22	0.40
2:B:125:THR:N	29:B:2143:HOH:O	2.54	0.40
1:N:416:ILE:HG22	1:N:464:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
1	N	512/514 (100%)	492 (96%)	20 (4%)	0	100	100
2	B	225/227 (99%)	209 (93%)	13 (6%)	3 (1%)	15	26
2	O	225/227 (99%)	210 (93%)	12 (5%)	3 (1%)	15	26
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
5	E	102/109 (94%)	100 (98%)	1 (1%)	1 (1%)	19	34
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	17	31
6	S	91/98 (93%)	84 (92%)	5 (6%)	2 (2%)	8	13
7	G	81/85 (95%)	66 (82%)	7 (9%)	8 (10%)	1	0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	1
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	3	4
8	U	73/85 (86%)	68 (93%)	4 (6%)	1 (1%)	14	24
9	I	69/73 (94%)	64 (93%)	4 (6%)	1 (1%)	14	24
9	V	69/73 (94%)	66 (96%)	2 (3%)	1 (1%)	14	24
10	J	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3478/3614 (96%)	3315 (95%)	132 (4%)	31 (1%)	21	37

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	39	SER
6	S	95	GLN
7	T	4	ALA
7	T	8	HIS
2	B	60	GLU
2	B	202	SER
7	G	6	GLY
7	G	8	HIS
7	G	37	LEU
7	G	40	GLY
2	O	59	GLN
2	O	202	SER
7	T	3	ALA
7	T	7	ASP
7	T	39	SER
7	T	40	GLY
8	U	47	GLY
7	G	3	ALA
8	H	46	LYS
2	O	60	GLU
7	T	6	GLY
5	E	79	LYS
9	I	36	LYS
9	V	36	LYS
8	H	45	ALA
8	H	47	GLY
6	S	94	HIS
2	B	130	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	416 (98%)	10 (2%)	58	83
1	N	426/426 (100%)	416 (98%)	10 (2%)	58	83
2	B	210/210 (100%)	199 (95%)	11 (5%)	29	51
2	O	210/210 (100%)	192 (91%)	18 (9%)	13	24
3	C	224/226 (99%)	218 (97%)	6 (3%)	52	79
3	P	224/226 (99%)	219 (98%)	5 (2%)	60	84
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	90
4	Q	128/129 (99%)	125 (98%)	3 (2%)	58	83
5	E	91/95 (96%)	89 (98%)	2 (2%)	60	84
5	R	91/95 (96%)	89 (98%)	2 (2%)	60	84
6	F	79/81 (98%)	76 (96%)	3 (4%)	40	67
6	S	79/81 (98%)	73 (92%)	6 (8%)	16	30
7	G	67/68 (98%)	60 (90%)	7 (10%)	9	16
7	T	67/68 (98%)	63 (94%)	4 (6%)	24	43
8	H	67/75 (89%)	61 (91%)	6 (9%)	12	22
8	U	67/75 (89%)	62 (92%)	5 (8%)	17	31
9	I	56/57 (98%)	53 (95%)	3 (5%)	27	49
9	V	56/57 (98%)	52 (93%)	4 (7%)	18	34
10	J	48/50 (96%)	46 (96%)	2 (4%)	36	62
10	W	48/50 (96%)	45 (94%)	3 (6%)	22	40
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	81
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	52
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	81
12	Y	39/40 (98%)	38 (97%)	1 (3%)	54	81
13	M	37/38 (97%)	33 (89%)	4 (11%)	8	15
13	Z	37/38 (97%)	34 (92%)	3 (8%)	15	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3022/3082 (98%)	2898 (96%)	124 (4%)	37 63

All (124) 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	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	377	PHE
1	A	382	SER
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	115	ASP
2	B	167	SER
3	C	29	SER
3	C	77	LYS
3	C	92	LEU
3	C	159	MET
3	C	192	VAL
3	C	230	ASN
4	D	15	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	53	THR
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU

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Mol	Chain	Res	Type
7	G	37	LEU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	27	ARG
8	H	29	CYS
8	H	40	GLU
8	H	51	SER
8	H	60	TYR
8	H	70	SER
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	27	THR
10	J	50	LEU
11	K	47	ARG
12	L	26	THR
13	M	13	LYS
13	M	34	LEU
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	338	MET
1	N	363	LEU
1	N	369	ASP
1	N	382	SER
1	N	484	THR
1	N	513	LEU
2	O	32	PHE
2	O	33	LEU
2	O	57	ASP
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER

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Mol	Chain	Res	Type
2	O	113	TYR
2	O	115	ASP
2	O	148	MET
2	O	167	SER
2	O	183	THR
2	O	205	SER
2	O	217	LYS
3	P	29	SER
3	P	41	THR
3	P	127	LEU
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	121	LYS
4	Q	143	ASN
5	R	70	VAL
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	17	ARG
7	T	18	PHE
7	T	38	HIS
7	T	84	LYS
8	U	27	ARG
8	U	29	CYS
8	U	52	VAL
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	10	ARG
9	V	21	ILE
9	V	29	LEU
10	W	4	ARG
10	W	50	LEU
10	W	54	SER
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG

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Mol	Chain	Res	Type
13	Z	13	LYS
13	Z	38	ASP
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	149	HIS
4	D	37	GLN
4	D	109	HIS
5	E	78	HIS
5	E	94	ASN
7	G	76	ASN
8	H	22	ASN
9	I	8	GLN
10	J	29	ASN
11	K	35	GLN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	143	ASN

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Mol	Chain	Res	Type
5	R	78	HIS
5	R	94	ASN
6	S	94	HIS
7	T	66	ASN
7	T	71	HIS
7	T	76	ASN
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	0.64	0	6,9,11	3.06	3 (50%)
2	FME	B	1	2	8,9,10	0.83	0	6,9,11	3.34	1 (16%)
7	TPO	G	11	7	8,10,11	1.72	2 (25%)	7,14,16	1.30	1 (14%)
1	FME	N	1	1	8,9,10	0.54	0	6,9,11	3.55	3 (50%)
2	FME	O	1	2	8,9,10	0.63	0	6,9,11	2.70	2 (33%)
7	TPO	T	11	7	8,10,11	1.60	1 (12%)	7,14,16	1.87	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	G	11	7	-	0/8/11/13	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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O2P	2.11	1.62	1.54
7	G	11	TPO	P-O1P	2.58	1.59	1.51
7	T	11	TPO	P-O1P	2.98	1.61	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-7.29	111.62	122.82
1	N	1	FME	CA-N-CN	-7.22	111.72	122.82
2	O	1	FME	CA-N-CN	-5.38	114.54	122.82
1	A	1	FME	O1-CN-N	-4.24	118.66	124.76
1	A	1	FME	CA-N-CN	-4.21	116.34	122.82
1	N	1	FME	O-C-CA	-2.58	118.63	125.44
7	T	11	TPO	O-C-CA	-2.32	119.31	125.44
7	G	11	TPO	O-C-CA	-2.30	119.36	125.44
2	O	1	FME	CE-SD-CG	2.30	108.23	100.37
7	T	11	TPO	CG2-CB-CA	3.95	121.20	113.17
1	A	1	FME	CE-SD-CG	4.01	114.05	100.37
1	N	1	FME	CE-SD-CG	4.01	114.07	100.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
2	B	1	FME	3	0
1	N	1	FME	1	0
2	O	1	FME	3	0
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	HEA	A	515	1	40,67,67	1.06	2 (5%)	41,103,103	2.73	18 (43%)
18	HEA	A	516	1,15	40,67,67	2.19	14 (35%)	41,103,103	4.60	23 (56%)
15	PER	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	A	521	-	50,50,50	1.06	2 (4%)	51,56,56	1.28	5 (9%)
19	PGV	A	524	-	50,50,50	1.15	2 (4%)	51,56,56	1.25	5 (9%)
23	CHD	B	1086	-	29,32,32	1.19	3 (10%)	48,51,51	5.34	32 (66%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.26	3 (5%)	55,59,59	1.24	5 (9%)
21	TGL	B	521	-	62,62,62	1.25	6 (9%)	65,65,65	1.73	10 (15%)
26	PEK	C	265	-	51,52,52	1.31	4 (7%)	52,57,57	1.29	4 (7%)
19	PGV	C	267	-	50,50,50	0.84	2 (4%)	51,56,56	1.21	5 (9%)
19	PGV	C	268	-	50,50,50	1.15	2 (4%)	51,56,56	1.34	4 (7%)
27	CDL	C	270	-	99,99,99	1.31	13 (13%)	101,111,111	1.34	11 (10%)
