



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 28, 2017 – 12:44 PM EST

PDB ID : 5XTC  
EMDB ID: : EMD-6772  
Title : Cryo-EM structure of human respiratory complex I transmembrane arm  
Authors : Gu, J.; Wu, M.; Yang, M.  
Deposited on : unknown  
Resolution : 3.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

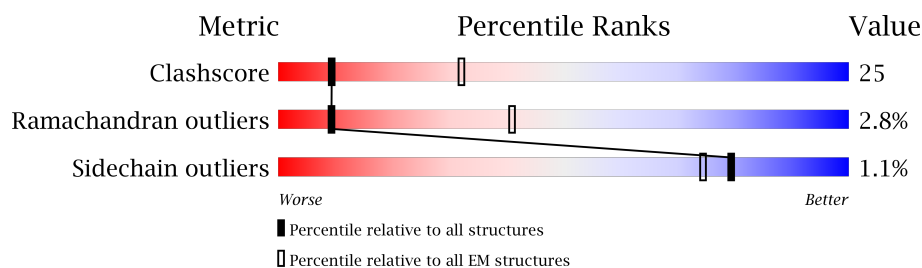
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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.




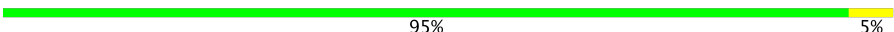
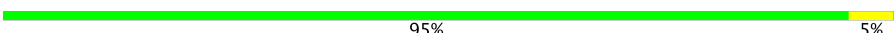

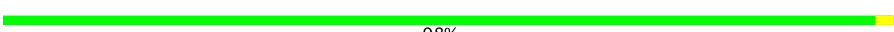
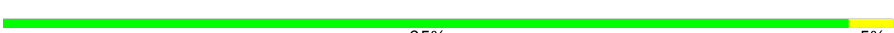






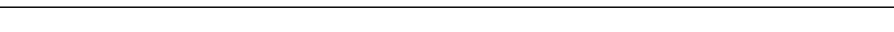

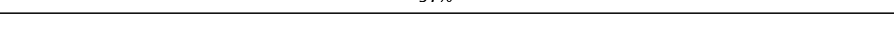
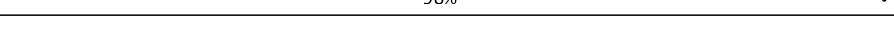
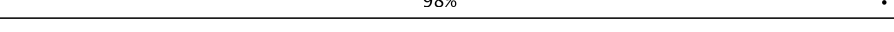
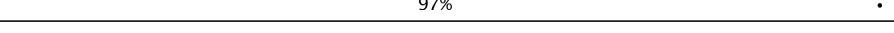
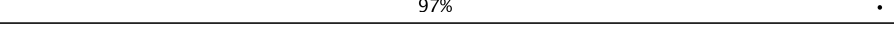

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	Q	46	
2	S	70	
3	U	83	
4	V	140	
5	W	116	
6	X	85	
7	Y	59	
8	Z	80	
9	a	138	

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Mol	Chain	Length	Quality of chain
10	b	128	 87% 9% . .
11	c	153	 95% 5% .
12	d	171	 95% 5% .
13	e	97	 97% .
14	f	47	 98% .
15	g	119	 95% 5% .
16	h	104	 94% 6% .
17	i	347	 98% .
18	j	115	 97% .
19	k	97	 93% 6% .
20	l	603	 94% 5% .
21	m	174	 94% 6% .
22	n	56	 96% .
23	o	128	 97% .
24	p	172	 98% .
25	r	459	 98% .
26	s	318	 97% .
27	u	169	 97% .
28	v	122	 86% 5% 9% .
29	w	320	 97% .

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 38835 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	46	Total	C	N	O	S	0	0
			381	247	65	68	1		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	116	Total	C	N	O	S	0	0
			956	614	167	170	5		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

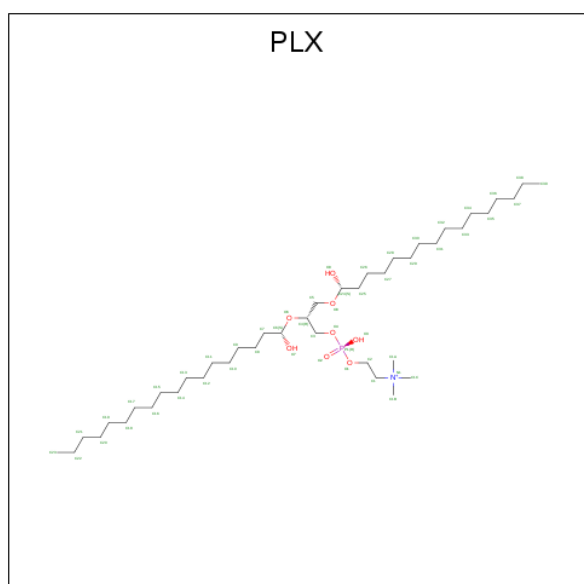
- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

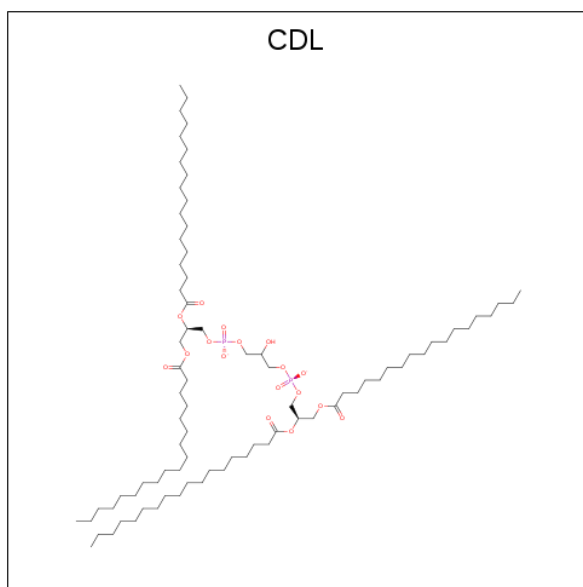
- Molecule 30 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY} METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).





Mol	Chain	Residues	Atoms					AltConf
30	U	1	Total	C	N	O	P	0
			52	42	1	8	1	
30	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
30	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
30	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
30	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
30	g	1	Total	C	N	O	P	0
			156	126	3	24	3	
30	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
30	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
30	s	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 31 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



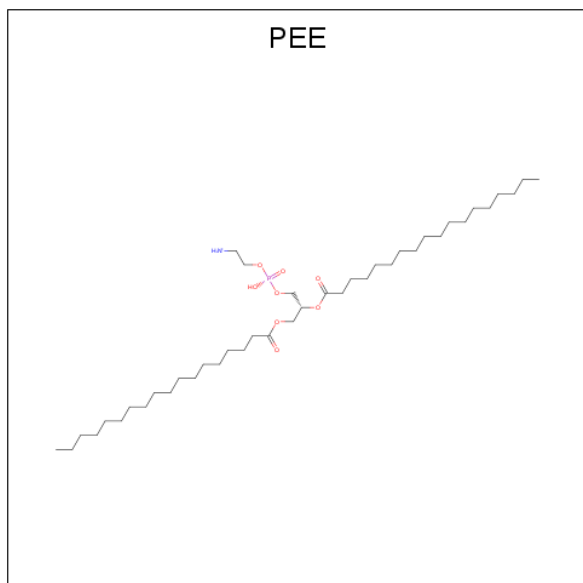
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			63	44	17	2	
31	i	1	Total	C	O	P	0
			64	45	17	2	
31	l	1	Total	C	O	P	0
			128	90	34	4	