23	CHD	C	271	-	29,32,32	0.75	0	48,51,51	4.76	32 (66%)
24	DMU	C	272	-	34,34,34	1.16	2 (5%)	45,45,45	3.43	23 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	C	525	-	29,32,32	1.19	2 (6%)	48,51,51	4.92	35 (72%)
21	TGL	D	523	-	62,62,62	1.42	6 (9%)	65,65,65	1.52	12 (18%)
26	PEK	G	1263	-	51,52,52	1.27	4 (7%)	52,57,57	1.27	4 (7%)
26	PEK	G	264	-	51,52,52	0.97	3 (5%)	52,57,57	1.28	4 (7%)
27	CDL	G	269	-	99,99,99	1.35	11 (11%)	101,111,111	1.28	10 (9%)
23	CHD	G	86	-	29,32,32	1.05	2 (6%)	48,51,51	5.05	33 (68%)
23	CHD	J	60	-	29,32,32	0.89	1 (3%)	48,51,51	4.90	33 (68%)
21	TGL	L	522	-	62,62,62	1.33	5 (8%)	65,65,65	1.49	8 (12%)
24	DMU	M	526	-	34,34,34	0.78	2 (5%)	45,45,45	3.18	23 (51%)
19	PGV	N	1266	-	50,50,50	0.93	3 (6%)	51,56,56	1.41	6 (11%)
19	PGV	N	1268	-	50,50,50	1.15	2 (4%)	51,56,56	1.39	5 (9%)
21	TGL	N	1521	-	62,62,62	1.43	7 (11%)	65,65,65	1.68	13 (20%)
21	TGL	N	1522	-	62,62,62	1.47	7 (11%)	65,65,65	1.40	10 (15%)
19	PGV	N	1524	-	50,50,50	1.09	2 (4%)	51,56,56	1.27	5 (9%)
18	HEA	N	515	1	40,67,67	0.86	0	41,103,103	2.60	16 (39%)
18	HEA	N	516	1,15	40,67,67	1.28	6 (15%)	41,103,103	2.08	11 (26%)
15	PER	N	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	O	1230	-	51,51,51	1.20	3 (5%)	55,59,59	1.09	3 (5%)
21	TGL	O	1523	-	62,62,62	1.37	6 (9%)	65,65,65	1.24	9 (13%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
26	PEK	P	1264	-	51,52,52	0.99	4 (7%)	52,57,57	1.53	7 (13%)
26	PEK	P	1265	-	51,52,52	1.65	5 (9%)	52,57,57	1.40	7 (13%)
19	PGV	P	1267	-	50,50,50	0.87	2 (4%)	51,56,56	1.03	4 (7%)
27	CDL	P	1270	-	99,99,99	1.31	10 (10%)	101,111,111	1.30	12 (11%)
23	CHD	P	1271	-	29,32,32	0.75	0	48,51,51	4.90	30 (62%)
24	DMU	P	1272	-	34,34,34	1.17	2 (5%)	45,45,45	3.34	24 (53%)
23	CHD	P	1525	-	29,32,32	0.89	1 (3%)	48,51,51	5.18	37 (77%)
27	CDL	T	1269	-	99,99,99	1.29	12 (12%)	101,111,111	1.44	12 (11%)
26	PEK	T	263	-	51,52,52	1.43	5 (9%)	52,57,57	1.43	5 (9%)
23	CHD	W	1060	-	29,32,32	1.06	2 (6%)	48,51,51	5.12	34 (70%)
24	DMU	Z	1526	-	34,34,34	0.94	2 (5%)	45,45,45	3.22	19 (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
18	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	A	520	18,14	-	0/0/0/0	0/0/0/0
19	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	PGV	A	524	-	-	1/55/55/55	0/0/0/0
23	CHD	B	1086	-	1/1/12/12	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	230	-	-	0/55/55/55	0/0/0/0
21	TGL	B	521	-	-	0/65/65/65	0/0/0/0
26	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
27	CDL	C	270	-	-	0/110/110/110	0/0/0/0
23	CHD	C	271	-	2/2/12/12	0/7/74/74	0/4/4/4
24	DMU	C	272	-	5/5/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	1/1/12/12	0/7/74/74	0/4/4/4
21	TGL	D	523	-	-	0/65/65/65	0/0/0/0
26	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	PEK	G	264	-	-	0/56/56/56	0/0/0/0
27	CDL	G	269	-	-	1/110/110/110	0/0/0/0
23	CHD	G	86	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	J	60	-	1/1/12/12	0/7/74/74	0/4/4/4
21	TGL	L	522	-	-	0/65/65/65	0/0/0/0
24	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	PGV	N	1268	-	-	0/55/55/55	0/0/0/0
21	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
21	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	1/55/55/55	0/0/0/0
18	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
18	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	PER	N	520	18,14	-	0/0/0/0	0/0/0/0
22	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
21	TGL	O	1523	-	-	0/65/65/65	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
26	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
26	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
27	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
23	CHD	P	1271	-	2/2/12/12	0/7/74/74	0/4/4/4
24	DMU	P	1272	-	5/5/10/10	0/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	P	1525	-	1/1/12/12	0/7/74/74	0/4/4/4
27	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
26	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1060	-	1/1/12/12	0/7/74/74	0/4/4/4
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C4B-NB	-4.39	1.30	1.36
18	A	516	HEA	C4A-NA	-4.30	1.30	1.36
23	B	1086	CHD	C13-C14	-3.22	1.49	1.55
26	P	1264	PEK	O03-C01	-3.13	1.38	1.45
27	C	270	CDL	C59-C58	-3.11	1.33	1.51
21	L	522	TGL	C20-CA9	-3.11	1.33	1.51
18	A	515	HEA	C4A-NA	-3.10	1.32	1.36
21	N	1521	TGL	C10-CB9	-3.09	1.33	1.51
21	L	522	TGL	C10-CB9	-3.05	1.33	1.51
24	Z	1526	DMU	C3-C4	-3.00	1.44	1.52
21	N	1522	TGL	C20-CA9	-3.00	1.34	1.51
27	P	1270	CDL	C59-C58	-2.96	1.34	1.51
27	P	1270	CDL	C62-C61	-2.93	1.34	1.51
27	G	269	CDL	C42-C41	-2.93	1.34	1.51
21	N	1522	TGL	C10-CB9	-2.90	1.34	1.51
27	G	269	CDL	C39-C38	-2.88	1.34	1.51
21	D	523	TGL	C15-CC9	-2.87	1.34	1.51
27	G	269	CDL	C59-C58	-2.87	1.34	1.51
27	C	270	CDL	C79-C78	-2.87	1.34	1.51
21	B	521	TGL	C10-CB9	-2.84	1.35	1.51
21	O	1523	TGL	C15-CC9	-2.83	1.35	1.51
27	P	1270	CDL	C22-C21	-2.80	1.35	1.51
27	P	1270	CDL	C19-C18	-2.78	1.35	1.51
27	T	1269	CDL	C62-C61	-2.78	1.35	1.51
27	G	269	CDL	C19-C18	-2.77	1.35	1.51
21	N	1521	TGL	C20-CA9	-2.76	1.35	1.51
21	O	1523	TGL	C10-CB9	-2.74	1.35	1.51
27	T	1269	CDL	C19-C18	-2.74	1.35	1.51
27	C	270	CDL	C62-C61	-2.73	1.35	1.51
27	G	269	CDL	C62-C61	-2.72	1.35	1.51
27	C	270	CDL	C22-C21	-2.71	1.35	1.51
21	B	521	TGL	C20-CA9	-2.71	1.35	1.51
27	T	1269	CDL	C42-C41	-2.69	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	270	CDL	C39-C38	-2.64	1.36	1.51
24	M	526	DMU	C3-C4	-2.63	1.45	1.52
21	D	523	TGL	C20-CA9	-2.63	1.36	1.51
27	T	1269	CDL	C39-C38	-2.61	1.36	1.51
26	G	264	PEK	O03-C01	-2.61	1.39	1.45
21	D	523	TGL	C10-CB9	-2.60	1.36	1.51
23	B	1086	CHD	C10-C5	-2.59	1.51	1.55
23	C	525	CHD	C13-C14	-2.58	1.51	1.55
21	N	1522	TGL	C15-CC9	-2.57	1.36	1.51
27	T	1269	CDL	C59-C58	-2.56	1.36	1.51
27	C	270	CDL	C42-C41	-2.56	1.36	1.51
27	C	270	CDL	C19-C18	-2.50	1.37	1.51
27	C	270	CDL	C82-C81	-2.49	1.37	1.51
21	N	1521	TGL	C15-CC9	-2.47	1.37	1.51
21	O	1523	TGL	C20-CA9	-2.47	1.37	1.51
27	G	269	CDL	C82-C81	-2.40	1.37	1.51
27	T	1269	CDL	C22-C21	-2.39	1.37	1.51
21	B	521	TGL	C15-CC9	-2.38	1.37	1.51
23	P	1525	CHD	C13-C14	-2.37	1.51	1.55
27	P	1270	CDL	C39-C38	-2.36	1.37	1.51
27	T	1269	CDL	C82-C81	-2.33	1.38	1.51
18	N	516	HEA	C3C-C2C	-2.23	1.37	1.40
23	B	1086	CHD	C13-C12	-2.19	1.51	1.54
27	C	270	CDL	OB6-CB4	-2.09	1.41	1.46
23	G	86	CHD	C10-C5	-2.08	1.51	1.55
26	P	1264	PEK	O01-C02	-2.06	1.41	1.46
27	P	1270	CDL	C42-C41	-2.06	1.39	1.51
27	G	269	CDL	C22-C21	-2.05	1.39	1.51
24	M	526	DMU	O16-C6	2.03	1.43	1.40
26	G	1263	PEK	C01-C02	2.04	1.56	1.50
27	T	1269	CDL	CB6-CB4	2.05	1.56	1.50
26	T	263	PEK	C9-C8	2.05	1.43	1.31
26	G	1263	PEK	C03-C02	2.09	1.56	1.50
23	J	60	CHD	C11-C9	2.09	1.57	1.53
26	C	265	PEK	P-O12	2.11	1.68	1.59
21	N	1522	TGL	CG1-CG2	2.13	1.56	1.50
18	A	515	HEA	O11-C11	2.16	1.47	1.42
18	N	516	HEA	C4D-CHA	2.18	1.45	1.39
19	N	1266	PGV	C01-C02	2.18	1.56	1.50
18	N	516	HEA	C22-C23	2.19	1.39	1.32
24	P	1272	DMU	O1-C10	2.19	1.47	1.41
26	P	1265	PEK	C10-C9	2.26	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C20-C19	2.27	1.56	1.51
26	T	263	PEK	C01-C02	2.27	1.57	1.50
26	T	263	PEK	C03-C02	2.29	1.57	1.50
23	G	86	CHD	C11-C9	2.30	1.57	1.53
18	A	516	HEA	C4C-CHD	2.31	1.46	1.39
23	W	1060	CHD	C20-C17	2.33	1.58	1.54
18	A	516	HEA	C3C-CAC	2.35	1.52	1.47
24	Z	1526	DMU	O16-C6	2.39	1.44	1.40
24	C	272	DMU	O1-C10	2.40	1.48	1.41
18	A	516	HEA	C18-C19	2.42	1.37	1.33
18	N	516	HEA	C4C-CHD	2.45	1.46	1.39
26	P	1264	PEK	O03-C21	2.47	1.40	1.33
18	A	516	HEA	C14-C15	2.51	1.37	1.33
19	P	1267	PGV	O01-C1	2.56	1.41	1.34
18	A	516	HEA	OMA-CMA	2.56	1.29	1.21
18	A	516	HEA	C3A-CMA	2.59	1.52	1.46
26	C	265	PEK	C7-C6	2.60	1.65	1.51
19	N	1266	PGV	O01-C1	2.61	1.42	1.34
18	N	516	HEA	C18-C19	2.76	1.38	1.33
26	P	1265	PEK	C6-C5	2.81	1.47	1.31
26	G	264	PEK	O03-C21	2.83	1.41	1.33
23	W	1060	CHD	C11-C9	2.99	1.58	1.53
18	A	516	HEA	CAD-C3D	3.00	1.57	1.52
19	C	267	PGV	O01-C1	3.00	1.43	1.34
18	N	516	HEA	O11-C11	3.09	1.50	1.42
23	C	525	CHD	C18-C13	3.19	1.59	1.54
18	A	516	HEA	C1C-CHC	3.28	1.48	1.39
26	P	1264	PEK	O01-C1	3.47	1.44	1.34
21	B	521	TGL	OG3-CC1	3.49	1.43	1.33
21	L	522	TGL	OG3-CC1	3.63	1.44	1.33
19	C	267	PGV	O03-C19	3.69	1.44	1.33
19	A	524	PGV	O01-C1	3.70	1.45	1.34
21	N	1521	TGL	CA6-CA5	3.71	1.73	1.51
26	G	264	PEK	O01-C1	3.72	1.45	1.34
27	C	270	CDL	OB6-CB5	3.77	1.45	1.34
22	O	1230	PSC	O03-C19	3.81	1.44	1.33
19	N	1524	PGV	O01-C1	3.90	1.46	1.34
19	P	1267	PGV	O03-C19	3.92	1.45	1.33
22	B	230	PSC	C13-C12	3.99	1.54	1.31
22	O	1230	PSC	O01-C1	4.00	1.46	1.34
27	P	1270	CDL	OB6-CB5	4.09	1.46	1.34
24	C	272	DMU	O16-C6	4.09	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	1269	CDL	OA8-CA7	4.10	1.45	1.33
18	A	516	HEA	CAA-C2A	4.15	1.60	1.52
19	N	1268	PGV	O03-C19	4.20	1.46	1.33
22	O	1230	PSC	C13-C12	4.21	1.56	1.31
27	G	269	CDL	OA8-CA7	4.22	1.46	1.33
19	N	1266	PGV	O03-C19	4.22	1.46	1.33
19	C	268	PGV	O03-C19	4.23	1.46	1.33
21	N	1522	TGL	OG3-CC1	4.24	1.46	1.33
21	N	1521	TGL	OG3-CC1	4.24	1.46	1.33
21	B	521	TGL	OG2-CB1	4.29	1.47	1.34
27	C	270	CDL	OB8-CB7	4.31	1.46	1.33
19	A	521	PGV	O01-C1	4.32	1.47	1.34
27	T	1269	CDL	OA6-CA5	4.33	1.47	1.34
24	P	1272	DMU	O16-C6	4.41	1.48	1.40
22	B	230	PSC	O03-C19	4.45	1.46	1.33
26	C	265	PEK	O01-C1	4.48	1.47	1.34
18	A	516	HEA	C1B-CHB	4.51	1.52	1.39
19	A	521	PGV	O03-C19	4.51	1.46	1.33
21	N	1521	TGL	OG2-CB1	4.52	1.47	1.34
21	O	1523	TGL	OG3-CC1	4.55	1.47	1.33
27	C	270	CDL	OA6-CA5	4.56	1.48	1.34
21	B	521	TGL	OG1-CA1	4.56	1.47	1.33
27	P	1270	CDL	OA6-CA5	4.56	1.48	1.34
27	P	1270	CDL	OB8-CB7	4.59	1.47	1.33
27	G	269	CDL	OB6-CB5	4.64	1.48	1.34
26	G	1263	PEK	O01-C1	4.65	1.48	1.34
21	O	1523	TGL	OG1-CA1	4.68	1.47	1.33
26	P	1265	PEK	O01-C1	4.75	1.48	1.34
27	T	1269	CDL	OB8-CB7	4.81	1.47	1.33
27	T	1269	CDL	OB6-CB5	4.82	1.48	1.34
21	D	523	TGL	OG1-CA1	4.83	1.47	1.33
27	G	269	CDL	OA6-CA5	4.85	1.48	1.34
27	G	269	CDL	OB8-CB7	4.88	1.48	1.33
22	B	230	PSC	O01-C1	4.89	1.49	1.34
21	D	523	TGL	OG2-CB1	4.93	1.49	1.34
21	O	1523	TGL	OG2-CB1	4.93	1.49	1.34
26	T	263	PEK	O01-C1	4.95	1.49	1.34
21	L	522	TGL	OG2-CB1	4.97	1.49	1.34
27	C	270	CDL	OA8-CA7	4.97	1.48	1.33
21	N	1521	TGL	OG1-CA1	4.99	1.48	1.33
26	P	1265	PEK	O03-C21	5.02	1.48	1.33
19	C	268	PGV	O01-C1	5.02	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	265	PEK	O03-C21	5.08	1.48	1.33
19	N	1524	PGV	O03-C19	5.10	1.48	1.33
19	N	1268	PGV	O01-C1	5.18	1.49	1.34
27	P	1270	CDL	OA8-CA7	5.22	1.49	1.33
21	L	522	TGL	OG1-CA1	5.28	1.49	1.33
26	G	1263	PEK	O03-C21	5.33	1.49	1.33
21	N	1522	TGL	OG2-CB1	5.35	1.50	1.34
21	D	523	TGL	OG3-CC1	5.40	1.49	1.33
21	N	1522	TGL	OG1-CA1	5.50	1.49	1.33
19	A	524	PGV	O03-C19	5.58	1.50	1.33
18	A	516	HEA	C1A-NA	5.79	1.44	1.36
26	T	263	PEK	O03-C21	5.84	1.50	1.33
26	P	1265	PEK	C7-C6	6.84	1.88	1.51

All (608) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C18-C13-C12	-14.56	94.89	109.09
18	A	516	HEA	CAD-C3D-C4D	-13.81	112.02	127.01
23	G	86	CHD	C18-C13-C12	-10.07	99.27	109.09
23	W	1060	CHD	C6-C5-C4	-8.49	101.57	111.05
23	B	1086	CHD	C19-C10-C9	-8.01	99.18	111.18
23	G	86	CHD	C19-C10-C9	-7.71	99.62	111.18
23	C	525	CHD	C18-C13-C12	-7.52	101.76	109.09
18	A	516	HEA	CAA-CBA-CGA	-7.38	99.23	112.75
23	P	1525	CHD	C19-C10-C9	-7.32	100.20	111.18
18	A	516	HEA	CMB-C2B-C3B	-7.09	110.64	125.14
23	P	1271	CHD	C17-C13-C12	-6.89	111.57	117.68
23	B	1086	CHD	C18-C13-C17	-6.88	100.37	111.22
23	G	86	CHD	C18-C13-C17	-6.79	100.50	111.22
23	P	1525	CHD	C18-C13-C12	-6.65	102.61	109.09
23	P	1525	CHD	C18-C13-C14	-6.40	101.13	111.22
23	P	1525	CHD	C6-C5-C4	-6.24	104.08	111.05
23	J	60	CHD	C6-C5-C4	-6.10	104.23	111.05
23	C	525	CHD	C19-C10-C9	-6.08	102.06	111.18
18	A	516	HEA	CAA-C2A-C3A	-5.88	111.86	128.66
23	P	1525	CHD	C18-C13-C17	-5.48	102.57	111.22
23	P	1525	CHD	C23-C22-C20	-5.43	108.35	114.75
23	G	86	CHD	O12-C12-C13	-5.39	102.37	111.11
23	C	525	CHD	C6-C5-C4	-5.36	105.06	111.05
18	A	516	HEA	C4B-C3B-C11	-5.29	121.27	127.01
23	J	60	CHD	C18-C13-C12	-5.23	103.99	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C18-C13-C17	-5.21	103.00	111.22
23	C	525	CHD	O12-C12-C13	-5.15	102.76	111.11
18	A	516	HEA	CBA-CAA-C2A	-5.13	103.33	112.53
18	A	516	HEA	CMD-C2D-C3D	-5.12	114.53	125.24
23	B	1086	CHD	O7-C7-C6	-5.06	97.68	110.06
23	P	1271	CHD	C18-C13-C12	-4.98	104.23	109.09
21	L	522	TGL	OG3-CC1-OC1	-4.97	110.66	123.49
18	N	516	HEA	OMA-CMA-C3A	-4.91	115.19	125.11
23	W	1060	CHD	C18-C13-C12	-4.85	104.36	109.09
18	A	516	HEA	O11-C11-C12	-4.83	97.92	109.73
23	P	1525	CHD	O7-C7-C6	-4.80	98.31	110.06
26	P	1264	PEK	O03-C01-C02	-4.79	95.79	108.69
23	G	86	CHD	C6-C5-C4	-4.75	105.74	111.05
23	W	1060	CHD	C19-C10-C5	-4.73	101.89	110.25
18	N	516	HEA	CAD-CBD-CGD	-4.51	104.48	112.75
23	W	1060	CHD	C1-C10-C9	-4.49	104.20	111.45
23	B	1086	CHD	C6-C5-C4	-4.36	106.18	111.05
23	C	525	CHD	C18-C13-C14	-4.34	104.38	111.22
23	P	1525	CHD	O12-C12-C11	-4.30	100.25	109.06
26	P	1265	PEK	C7-C6-C5	-4.29	98.48	125.00
19	A	521	PGV	O03-C19-O04	-4.28	112.44	123.49
19	N	1266	PGV	O03-C19-O04	-4.27	112.48	123.49
23	W	1060	CHD	O7-C7-C6	-4.16	99.87	110.06
18	A	515	HEA	C26-C15-C14	-4.15	115.36	123.50
18	N	515	HEA	C27-C19-C18	-4.05	115.55	123.50
23	C	271	CHD	C6-C5-C4	-3.95	106.63	111.05
26	P	1264	PEK	C24-C23-C22	-3.95	98.80	113.29
23	C	271	CHD	C19-C10-C1	-3.94	101.57	108.20