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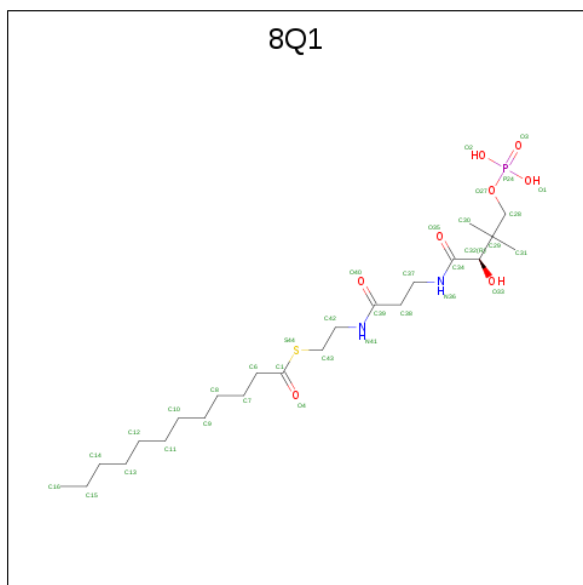
Mol	Chain	Residues	Atoms				AltConf
31	l	1	Total	C	O	P	0
			128	90	34	4	
31	n	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 32 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
32	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	l	1	Total	C	N	O	P	0
			100	80	2	16	2	
32	l	1	Total	C	N	O	P	0
			100	80	2	16	2	

- Molecule 33 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula:  $C_{23}H_{45}N_2O_8PS$ ).




Mol	Chain	Residues	Atoms						AltConf
33	p	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q:  76% 22% .




- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  74% 24% .



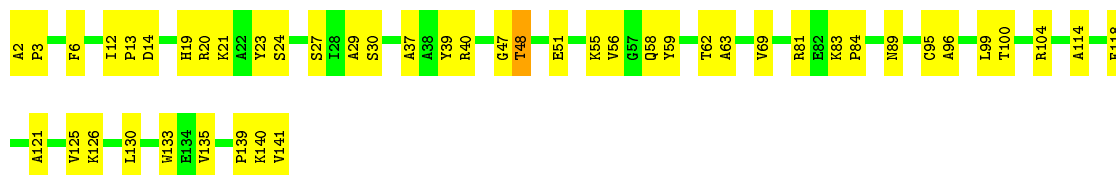
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  84% 16% .




- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  66% 33% .

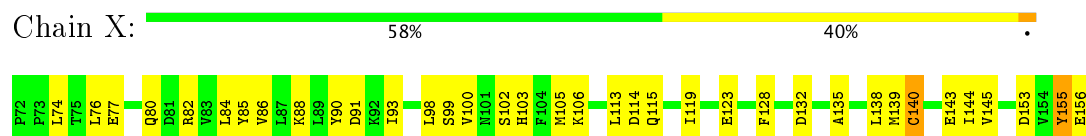


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

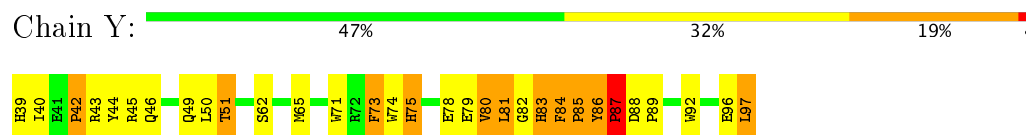
Chain W:  79% 20% .



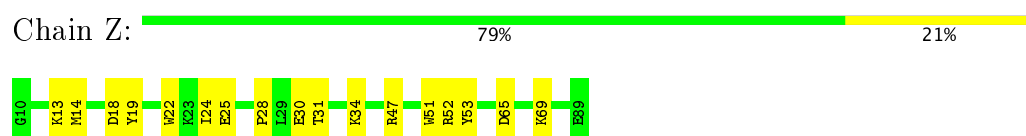
- Molecule 6: Acyl carrier protein, mitochondrial



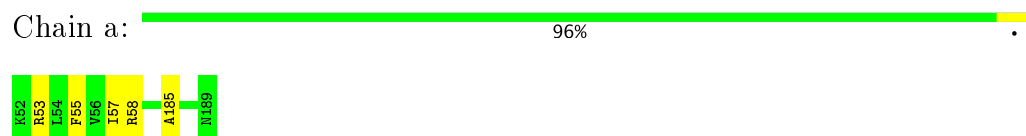
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