18	A	515	HEA	CAA-C2A-C1A	-3.87	122.80	127.01
23	P	1525	CHD	C1-C10-C9	-3.81	105.30	111.45
23	J	60	CHD	C19-C10-C5	-3.79	103.57	110.25
21	N	1521	TGL	CG1-OG1-CA1	-3.76	106.33	116.85
23	P	1271	CHD	C19-C10-C5	-3.68	103.76	110.25
23	P	1525	CHD	C22-C20-C17	-3.67	102.54	110.24
23	B	1086	CHD	C19-C10-C5	-3.66	103.78	110.25
23	B	1086	CHD	C1-C10-C9	-3.55	105.72	111.45
26	C	265	PEK	O03-C21-O04	-3.55	114.33	123.49
18	A	515	HEA	C1A-C2A-C3A	-3.52	103.55	107.07
26	P	1264	PEK	O01-C1-O02	-3.52	114.23	123.67
23	G	86	CHD	C18-C13-C14	-3.51	105.68	111.22
24	M	526	DMU	O7-C10-C5	-3.51	99.56	108.10
18	N	515	HEA	C12-C13-C14	-3.51	102.58	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	516	HEA	C1A-C2A-C3A	-3.48	103.59	107.07
26	G	264	PEK	O01-C1-O02	-3.47	114.36	123.67
26	G	264	PEK	O03-C01-C02	-3.43	99.47	108.69
23	C	271	CHD	C23-C22-C20	-3.42	110.72	114.75
23	J	60	CHD	C1-C10-C9	-3.40	105.96	111.45
21	N	1521	TGL	CA6-CA5-CA4	-3.39	97.02	114.53
23	C	271	CHD	C18-C13-C12	-3.38	105.79	109.09
23	W	1060	CHD	C23-C22-C20	-3.38	110.77	114.75
23	G	86	CHD	C1-C10-C9	-3.37	106.01	111.45
23	P	1525	CHD	O12-C12-C13	-3.37	105.65	111.11
18	A	515	HEA	C12-C13-C14	-3.24	103.32	112.40
18	N	516	HEA	CAD-C3D-C4D	-3.24	123.49	127.01
23	G	86	CHD	O12-C12-C11	-3.20	102.52	109.06
23	B	1086	CHD	C18-C13-C14	-3.20	106.18	111.22
18	N	516	HEA	C20-C19-C18	-3.19	115.00	121.05
18	N	515	HEA	C21-C20-C19	-3.19	102.33	112.71
23	G	86	CHD	O7-C7-C6	-3.19	102.26	110.06
23	P	1271	CHD	C19-C10-C9	-3.18	106.41	111.18
18	A	516	HEA	C13-C14-C15	-3.11	121.00	127.76
23	B	1086	CHD	O12-C12-C13	-3.11	106.07	111.11
18	A	515	HEA	C20-C21-C22	-3.09	103.59	111.69
19	N	1268	PGV	O03-C19-O04	-3.05	115.62	123.49
23	C	271	CHD	O7-C7-C6	-3.05	102.59	110.06
27	P	1270	CDL	OB8-CB7-OB9	-3.02	115.69	123.49
27	T	1269	CDL	OA6-CA5-OA7	-3.02	115.57	123.67
18	N	516	HEA	CMB-C2B-C1B	-3.00	123.39	128.36
27	C	270	CDL	OB8-CB7-OB9	-3.00	115.75	123.49
21	N	1522	TGL	OG3-CC1-OC1	-2.99	115.78	123.49
22	O	1230	PSC	O01-C1-O02	-2.96	115.73	123.67
21	B	521	TGL	CG1-OG1-CA1	-2.95	108.59	116.85
26	G	264	PEK	C24-C23-C22	-2.89	102.68	113.29
21	B	521	TGL	OG3-CC1-OC1	-2.87	116.08	123.49
18	A	515	HEA	CMC-C2C-C1C	-2.87	123.62	128.36
19	N	1268	PGV	C03-C02-C01	-2.84	105.43	112.07
19	C	268	PGV	O03-C19-O04	-2.83	116.19	123.49
23	W	1060	CHD	C18-C13-C14	-2.79	106.82	111.22
18	N	515	HEA	C26-C15-C14	-2.76	118.08	123.50
23	C	525	CHD	O7-C7-C6	-2.75	103.32	110.06
19	N	1266	PGV	O01-C1-O02	-2.75	116.30	123.67
23	P	1271	CHD	O7-C7-C6	-2.73	103.37	110.06
24	Z	1526	DMU	O7-C10-C5	-2.72	101.49	108.10
26	P	1265	PEK	O03-C21-O04	-2.71	116.50	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C19-C10-C5	-2.70	105.49	110.25
27	T	1269	CDL	OA8-CA7-OA9	-2.67	116.61	123.49
19	N	1266	PGV	C01-O03-C19	-2.64	109.48	116.85
18	N	515	HEA	CAD-C3D-C4D	-2.63	124.16	127.01
18	A	515	HEA	OMA-CMA-C3A	-2.61	119.84	125.11
19	N	1266	PGV	C15-C14-C13	-2.59	103.75	113.86
18	A	515	HEA	O11-C11-C3B	-2.52	104.38	111.82
23	P	1271	CHD	C6-C5-C4	-2.52	108.23	111.05
21	N	1521	TGL	CA7-CA6-CA5	-2.51	101.58	114.53
24	M	526	DMU	O7-C10-O1	-2.50	104.34	110.68
26	P	1265	PEK	C8-C7-C6	-2.50	103.68	112.00
19	C	267	PGV	O03-C19-O04	-2.49	117.08	123.49
21	O	1523	TGL	OG1-CA1-OA1	-2.47	117.11	123.49
26	P	1264	PEK	C3-C2-C1	-2.46	103.93	113.59
21	N	1521	TGL	CB7-CB6-CB5	-2.45	101.90	114.53
23	P	1271	CHD	C23-C22-C20	-2.44	111.87	114.75
27	G	269	CDL	OA6-CA5-OA7	-2.44	117.12	123.67
18	A	516	HEA	CMC-C2C-C3C	-2.42	120.36	125.09
23	J	60	CHD	C23-C22-C20	-2.42	111.91	114.75
23	J	60	CHD	O7-C7-C6	-2.41	104.15	110.06
23	P	1271	CHD	C19-C10-C1	-2.41	104.15	108.20
19	P	1267	PGV	O03-C19-O04	-2.39	117.33	123.49
27	C	270	CDL	CA6-CA4-CA3	-2.38	106.49	112.07
21	D	523	TGL	CG3-CG2-CG1	-2.35	106.58	112.07
27	G	269	CDL	OB8-CB7-OB9	-2.35	117.43	123.49
27	P	1270	CDL	C78-C77-C76	-2.33	102.51	114.53
21	N	1522	TGL	C24-C23-C22	-2.33	102.51	114.53
23	C	271	CHD	C19-C10-C5	-2.30	106.19	110.25
23	C	271	CHD	O12-C12-C11	-2.30	104.37	109.06
23	G	86	CHD	C19-C10-C5	-2.28	106.23	110.25
19	N	1524	PGV	O03-C19-O04	-2.27	117.62	123.49
21	N	1522	TGL	CB9-CB8-CB7	-2.26	102.84	114.53
18	A	515	HEA	C25-C23-C22	-2.25	115.36	122.61
19	P	1267	PGV	C8-C9-C10	-2.24	105.11	113.86
27	C	270	CDL	OA8-CA7-OA9	-2.24	117.71	123.49
18	N	515	HEA	C16-C15-C14	-2.23	116.81	121.05
27	C	270	CDL	C52-C51-CB5	-2.23	104.82	113.59
27	T	1269	CDL	CA4-OA6-CA5	-2.22	112.55	117.89
26	P	1264	PEK	O01-C02-C01	-2.22	100.55	108.36
22	B	230	PSC	O01-C1-O02	-2.21	117.74	123.67
21	B	521	TGL	CB7-CB6-CB5	-2.21	103.14	114.53
27	P	1270	CDL	OA8-CA7-OA9	-2.20	117.81	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1268	PGV	O02-C1-C2	-2.19	114.94	123.72
23	C	525	CHD	C23-C22-C20	-2.18	112.18	114.75
23	C	525	CHD	C1-C10-C9	-2.16	107.97	111.45
18	N	515	HEA	C17-C18-C19	-2.16	123.07	127.76
21	N	1521	TGL	OG1-CA1-OA1	-2.15	117.94	123.49
23	W	1060	CHD	C19-C10-C1	-2.15	104.58	108.20
23	C	271	CHD	C18-C13-C17	-2.15	107.83	111.22
19	C	267	PGV	C9-C10-C11	-2.14	101.20	112.45
23	P	1525	CHD	O7-C7-C8	-2.14	104.54	109.26
18	A	515	HEA	C16-C15-C14	-2.13	117.01	121.05
18	N	515	HEA	CAA-CBA-CGA	-2.10	108.90	112.75
21	O	1523	TGL	OG3-CC1-OC1	-2.10	118.08	123.49
19	P	1267	PGV	C27-C26-C25	-2.09	103.71	114.53
27	G	269	CDL	OA8-CA7-OA9	-2.08	118.12	123.49
23	B	1086	CHD	O7-C7-C8	-2.08	104.67	109.26
18	A	516	HEA	C26-C15-C14	-2.07	119.44	123.50
18	N	515	HEA	CMB-C2B-C1B	-2.06	124.96	128.36
18	N	516	HEA	C13-C14-C15	-2.04	123.34	127.76
19	C	267	PGV	C27-C26-C25	-2.02	104.08	114.53
22	B	230	PSC	C32-C31-C30	-2.02	104.10	114.53
23	C	271	CHD	C22-C23-C24	-2.02	104.78	113.02
22	B	230	PSC	C29-C28-C27	-2.02	104.11	114.53
27	C	270	CDL	C57-C56-C55	-2.02	104.11	114.53
19	A	521	PGV	C26-C25-C24	-2.01	104.15	114.53
27	P	1270	CDL	OA6-CA5-OA7	-2.01	118.28	123.67
23	C	525	CHD	C22-C20-C17	-2.01	106.02	110.24
23	C	525	CHD	C19-C10-C5	-2.00	106.72	110.25
18	N	516	HEA	CMD-C2D-C3D	2.01	129.43	125.24
23	G	86	CHD	C13-C14-C8	2.01	117.34	114.75
18	A	515	HEA	C3C-C4C-NC	2.02	111.82	109.21
22	O	1230	PSC	O03-C19-C20	2.02	118.05	111.90
18	A	516	HEA	C16-C17-C18	2.02	116.97	111.69
27	T	1269	CDL	CA6-OA8-CA7	2.03	122.52	116.85
27	G	269	CDL	C83-C82-C81	2.04	125.05	114.53
18	A	516	HEA	C20-C21-C22	2.04	117.02	111.69
24	P	1272	DMU	O7-C3-C2	2.04	112.43	107.17
26	P	1265	PEK	O03-C01-C02	2.04	114.18	108.69
21	N	1521	TGL	C15-CC9-CC8	2.05	125.09	114.53
23	B	1086	CHD	C14-C8-C7	2.05	114.58	111.74
24	M	526	DMU	C11-C9-C8	2.07	118.11	113.02
21	O	1523	TGL	C11-C10-CB9	2.07	125.22	114.53
27	P	1270	CDL	C20-C19-C18	2.07	125.24	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	267	PGV	O03-C19-C20	2.08	118.24	111.90
21	L	522	TGL	CG2-OG2-CB1	2.09	122.91	117.89
24	P	1272	DMU	O7-C10-O1	2.10	116.00	110.68
19	C	268	PGV	O03-C01-C02	2.11	114.36	108.69
27	P	1270	CDL	C39-C38-C37	2.11	125.41	114.53
24	M	526	DMU	O5-C6-O16	2.13	115.17	110.05
22	B	230	PSC	O03-C19-C20	2.13	118.39	111.90
24	M	526	DMU	O55-C2-C1	2.13	115.14	110.34
24	P	1272	DMU	O4-C7-C5	2.14	115.16	110.34
21	D	523	TGL	CG1-OG1-CA1	2.18	122.94	116.85
19	A	524	PGV	O01-C02-C01	2.18	116.05	108.36
21	D	523	TGL	C20-CA9-CA8	2.20	125.91	114.53
21	L	522	TGL	OG2-CB1-CB2	2.23	116.38	111.53
23	B	1086	CHD	C2-C1-C10	2.24	116.84	112.84
23	C	525	CHD	O3-C3-C4	2.25	114.33	109.86
23	C	271	CHD	C13-C14-C8	2.25	117.65	114.75
24	C	272	DMU	O5-C6-O16	2.26	115.49	110.05
21	D	523	TGL	C10-CB9-CB8	2.27	126.24	114.53
24	C	272	DMU	C10-C5-C7	2.27	114.45	109.97
21	N	1522	TGL	C15-CC9-CC8	2.30	126.40	114.53
27	P	1270	CDL	OB6-CB5-C51	2.30	116.53	111.53
18	A	515	HEA	C13-C12-C11	2.30	117.58	114.51
21	D	523	TGL	C11-C10-CB9	2.31	126.45	114.53
19	P	1267	PGV	O03-C19-C20	2.31	118.94	111.90
27	C	270	CDL	CA6-OA8-CA7	2.32	123.33	116.85
27	C	270	CDL	C39-C38-C37	2.33	126.57	114.53
27	T	1269	CDL	C43-C42-C41	2.34	126.61	114.53
19	A	521	PGV	O12-P-O13	2.37	118.80	109.62
23	J	60	CHD	C13-C14-C8	2.37	117.81	114.75
19	A	524	PGV	C02-O01-C1	2.39	123.62	117.89
27	G	269	CDL	OB8-CB7-C71	2.41	119.24	111.90
21	N	1522	TGL	CG3-OG3-CC1	2.44	123.68	116.85
21	O	1523	TGL	OG2-CG2-CG3	2.45	116.99	108.36
21	O	1523	TGL	C21-C20-CA9	2.45	127.19	114.53
18	N	515	HEA	C4B-C3B-C11	2.45	129.67	127.01
21	D	523	TGL	CG2-OG2-CB1	2.46	123.78	117.89
21	N	1521	TGL	OG3-CC1-CC2	2.46	119.39	111.90
19	N	1524	PGV	C02-O01-C1	2.46	123.80	117.89
18	A	516	HEA	C17-C16-C15	2.48	120.79	112.71
21	B	521	TGL	OG1-CG1-CG2	2.48	115.36	108.69
24	M	526	DMU	O7-C3-C4	2.48	115.84	109.32
24	Z	1526	DMU	C6-O5-C4	2.49	118.57	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	86	CHD	C5-C6-C7	2.49	117.21	114.44
18	A	516	HEA	O11-C11-C3B	2.49	119.18	111.82
27	T	1269	CDL	CB6-OB8-CB7	2.49	123.82	116.85
23	J	60	CHD	C17-C13-C12	2.50	119.89	117.68
23	P	1525	CHD	O3-C3-C4	2.50	114.83	109.86
23	W	1060	CHD	C16-C17-C20	2.50	116.52	112.05
27	T	1269	CDL	C82-C81-C80	2.51	127.47	114.53
27	C	270	CDL	OA8-CA6-CA4	2.51	115.44	108.69
21	D	523	TGL	OG1-CA1-CA2	2.52	119.59	111.90
21	B	521	TGL	OG3-CC1-CC2	2.53	119.60	111.90
26	P	1265	PEK	C01-O03-C21	2.53	123.93	116.85
27	P	1270	CDL	OA8-CA6-CA4	2.54	115.53	108.69
27	P	1270	CDL	CA6-OA8-CA7	2.54	123.96	116.85
27	G	269	CDL	OA8-CA7-C31	2.54	119.65	111.90
24	P	1272	DMU	C11-C9-C8	2.55	119.31	113.02
23	C	525	CHD	C5-C6-C7	2.56	117.29	114.44
24	M	526	DMU	C10-O7-C3	2.57	124.71	118.01
18	N	516	HEA	CMB-C2B-C3B	2.58	130.43	125.14
18	N	515	HEA	CMB-C2B-C3B	2.59	130.44	125.14
18	N	516	HEA	C3C-C4C-NC	2.60	112.57	109.21
23	B	1086	CHD	C16-C17-C20	2.61	116.71	112.05
24	C	272	DMU	C57-C4-C3	2.63	120.89	113.25
18	N	515	HEA	CMD-C2D-C3D	2.63	130.74	125.24
23	P	1525	CHD	C16-C17-C20	2.64	116.75	112.05
24	P	1272	DMU	O5-C6-O16	2.65	116.42	110.05
23	J	60	CHD	C16-C17-C20	2.67	116.81	112.05
23	W	1060	CHD	C13-C14-C8	2.69	118.21	114.75
18	A	515	HEA	CMD-C2D-C3D	2.70	130.89	125.24
24	P	1272	DMU	C57-C4-C3	2.71	121.14	113.25
24	P	1272	DMU	O16-C18-C19	2.72	120.69	109.88
21	L	522	TGL	CG1-OG1-CA1	2.72	124.46	116.85
21	O	1523	TGL	OG1-CA1-CA2	2.73	120.20	111.90
21	N	1522	TGL	OG1-CG1-CG2	2.74	116.06	108.69
23	B	1086	CHD	C15-C14-C8	2.75	122.31	118.32
23	G	86	CHD	C16-C17-C13	2.75	106.33	103.60
24	M	526	DMU	O7-C3-C2	2.76	114.28	107.17
26	C	265	PEK	C01-O03-C21	2.80	124.69	116.85
24	M	526	DMU	C6-O5-C4	2.82	119.22	113.75
19	A	524	PGV	O01-C1-C2	2.83	117.69	111.53
23	B	1086	CHD	C16-C17-C13	2.84	106.42	103.60
23	W	1060	CHD	C11-C9-C8	2.84	114.77	110.73
21	L	522	TGL	OG1-CG1-CG2	2.84	116.34	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	C10-C5-C7	2.85	115.58	109.97
24	C	272	DMU	C18-O16-C6	2.85	118.92	113.94
26	G	1263	PEK	C01-O03-C21	2.85	124.81	116.85
24	Z	1526	DMU	C10-O1-C9	2.85	119.28	113.75
19	A	521	PGV	O01-C1-C2	2.86	117.73	111.53
23	P	1525	CHD	C5-C6-C7	2.86	117.62	114.44
26	T	263	PEK	C02-O01-C1	2.86	124.75	117.89
19	N	1266	PGV	O03-C01-C02	2.87	116.40	108.69
23	P	1525	CHD	C15-C14-C8	2.87	122.49	118.32
18	A	516	HEA	C3C-C4C-NC	2.88	112.93	109.21
24	M	526	DMU	C1-C2-C3	2.90	115.97	109.60
21	N	1522	TGL	OG3-CC1-CC2	2.94	120.86	111.90
27	G	269	CDL	CB6-OB8-CB7	2.94	125.08	116.85
18	A	516	HEA	C16-C15-C14	2.98	126.70	121.05
27	T	1269	CDL	OA8-CA7-C31	3.00	121.03	111.90
21	D	523	TGL	C21-C20-CA9	3.00	130.02	114.53
18	A	515	HEA	CMC-C2C-C3C	3.00	130.96	125.09
24	Z	1526	DMU	C1-C2-C3	3.00	116.20	109.60
24	C	272	DMU	C11-C9-C8	3.03	120.49	113.02
23	B	1086	CHD	C11-C12-C13	3.03	114.28	111.20
23	J	60	CHD	C21-C20-C22	3.04	115.42	110.35
23	P	1525	CHD	C2-C1-C10	3.04	118.27	112.84
24	Z	1526	DMU	O5-C6-O16	3.05	117.41	110.05
21	O	1523	TGL	CG3-OG3-CC1	3.06	125.41	116.85
21	O	1523	TGL	OG2-CB1-CB2	3.07	118.20	111.53
21	L	522	TGL	CC3-CC2-CC1	3.09	125.74	113.59
23	C	525	CHD	C11-C9-C10	3.11	117.03	113.79
18	A	515	HEA	C12-C11-C3B	3.12	119.05	112.59
24	M	526	DMU	C57-C4-C3	3.14	122.39	113.25
23	C	525	CHD	C9-C8-C7	3.19	115.69	111.92
26	P	1264	PEK	O01-C1-C2	3.19	118.46	111.53
24	C	272	DMU	O7-C3-C2	3.20	115.43	107.17
23	C	271	CHD	C14-C13-C12	3.20	110.26	107.39
18	A	516	HEA	C12-C11-C3B	3.21	119.23	112.59
24	P	1272	DMU	C6-O5-C4	3.21	119.97	113.75
26	G	1263	PEK	O03-C01-C02	3.21	117.34	108.69
27	C	270	CDL	OB8-CB7-C71	3.21	121.69	111.90
26	T	263	PEK	C01-O03-C21	3.25	125.95	116.85
23	C	525	CHD	C15-C14-C8	3.26	123.05	118.32
27	P	1270	CDL	OA8-CA7-C31	3.27	121.87	111.90
27	G	269	CDL	CA6-OA8-CA7	3.28	126.02	116.85
23	P	1271	CHD	C17-C13-C14	3.30	103.39	100.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	CMC-C2C-C1C	3.30	133.82	128.36
23	C	525	CHD	C13-C17-C20	3.30	123.53	119.50
23	C	271	CHD	C9-C10-C5	3.31	113.56	108.67
24	C	272	DMU	C6-O5-C4	3.31	120.16	113.75
23	C	525	CHD	C1-C2-C3	3.31	115.80	110.43
27	T	1269	CDL	C83-C82-C81	3.36	131.88	114.53
21	N	1522	TGL	OG1-CA1-CA2	3.38	122.21	111.90
24	M	526	DMU	C6-C1-C2	3.39	116.65	109.97
23	C	271	CHD	C17-C13-C14	3.39	103.48	100.05
26	T	263	PEK	O03-C21-C22	3.41	122.30	111.90
23	G	86	CHD	C11-C9-C10	3.43	117.35	113.79
21	N	1521	TGL	OG2-CG2-CG3	3.43	120.45	108.36
23	G	86	CHD	C15-C14-C8	3.44	123.32	118.32
21	N	1522	TGL	CG1-OG1-CA1	3.45	126.48	116.85
24	Z	1526	DMU	O55-C2-C3	3.47	118.09	109.87
24	C	272	DMU	O4-C7-C5	3.48	118.17	110.34
23	C	525	CHD	C16-C17-C20	3.48	118.26	112.05