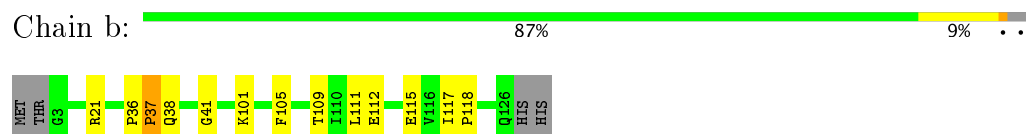
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



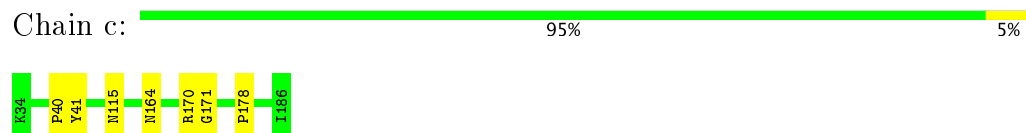
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



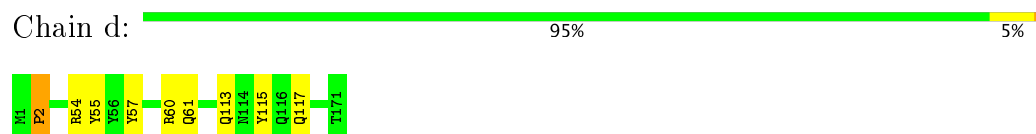
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  97% .



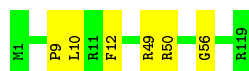
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  98% .



- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  95% 5% .



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  94% 6% .



- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

Chain i:  98% .



- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j:  97% .



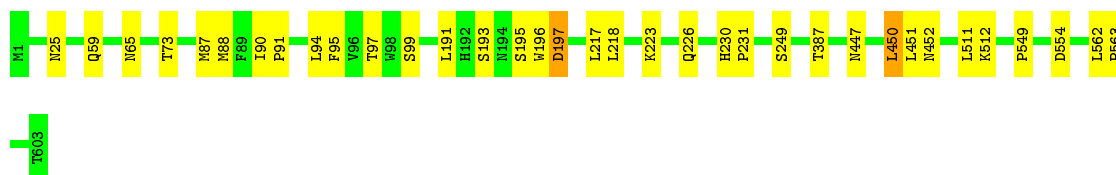
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  93% 6% .



- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

Chain l:  94% 5% .



- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

Chain m: 94% 6%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 96% .



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o: 97% .



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p: 98% .



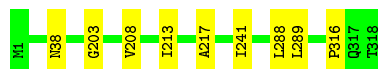
- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

Chain r: 98% .



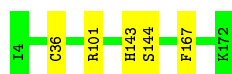
- Molecule 26: NADH-ubiquinone oxidoreductase chain 1

Chain s: 97% .



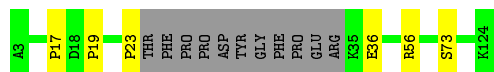
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 97% .



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 86% 5% 9%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w: 97% .