19	C	267	PGV	O01-C1-C2	3.48	119.10	111.53
21	N	1521	TGL	OG2-CB1-CB2	3.50	119.14	111.53
21	B	521	TGL	OG1-CA1-CA2	3.51	122.61	111.90
27	C	270	CDL	OA8-CA7-C31	3.53	122.64	111.90
21	N	1522	TGL	OG2-CB1-CB2	3.54	119.22	111.53
23	P	1525	CHD	C14-C8-C9	3.55	114.50	109.62
23	P	1525	CHD	C16-C17-C13	3.56	107.14	103.60
21	L	522	TGL	OG1-CA1-CA2	3.57	122.77	111.90
26	G	1263	PEK	O03-C21-C22	3.60	122.86	111.90
26	G	264	PEK	O01-C1-C2	3.61	119.38	111.53
23	G	86	CHD	C14-C8-C9	3.62	114.61	109.62
23	P	1271	CHD	C9-C10-C5	3.63	114.05	108.67
21	O	1523	TGL	OG3-CC1-CC2	3.64	123.00	111.90
23	G	86	CHD	C9-C11-C12	3.65	118.98	114.36
23	J	60	CHD	C11-C9-C8	3.67	115.94	110.73
24	P	1272	DMU	C10-O1-C9	3.67	120.87	113.75
21	N	1521	TGL	OG1-CA1-CA2	3.69	123.14	111.90
23	P	1525	CHD	C9-C11-C12	3.72	119.06	114.36
24	C	272	DMU	C1-C2-C3	3.73	117.78	109.60
21	B	521	TGL	OG2-CB1-CB2	3.73	119.64	111.53
21	D	523	TGL	OG1-CG1-CG2	3.75	118.77	108.69
26	P	1264	PEK	C2-C3-C4	3.75	120.77	113.30
21	D	523	TGL	OG2-CB1-CB2	3.77	119.72	111.53
23	B	1086	CHD	C5-C6-C7	3.77	118.64	114.44
24	C	272	DMU	C10-O1-C9	3.77	121.06	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C14-C8-C9	3.78	114.82	109.62
19	N	1524	PGV	C01-O03-C19	3.78	127.42	116.85
24	C	272	DMU	O7-C10-C5	3.80	117.36	108.10
24	M	526	DMU	C8-C7-C5	3.80	117.89	110.79
23	P	1525	CHD	C11-C9-C10	3.82	117.76	113.79
24	P	1272	DMU	O7-C3-C4	3.82	119.36	109.32
23	J	60	CHD	C22-C20-C17	3.82	118.27	110.24
24	Z	1526	DMU	C10-C5-C7	3.84	117.53	109.97
26	T	263	PEK	O03-C01-C02	3.84	119.04	108.69
24	C	272	DMU	C6-C1-C2	3.85	117.56	109.97
21	N	1521	TGL	OG1-CG1-CG2	3.86	119.07	108.69
19	N	1524	PGV	O03-C19-C20	3.87	123.69	111.90
24	P	1272	DMU	C2-C3-C4	3.87	119.59	110.84
21	L	522	TGL	OG3-CC1-CC2	3.88	123.72	111.90
23	G	86	CHD	C9-C8-C7	3.89	116.52	111.92
24	Z	1526	DMU	C6-C1-C2	3.90	117.65	109.97
19	A	524	PGV	C01-O03-C19	3.90	127.75	116.85
23	C	525	CHD	C16-C17-C13	3.93	107.50	103.60
27	P	1270	CDL	OB8-CB7-C71	3.94	123.90	111.90
26	C	265	PEK	O01-C1-C2	3.94	120.09	111.53
23	P	1271	CHD	C16-C17-C20	3.95	119.09	112.05
19	N	1524	PGV	O01-C1-C2	3.95	120.12	111.53
27	T	1269	CDL	OB8-CB6-CB4	3.96	119.34	108.69
26	P	1265	PEK	O03-C21-C22	4.00	124.09	111.90
24	P	1272	DMU	O5-C4-C57	4.01	116.50	106.36
24	P	1272	DMU	C6-C1-C2	4.01	117.88	109.97
24	P	1272	DMU	O7-C10-C5	4.02	117.88	108.10
19	A	524	PGV	O03-C19-C20	4.02	124.15	111.90
21	D	523	TGL	CG3-OG3-CC1	4.05	128.18	116.85
24	M	526	DMU	C7-C8-C9	4.09	117.32	110.20
24	P	1272	DMU	C1-C2-C3	4.10	118.60	109.60
24	C	272	DMU	O7-C3-C4	4.13	120.19	109.32
23	P	1525	CHD	C13-C17-C20	4.14	124.55	119.50
24	M	526	DMU	O1-C9-C11	4.16	116.86	106.36
23	P	1271	CHD	C9-C11-C12	4.16	119.61	114.36
24	C	272	DMU	C7-C8-C9	4.16	117.45	110.20
23	B	1086	CHD	C11-C9-C10	4.16	118.12	113.79
26	P	1265	PEK	O01-C1-C2	4.16	120.58	111.53
23	C	525	CHD	C9-C11-C12	4.17	119.63	114.36
23	W	1060	CHD	C17-C13-C12	4.19	121.39	117.68
24	C	272	DMU	C2-C3-C4	4.19	120.31	110.84
24	Z	1526	DMU	C8-C7-C5	4.21	118.65	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	O5-C4-C57	4.23	117.05	106.36
23	C	271	CHD	C16-C17-C20	4.25	119.63	112.05
24	C	272	DMU	O5-C4-C57	4.27	117.14	106.36
24	M	526	DMU	C10-C5-C7	4.28	118.41	109.97
21	D	523	TGL	OG3-CC1-CC2	4.30	125.01	111.90
23	B	1086	CHD	C11-C9-C8	4.30	116.85	110.73
21	B	521	TGL	CG3-OG3-CC1	4.39	129.12	116.85
23	P	1271	CHD	C14-C13-C12	4.40	111.33	107.39
23	P	1525	CHD	C17-C13-C14	4.46	104.56	100.05
23	B	1086	CHD	C14-C8-C9	4.46	115.76	109.62
22	O	1230	PSC	O01-C1-C2	4.48	121.25	111.53
18	N	515	HEA	C12-C11-C3B	4.48	121.86	112.59
19	A	521	PGV	O03-C19-C20	4.49	125.58	111.90
23	G	86	CHD	C2-C1-C10	4.49	120.86	112.84
24	P	1272	DMU	C7-C8-C9	4.50	118.04	110.20
26	C	265	PEK	O03-C21-C22	4.52	125.66	111.90
19	C	268	PGV	O03-C19-C20	4.58	125.87	111.90
23	W	1060	CHD	C9-C8-C7	4.59	117.34	111.92
21	B	521	TGL	OG2-CG2-CG3	4.60	124.56	108.36
23	B	1086	CHD	C4-C3-C2	4.60	116.39	110.52
21	N	1521	TGL	CG2-OG2-CB1	4.62	128.98	117.89
21	N	1521	TGL	CG3-OG3-CC1	4.64	129.84	116.85
23	P	1525	CHD	C9-C8-C7	4.66	117.42	111.92
24	Z	1526	DMU	O7-C3-C2	4.67	119.23	107.17
27	G	269	CDL	OB6-CB5-C51	4.68	121.69	111.53
23	P	1271	CHD	C1-C2-C3	4.70	118.06	110.43
24	Z	1526	DMU	C2-C3-C4	4.76	121.61	110.84
23	C	271	CHD	C9-C11-C12	4.82	120.45	114.36
23	B	1086	CHD	C15-C14-C13	4.83	108.41	103.60
24	C	272	DMU	O1-C9-C11	4.85	118.61	106.36
24	Z	1526	DMU	C7-C8-C9	4.85	118.66	110.20
23	C	525	CHD	C11-C9-C8	4.86	117.64	110.73
23	C	525	CHD	C17-C13-C14	4.88	104.98	100.05
27	P	1270	CDL	OA6-CA5-C11	4.88	122.14	111.53
23	P	1271	CHD	C13-C17-C20	4.89	125.45	119.50
23	P	1525	CHD	C1-C2-C3	4.91	118.40	110.43
19	N	1268	PGV	O03-C19-C20	4.92	126.90	111.90
23	G	86	CHD	C16-C17-C20	5.02	121.00	112.05
23	W	1060	CHD	C1-C10-C5	5.02	116.06	107.81
26	G	1263	PEK	O01-C1-C2	5.03	122.45	111.53
19	N	1266	PGV	O03-C19-C20	5.09	127.42	111.90
27	G	269	CDL	OA6-CA5-C11	5.10	122.62	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	CAD-C3D-C2D	5.10	143.58	129.00
24	M	526	DMU	O5-C4-C3	5.12	120.55	109.75
24	P	1272	DMU	O1-C9-C11	5.15	119.37	106.36
27	T	1269	CDL	OB6-CB5-C51	5.17	122.77	111.53
23	G	86	CHD	C11-C12-C13	5.19	116.47	111.20
23	J	60	CHD	C15-C14-C8	5.20	125.87	118.32
23	C	525	CHD	C2-C1-C10	5.24	122.19	112.84
24	Z	1526	DMU	O5-C4-C57	5.26	119.65	106.36
23	J	60	CHD	C9-C10-C5	5.27	116.47	108.67
26	T	263	PEK	O01-C1-C2	5.27	122.98	111.53
27	C	270	CDL	OA6-CA5-C11	5.29	123.02	111.53
23	J	60	CHD	C1-C10-C5	5.30	116.51	107.81
24	P	1272	DMU	C8-C7-C5	5.30	120.68	110.79
23	P	1525	CHD	C11-C12-C13	5.30	116.59	111.20
23	P	1271	CHD	C2-C1-C10	5.37	122.43	112.84
23	J	60	CHD	C9-C8-C7	5.39	118.29	111.92
23	W	1060	CHD	C22-C20-C17	5.40	121.58	110.24
23	G	86	CHD	C1-C2-C3	5.41	119.21	110.43
27	T	1269	CDL	OA6-CA5-C11	5.42	123.32	111.53
22	B	230	PSC	O01-C1-C2	5.45	123.38	111.53
24	M	526	DMU	C2-C3-C4	5.50	123.28	110.84
24	P	1272	DMU	O5-C6-C1	5.51	121.57	110.28
23	P	1271	CHD	C4-C5-C10	5.55	118.77	112.66
23	C	271	CHD	C11-C9-C8	5.55	118.62	110.73
23	J	60	CHD	C11-C12-C13	5.56	116.84	111.20
19	C	268	PGV	O01-C1-C2	5.56	123.61	111.53
23	P	1525	CHD	C6-C7-C8	5.56	117.37	111.47
23	J	60	CHD	C11-C9-C10	5.56	119.58	113.79
23	G	86	CHD	C4-C3-C2	5.57	117.62	110.52
23	W	1060	CHD	C2-C1-C10	5.58	122.80	112.84
23	C	271	CHD	C1-C2-C3	5.59	119.50	110.43
23	W	1060	CHD	C14-C13-C12	5.60	112.41	107.39
23	J	60	CHD	C2-C1-C10	5.62	122.86	112.84
18	N	516	HEA	C27-C19-C20	5.64	124.02	115.41
23	C	271	CHD	C5-C4-C3	5.69	121.37	112.91
23	C	271	CHD	C2-C1-C10	5.71	123.03	112.84
21	B	521	TGL	CG2-OG2-CB1	5.72	131.62	117.89