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEE, 8Q1, PLX

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  > 2$	RMSZ	# $ Z  > 2$
1	Q	0.33	0/398	0.51	0/548
10	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
11	c	0.58	0/1287	0.58	0/1761
12	d	0.63	0/1445	0.65	1/1945 (0.1%)
13	e	0.61	0/835	0.61	0/1134
14	f	0.48	0/418	0.58	0/566
15	g	0.64	0/1035	0.63	0/1398
16	h	0.62	0/884	0.65	0/1182
17	i	0.67	0/2808	0.77	2/3843 (0.1%)
18	j	0.55	0/945	0.69	1/1292 (0.1%)
19	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
2	S	0.60	0/583	0.64	0/785
20	l	0.61	2/4840 (0.0%)	0.69	3/6611 (0.0%)
21	m	0.68	0/1346	0.67	0/1832
22	n	0.49	0/484	0.62	0/652
23	o	0.54	0/1093	0.60	0/1479
24	p	0.58	0/1549	0.59	0/2098
25	r	0.70	0/3723	0.76	2/5089 (0.0%)
26	s	0.62	0/2580	0.73	0/3539
27	u	0.57	0/1433	0.60	0/1937
28	v	0.48	0/934	0.67	3/1241 (0.2%)
29	w	0.44	0/2533	0.56	0/3440
3	U	0.52	0/670	0.63	0/920
4	V	0.51	0/1065	0.61	0/1450
5	W	0.60	0/980	0.66	0/1327
6	X	0.57	0/698	0.61	0/942
7	Y	0.52	0/559	0.73	3/763 (0.4%)
8	Z	0.45	0/669	0.53	0/899
9	a	0.68	0/1209	0.65	0/1639
All	All	0.60	4/38849 (0.0%)	0.67	20/52811 (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
29	w	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	118	PRO	N-CD	5.14	1.55	1.47
19	k	2	PRO	N-CD	5.14	1.55	1.47
20	l	231	PRO	N-CD	5.04	1.54	1.47
20	l	91	PRO	N-CD	5.00	1.54	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	323	THR	C-N-CD	-7.37	104.39	120.60
7	Y	92	TRP	N-CA-C	-6.98	92.15	111.00
12	d	2	PRO	N-CA-CB	6.75	111.41	103.30
7	Y	87	PRO	CA-N-CD	-6.58	102.30	111.50
10	b	36	PRO	C-N-CD	6.21	141.45	128.40
17	i	323	THR	C-N-CA	6.05	147.40	122.00
28	v	17	PRO	N-CA-CB	5.92	110.40	103.30
20	l	197	ASP	C-N-CD	5.90	140.78	128.40
28	v	23	PRO	N-CA-CB	5.90	110.38	103.30
10	b	105	PHE	C-N-CD	5.81	140.60	128.40
19	k	1	MET	C-N-CD	5.75	140.47	128.40
20	l	90	ILE	C-N-CD	5.71	140.39	128.40
20	l	230	HIS	C-N-CD	5.69	140.34	128.40
10	b	117	ILE	C-N-CD	5.68	140.32	128.40
28	v	19	PRO	N-CA-CB	5.65	110.08	103.30
10	b	37	PRO	CA-N-CD	-5.42	103.92	111.50
18	j	98	LEU	CB-CG-CD2	-5.39	101.84	111.00
7	Y	86	TYR	C-N-CD	5.12	139.15	128.40
25	r	238	LEU	CB-CG-CD2	-5.09	102.34	111.00
25	r	408	LEU	CA-CB-CG	-5.08	103.61	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	w	338	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	381	0	355	9	0
2	S	568	0	567	13	0
3	U	647	0	653	9	0
4	V	1038	0	1027	34	0
5	W	956	0	949	21	0
6	X	686	0	676	24	0
7	Y	533	0	475	45	0
8	Z	648	0	627	13	0
9	a	1174	0	1177	0	0
10	b	1059	0	1079	0	0
11	c	1236	0	1092	0	0
12	d	1418	0	1375	0	0
13	e	810	0	772	0	0
14	f	405	0	407	0	0
15	g	1004	0	1008	0	0
16	h	863	0	861	0	0
17	i	2735	0	2893	0	0
18	j	919	0	968	0	0
19	k	740	0	792	0	0
20	l	4717	0	4893	0	0
21	m	1313	0	1330	0	0
22	n	473	0	480	0	0
23	o	1066	0	1086	0	0
24	p	1495	0	1440	0	0
25	r	3629	0	3825	0	0
26	s	2509	0	2617	0	0
27	u	1394	0	1367	0	0
28	v	921	0	892	0	0
29	w	2474	0	2304	0	0
30	U	52	0	88	1	0
30	V	52	0	88	2	0
30	b	52	0	88	0	0
30	g	156	0	264	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	r	104	0	176	0	0
30	s	52	0	88	0	0
31	V	63	0	68	8	0
31	i	64	0	72	0	0
31	l	128	0	144	0	0
31	n	64	0	72	0	0
32	V	51	0	82	12	0
32	W	51	0	82	5	0
32	l	100	0	157	0	0
33	p	35	0	0	0	0
All	All	38835	0	39456	181	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 25.