23	G	86	CHD	C17-C13-C14	5.72	105.84	100.05
23	C	271	CHD	C1-C10-C5	5.74	117.25	107.81
24	C	272	DMU	C8-C7-C5	5.74	121.51	110.79
23	P	1525	CHD	C5-C4-C3	5.75	121.47	112.91
24	C	272	DMU	O5-C6-C1	5.75	122.08	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1060	CHD	C5-C4-C3	5.75	121.47	112.91
24	C	272	DMU	O5-C4-C3	5.78	121.95	109.75
23	J	60	CHD	C4-C3-C2	5.78	117.89	110.52
23	C	271	CHD	C14-C8-C7	5.80	119.79	111.74
24	Z	1526	DMU	O5-C4-C3	5.81	122.02	109.75
23	W	1060	CHD	C9-C10-C5	5.81	117.28	108.67
23	P	1271	CHD	C5-C4-C3	5.82	121.57	112.91
23	P	1525	CHD	C11-C9-C8	5.82	119.00	110.73
18	A	515	HEA	C4B-C3B-C11	5.83	133.34	127.01
23	C	525	CHD	C6-C7-C8	5.85	117.68	111.47
19	N	1268	PGV	O01-C1-C2	5.90	124.36	111.53
23	G	86	CHD	C11-C9-C8	5.95	119.18	110.73
23	W	1060	CHD	C15-C14-C8	5.95	126.96	118.32
24	P	1272	DMU	O5-C4-C3	5.96	122.34	109.75
24	C	272	DMU	O1-C9-C8	5.98	120.90	109.68
23	W	1060	CHD	C4-C3-C2	6.00	118.17	110.52
23	C	525	CHD	C11-C12-C13	6.00	117.30	111.20
18	A	516	HEA	OMA-CMA-C3A	6.04	137.32	125.11
23	C	271	CHD	C13-C17-C20	6.06	126.88	119.50
24	Z	1526	DMU	O1-C9-C11	6.09	121.74	106.36
23	J	60	CHD	C1-C2-C3	6.11	120.34	110.43
23	W	1060	CHD	C1-C2-C3	6.11	120.34	110.43
23	J	60	CHD	C5-C4-C3	6.15	122.06	112.91
23	B	1086	CHD	C9-C11-C12	6.18	122.17	114.36
24	P	1272	DMU	O1-C9-C8	6.19	121.30	109.68
23	W	1060	CHD	C6-C5-C10	6.19	119.48	112.66
23	C	525	CHD	C5-C4-C3	6.19	122.13	112.91
24	Z	1526	DMU	O16-C6-C1	6.24	115.91	108.04
23	C	271	CHD	C4-C3-C2	6.25	118.49	110.52
23	J	60	CHD	C6-C5-C10	6.32	119.61	112.66
18	N	515	HEA	C26-C15-C16	6.32	125.06	115.41
23	C	271	CHD	C6-C5-C10	6.34	119.64	112.66
23	G	86	CHD	C6-C7-C8	6.36	118.22	111.47
23	C	525	CHD	C15-C14-C13	6.38	109.94	103.60
23	P	1271	CHD	C6-C5-C10	6.40	119.71	112.66
23	J	60	CHD	C9-C11-C12	6.40	122.45	114.36
24	P	1272	DMU	O1-C10-C5	6.40	123.41	110.28
24	M	526	DMU	O1-C10-C5	6.43	123.46	110.28
23	W	1060	CHD	C11-C12-C13	6.46	117.76	111.20
23	C	271	CHD	C16-C17-C13	6.47	110.03	103.60
23	G	86	CHD	C15-C14-C13	6.48	110.04	103.60
24	Z	1526	DMU	O1-C10-C5	6.52	123.66	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C16-C17-C18	6.53	128.79	111.69
23	P	1271	CHD	C16-C17-C13	6.56	110.13	103.60
23	P	1271	CHD	C14-C8-C7	6.60	120.89	111.74
24	Z	1526	DMU	O1-C9-C8	6.60	122.06	109.68
24	Z	1526	DMU	O5-C6-C1	6.61	123.84	110.28
23	P	1271	CHD	C11-C9-C8	6.61	120.13	110.73
23	P	1271	CHD	C1-C10-C5	6.62	118.68	107.81
24	C	272	DMU	O1-C10-C5	6.63	123.88	110.28
23	J	60	CHD	C14-C13-C12	6.73	113.42	107.39
18	N	515	HEA	C27-C19-C20	6.79	125.77	115.41
23	J	60	CHD	C6-C7-C8	6.81	118.69	111.47
24	M	526	DMU	O5-C6-C1	6.83	124.28	110.28
23	C	271	CHD	C4-C5-C10	6.85	120.20	112.66
23	W	1060	CHD	C9-C11-C12	6.87	123.04	114.36
23	B	1086	CHD	C17-C13-C14	6.90	107.03	100.05
23	J	60	CHD	C4-C5-C10	6.92	120.28	112.66
23	W	1060	CHD	C11-C9-C10	7.03	121.10	113.79
24	M	526	DMU	O16-C6-C1	7.03	116.92	108.04
23	W	1060	CHD	C16-C17-C13	7.06	110.62	103.60
23	B	1086	CHD	C5-C4-C3	7.12	123.51	112.91
23	W	1060	CHD	C5-C6-C7	7.16	122.42	114.44
23	J	60	CHD	C5-C6-C7	7.18	122.44	114.44
18	N	515	HEA	C16-C17-C18	7.18	130.49	111.69
23	B	1086	CHD	C1-C2-C3	7.22	122.14	110.43
23	C	271	CHD	C15-C14-C13	7.27	110.83	103.60
23	J	60	CHD	C14-C8-C7	7.28	121.83	111.74
23	P	1271	CHD	C11-C12-C13	7.49	118.81	111.20
23	P	1271	CHD	C5-C6-C7	7.51	122.81	114.44
23	W	1060	CHD	C4-C5-C10	7.66	121.10	112.66
23	P	1271	CHD	C6-C7-C8	7.66	119.60	111.47
23	P	1271	CHD	C4-C3-C2	7.67	120.29	110.52
23	W	1060	CHD	C15-C14-C13	7.71	111.26	103.60
23	C	525	CHD	C4-C3-C2	7.78	120.44	110.52
23	C	271	CHD	C6-C7-C8	7.82	119.77	111.47
23	W	1060	CHD	C6-C7-C8	7.82	119.77	111.47
23	C	271	CHD	C5-C6-C7	7.84	123.19	114.44
23	P	1525	CHD	C15-C14-C13	7.90	111.46	103.60
23	G	86	CHD	C5-C4-C3	7.91	124.68	112.91
23	P	1271	CHD	C15-C14-C13	7.92	111.48	103.60
18	A	515	HEA	C26-C15-C16	8.00	127.63	115.41
23	P	1525	CHD	C4-C3-C2	8.12	120.87	110.52
23	B	1086	CHD	C6-C7-C8	8.16	120.13	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	O1-C9-C8	8.17	125.01	109.68
23	C	525	CHD	C14-C13-C12	8.24	114.77	107.39
23	W	1060	CHD	C14-C8-C7	8.31	123.26	111.74
23	J	60	CHD	C13-C17-C20	8.37	129.69	119.50
23	C	271	CHD	C11-C12-C13	8.52	119.85	111.20
23	P	1525	CHD	C17-C13-C12	8.57	125.28	117.68
23	G	86	CHD	C1-C10-C5	8.60	121.94	107.81
23	C	525	CHD	C17-C13-C12	8.63	125.33	117.68
18	A	516	HEA	CMB-C2B-C1B	8.76	142.85	128.36
23	B	1086	CHD	C6-C5-C10	8.77	122.31	112.66
23	C	271	CHD	C15-C14-C8	8.82	131.13	118.32
23	C	525	CHD	C1-C10-C5	8.93	122.48	107.81
23	J	60	CHD	C16-C17-C13	8.97	112.52	103.60
23	W	1060	CHD	C10-C9-C8	9.42	122.22	111.88
23	P	1525	CHD	C10-C9-C8	9.42	122.22	111.88
23	J	60	CHD	C15-C14-C13	9.44	112.99	103.60
23	G	86	CHD	C14-C13-C12	9.45	115.85	107.39
23	G	86	CHD	C10-C9-C8	9.66	122.48	111.88
23	G	86	CHD	C17-C13-C12	9.71	126.28	117.68
23	B	1086	CHD	C1-C10-C5	9.72	123.78	107.81
23	P	1525	CHD	C1-C10-C5	9.82	123.94	107.81
23	J	60	CHD	C10-C9-C8	9.91	122.76	111.88
24	P	1272	DMU	O16-C6-C1	10.03	120.71	108.04
23	W	1060	CHD	C13-C17-C20	10.11	131.81	119.50
23	P	1271	CHD	C15-C14-C8	10.11	133.00	118.32
23	B	1086	CHD	C17-C13-C12	10.30	126.81	117.68
24	C	272	DMU	O16-C6-C1	10.65	121.49	108.04
23	B	1086	CHD	C14-C13-C12	10.67	116.94	107.39
23	P	1525	CHD	C14-C13-C12	10.68	116.95	107.39
23	B	1086	CHD	C10-C9-C8	10.87	123.81	111.88
23	G	86	CHD	C6-C5-C10	11.04	124.82	112.66
23	C	525	CHD	C10-C9-C8	11.64	124.66	111.88
23	P	1525	CHD	C6-C5-C10	11.99	125.86	112.66
23	C	525	CHD	C6-C5-C10	12.78	126.73	112.66
23	P	1271	CHD	C10-C9-C8	13.45	126.64	111.88
23	C	271	CHD	C10-C9-C8	13.49	126.68	111.88
18	A	516	HEA	CAA-C2A-C1A	13.70	141.88	127.01

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	M	526	DMU	C2

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Mol	Chain	Res	Type	Atom
24	M	526	DMU	C4
24	M	526	DMU	C9
24	M	526	DMU	C6
24	M	526	DMU	C5
23	B	1086	CHD	C9
23	P	1525	CHD	C9
24	C	272	DMU	C2
24	C	272	DMU	C4
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C5
24	P	1272	DMU	C2
24	P	1272	DMU	C4
24	P	1272	DMU	C6
24	P	1272	DMU	C9
24	P	1272	DMU	C5
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C9
24	Z	1526	DMU	C6
24	Z	1526	DMU	C5
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
23	C	525	CHD	C9
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB
23	G	86	CHD	C9
23	J	60	CHD	C17
23	C	271	CHD	C14
23	C	271	CHD	C9
23	W	1060	CHD	C17
23	P	1271	CHD	C14
23	P	1271	CHD	C9

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C02-O01-C1-C2
19	N	1524	PGV	C02-O01-C1-C2
27	G	269	CDL	PB2-OB2-CB2-C1

There are no ring outliers.

40 monomers are involved in 244 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	7	0
18	A	516	HEA	5	0
15	A	520	PER	1	0
19	A	524	PGV	5	0
22	B	230	PSC	13	0
21	B	521	TGL	10	0
26	C	265	PEK	4	0
19	C	267	PGV	3	0
19	C	268	PGV	2	0
27	C	270	CDL	13	0
23	C	271	CHD	4	0
24	C	272	DMU	2	0
21	D	523	TGL	5	0
26	G	1263	PEK	12	0
26	G	264	PEK	4	0
27	G	269	CDL	17	0
23	G	86	CHD	2	0
23	J	60	CHD	2	0
21	L	522	TGL	13	0
19	N	1266	PGV	1	0
19	N	1268	PGV	2	0
21	N	1521	TGL	7	0
21	N	1522	TGL	19	0
19	N	1524	PGV	9	0
18	N	515	HEA	7	0
18	N	516	HEA	1	0
15	N	520	PER	1	0
22	O	1230	PSC	12	0
21	O	1523	TGL	6	0
26	P	1264	PEK	5	0
26	P	1265	PEK	8	0
19	P	1267	PGV	5	0
27	P	1270	CDL	9	0
23	P	1271	CHD	3	0
24	P	1272	DMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	1525	CHD	2	0
27	T	1269	CDL	17	0
26	T	263	PEK	14	0
23	W	1060	CHD	1	0
24	Z	1526	DMU	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.61	0 100 100	11, 17, 25, 51	0
1	N	513/514 (99%)	-0.63	1 (0%) 95 96	15, 23, 33, 56	0
2	B	226/227 (99%)	-0.75	0 100 100	12, 23, 49, 86	0
2	O	226/227 (99%)	-0.50	5 (2%) 65 69	20, 30, 60, 84	0
3	C	259/261 (99%)	-0.88	0 100 100	13, 21, 34, 58	0
3	P	259/261 (99%)	-0.81	1 (0%) 93 93	16, 24, 40, 64	0
4	D	144/147 (97%)	-0.61	0 100 100	14, 26, 48, 70	0
4	Q	144/147 (97%)	0.39	13 (9%) 12 12	27, 41, 63, 105	0
5	E	104/109 (95%)	-0.67	3 (2%) 55 60	18, 27, 54, 75	0
5	R	104/109 (95%)	-0.29	1 (0%) 84 86	23, 35, 57, 77	0
6	F	93/98 (94%)	-0.20	3 (3%) 51 56	15, 27, 49, 94	0
6	S	93/98 (94%)	0.09	4 (4%) 39 44	20, 33, 55, 102	0
7	G	83/85 (97%)	0.22	14 (16%) 2 2	15, 28, 99, 105	0
7	T	83/85 (97%)	0.41	15 (18%) 2 2	17, 33, 98, 102	0
8	H	75/85 (88%)	-0.14	3 (4%) 42 47	18, 29, 70, 78	0
8	U	75/85 (88%)	-0.00	3 (4%) 42 47	24, 34, 72, 79	0
9	I	71/73 (97%)	0.15	7 (9%) 9 10	21, 34, 60, 65	0
9	V	71/73 (97%)	0.36	6 (8%) 13 14	23, 45, 60, 70	0
10	J	57/59 (96%)	-0.24	5 (8%) 12 13	19, 32, 59, 82	0
10	W	57/59 (96%)	0.27	9 (15%) 3 2	25, 37, 68, 92	0
11	K	49/56 (87%)	-0.30	1 (2%) 68 72	19, 31, 43, 50	0
11	X	49/56 (87%)	0.92	7 (14%) 4 3	33, 42, 59, 71	0
12	L	46/47 (97%)	-0.58	1 (2%) 65 69	17, 26, 48, 74	0
12	Y	46/47 (97%)	-0.23	2 (4%) 39 44	26, 35, 60, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.24	5 (11%)	6	6	15, 24, 72, 97	0
13	Z	43/46 (93%)	0.32	5 (11%)	6	6	28, 36, 89, 106	0
All	All	3526/3614 (97%)	-0.40	114 (3%)	51	56	11, 26, 57, 106	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	18.4
4	Q	6	VAL	10.5
4	Q	4	SER	10.2
4	Q	8	SER	9.8
13	Z	43	SER	8.0
6	S	96	LEU	7.6
7	T	39	SER	7.2
4	Q	7	LYS	7.1
6	S	94	HIS	6.9
7	G	40	GLY	6.8
7	T	3	ALA	6.6
6	F	96	LEU	6.3
7	T	1	ALA	5.9
11	X	6	ALA	5.5
13	Z	41	LYS	5.3
7	G	8	HIS	5.2
10	W	52	TRP	5.2
6	F	95	GLN	5.2
13	Z	42	LYS	5.2
10	W	57	HIS	5.1
5	R	109	VAL	5.0
10	W	56	PRO	5.0
7	G	3	ALA	4.9
11	X	13	TYR	4.8
7	G	5	LYS	4.8
9	I	37	PHE	4.8
7	T	2	SER	4.7
13	M	43	SER	4.7
4	Q	35	ALA	4.6
12	Y	47	LYS	4.5
7	T	40	GLY	4.5
7	G	42	ARG	4.5
13	Z	39	ASN	4.4
7	T	5	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
6	S	95	GLN	4.2
6	S	93	PRO	4.1
8	U	44	THR	4.1
7	T	8	HIS	4.1
4	Q	147	LYS	4.1
13	Z	40	TYR	4.0
7	G	2	SER	3.9
6	F	94	HIS	3.9
11	X	7	PRO	3.8
10	W	1	PHE	3.8
9	V	37	PHE	3.7
7	T	42	ARG	3.7
13	M	42	LYS	3.7
8	H	47	GLY	3.5
7	G	36	TRP	3.5
2	O	113	TYR	3.5
1	N	513	LEU	3.5
7	T	36	TRP	3.4
7	T	10	GLY	3.4
8	U	47	GLY	3.3
7	T	4	ALA	3.2
2	O	226	MET	3.2
2	O	59	GLN	3.1
7	T	84	LYS	3.1
11	X	23	THR	3.1
7	G	4	ALA	3.1
9	I	26	MET	3.1
8	H	44	THR	3.1
9	I	33	THR	3.0
7	G	84	LYS	3.0
10	J	52	TRP	3.0
13	M	39	ASN	3.0
9	I	34	PHE	2.9
9	I	30	GLY	2.9
12	Y	45	LEU	2.9
5	E	7	THR	2.9
8	U	49	ASP	2.9
7	G	1	ALA	2.9
12	L	2	HIS	2.8
5	E	109	VAL	2.8
13	M	38	ASP	2.8
9	I	25	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	O	217	LYS	2.7
7	G	7	ASP	2.7
7	G	9	GLY	2.7
3	P	3	HIS	2.7
9	V	30	GLY	2.6
9	V	33	THR	2.6
13	M	40	TYR	2.6
4	Q	142	LYS	2.5
4	Q	51	LEU	2.5
7	T	41	HIS	2.5
7	G	41	HIS	2.4
11	X	16	ALA	2.4
7	T	12	GLY	2.4
10	J	1	PHE	2.3
10	J	56	PRO	2.3
10	W	55	PHE	2.3
5	E	9	GLU	2.3
4	Q	9	GLU	2.3
8	H	45	ALA	2.3
10	J	55	PHE	2.3
2	O	227	LEU	2.3
7	T	43	GLU	2.2
10	W	4	ARG	2.2
4	Q	33	LEU	2.2
4	Q	58	GLU	2.2
10	J	57	HIS	2.1
11	X	12	LYS	2.1
10	W	48	TYR	2.1
9	V	34	PHE	2.1
10	W	2	GLU	2.1
7	G	43	GLU	2.1
4	Q	39	ALA	2.1
11	K	6	ALA	2.1
10	W	26	ALA	2.1
9	V	36	LYS	2.0
9	V	25	PHE	2.0
11	X	47	ARG	2.0
9	I	29	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
7	TPO	G	11	11/12	0.51	0.33	-	74,81,102,102	0
1	FME	A	1	10/11	0.92	0.19	-	44,46,62,65	0
7	TPO	T	11	11/12	0.59	0.36	-	74,80,100,101	0
1	FME	N	1	10/11	0.92	0.19	-	48,50,63,64	0
2	FME	O	1	10/11	0.96	0.12	-	30,31,37,38	0
2	FME	B	1	10/11	0.98	0.13	-	19,21,26,33	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
19	PGV	A	524	51/51	0.81	0.26	8.79	30,65,100,103	0
27	CDL	C	270	100/100	0.80	0.30	7.49	40,86,103,105	0
27	CDL	P	1270	100/100	0.71	0.34	6.80	44,89,104,105	0
23	CHD	W	1060	29/29	0.72	0.50	6.72	97,100,102,103	0
23	CHD	J	60	29/29	0.68	0.48	5.68	95,98,101,103	0
21	TGL	B	521	63/63	0.84	0.24	5.62	31,58,87,89	0
24	DMU	C	272	33/33	0.62	0.35	5.55	64,101,103,105	0
21	TGL	N	1522	63/63	0.66	0.34	5.31	25,66,80,81	0
24	DMU	P	1272	33/33	0.57	0.40	5.03	74,102,105,106	0
21	TGL	L	522	63/63	0.79	0.28	4.44	25,61,74,78	0
21	TGL	N	1521	63/63	0.82	0.23	3.97	43,63,85,90	0
19	PGV	N	1266	51/51	0.98	0.20	3.85	15,28,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	PGV	C	267	51/51	0.96	0.18	3.65	13,24,55,58	0
26	PEK	G	264	53/53	0.96	0.18	3.52	15,31,57,58	0
19	PGV	N	1524	51/51	0.81	0.29	3.38	36,68,102,102	0
21	TGL	D	523	63/63	0.81	0.23	3.26	38,57,83,86	0
22	PSC	O	1230	52/52	0.74	0.29	3.08	38,82,113,115	0
19	PGV	N	1268	51/51	0.76	0.29	2.92	62,89,99,101	0
19	PGV	P	1267	51/51	0.96	0.18	2.83	16,28,59,60	0
15	PER	N	520	2/2	0.98	0.13	2.82	13,13,13,13	0
23	CHD	C	271	29/29	0.86	0.31	2.80	71,83,86,86	0
19	PGV	A	521	51/51	0.98	0.18	2.79	12,24,48,57	0
22	PSC	B	230	52/52	0.79	0.31	2.62	31,86,112,114	0
27	CDL	G	269	100/100	0.73	0.31	2.57	42,77,109,113	0
21	TGL	O	1523	63/63	0.77	0.23	2.57	34,64,86,90	0
26	PEK	P	1264	53/53	0.94	0.20	2.46	20,37,65,65	0
27	CDL	T	1269	100/100	0.72	0.27	2.32	43,76,109,113	0
15	PER	A	520	2/2	0.99	0.18	2.17	8,8,8,10	0
26	PEK	C	265	53/53	0.59	0.33	1.81	39,87,101,104	0
24	DMU	Z	1526	33/33	0.82	0.23	1.76	32,50,66,68	0
26	PEK	P	1265	53/53	0.72	0.30	1.76	32,83,103,103	0
26	PEK	T	263	53/53	0.64	0.38	1.44	35,81,112,112	0
19	PGV	C	268	51/51	0.77	0.26	1.40	53,87,97,98	0
23	CHD	P	1271	29/29	0.82	0.27	1.36	74,82,84,84	0
26	PEK	G	1263	53/53	0.67	0.37	1.33	46,88,115,116	0
18	HEA	N	515	60/60	0.98	0.16	1.04	14,25,37,39	0
24	DMU	M	526	33/33	0.91	0.16	0.85	15,38,57,59	0
18	HEA	A	515	60/60	0.99	0.16	0.43	8,17,40,45	0
23	CHD	C	525	29/29	0.96	0.10	0.40	14,24,31,33	0
16	MG	N	1518	1/1	0.85	0.13	0.11	26,26,26,26	0
18	HEA	N	516	60/60	0.98	0.12	-0.09	9,20,26,28	0
23	CHD	P	1525	29/29	0.95	0.10	-0.13	17,27,31,35	0
23	CHD	B	1086	29/29	0.97	0.10	-0.27	11,20,27,33	0
20	CUA	B	228	2/2	0.99	0.09	-0.28	17,17,17,18	0
18	HEA	A	516	60/60	0.99	0.12	-0.35	9,16,24,27	0
23	CHD	G	86	29/29	0.98	0.08	-0.39	17,21,25,26	0
17	NA	A	519	1/1	0.96	0.07	-1.36	16,16,16,16	0
28	ZN	F	99	1/1	1.00	0.07	-1.48	26,26,26,26	0
28	ZN	S	99	1/1	0.99	0.05	-1.60	28,28,28,28	0
16	MG	A	518	1/1	0.96	0.08	-2.27	21,21,21,21	0
20	CUA	O	228	2/2	0.98	0.07	-2.29	25,25,25,26	0
17	NA	N	1519	1/1	0.97	0.04	-2.85	24,24,24,24	0
14	CU	A	517	1/1	1.00	0.09	-	17,17,17,17	0
25	UNX	C	262	1/1	0.82	0.21	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	CU	N	517	1/1	1.00	0.10	-	18,18,18,18	0
25	UNX	P	1262	1/1	0.74	0.30	-	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.