All (181) 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)
7:Y:84:PHE:CD1	7:Y:85:PRO:HD3	1.84	1.13
7:Y:71:TRP:CH2	7:Y:75:HIS:CD2	2.42	1.08
7:Y:71:TRP:CH2	7:Y:75:HIS:HD2	1.76	1.04
32:V:202:PEE:C25	32:V:202:PEE:H60	1.92	0.99
6:X:99:SER:HG	6:X:102:SER:HG	1.09	0.96
7:Y:83:HIS:O	7:Y:84:PHE:HB2	1.67	0.91
7:Y:84:PHE:CG	7:Y:85:PRO:CD	2.57	0.87
7:Y:84:PHE:CD1	7:Y:85:PRO:CD	2.58	0.86
32:W:201:PEE:N	32:W:201:PEE:O2P	2.08	0.85
4:V:84:PRO:O	4:V:89:ASN:ND2	2.10	0.84
7:Y:74:TRP:HZ3	7:Y:75:HIS:HD1	1.29	0.80
7:Y:74:TRP:CE3	7:Y:75:HIS:HA	2.16	0.79
7:Y:83:HIS:O	7:Y:84:PHE:CB	2.31	0.78
7:Y:84:PHE:CG	7:Y:85:PRO:HD2	2.19	0.77
7:Y:96:GLU:O	7:Y:97:LEU:HD23	1.84	0.77
4:V:40:ARG:HH22	4:V:55:LYS:HD3	1.50	0.75
7:Y:71:TRP:CZ2	7:Y:75:HIS:CD2	2.74	0.74
7:Y:84:PHE:CG	7:Y:85:PRO:HD3	2.22	0.74
32:V:202:PEE:H41	32:V:202:PEE:H60	1.67	0.74
32:V:202:PEE:H32	32:V:202:PEE:H39	1.70	0.73
7:Y:43:ARG:HG3	7:Y:46:GLN:HB2	1.72	0.72
32:V:202:PEE:H42	32:V:202:PEE:H60	1.73	0.71
7:Y:86:TYR:HB3	7:Y:87:PRO:CA	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:91:ASP:OD1	8:Z:47:ARG:NH1	2.24	0.70
7:Y:86:TYR:CB	7:Y:87:PRO:HA	2.22	0.69
6:X:84:LEU:HD22	6:X:98:LEU:HD21	1.74	0.69
32:W:201:PEE:H24	32:W:201:PEE:H53	1.74	0.69
4:V:81:ARG:HG2	4:V:83:LYS:HG3	1.75	0.68
7:Y:86:TYR:HB3	7:Y:87:PRO:HA	1.75	0.68
7:Y:84:PHE:CD2	7:Y:85:PRO:HD2	2.30	0.67
5:W:86:MET:SD	5:W:128:ARG:NH1	2.66	0.66
7:Y:81:LEU:HD23	7:Y:81:LEU:C	2.15	0.66
7:Y:79:GLU:O	7:Y:80:VAL:HG13	1.96	0.64
4:V:27:SER:O	4:V:30:SER:OG	2.14	0.63
32:V:202:PEE:H32	32:V:202:PEE:C24	2.25	0.63
7:Y:74:TRP:HE3	7:Y:75:HIS:HA	1.62	0.63
8:Z:24:ILE:HD11	8:Z:47:ARG:HG2	1.80	0.62
7:Y:96:GLU:O	7:Y:97:LEU:HB2	1.98	0.62
7:Y:81:LEU:HD23	7:Y:82:GLY:N	2.14	0.61
6:X:138:LEU:HD21	6:X:144:ILE:HG12	1.83	0.61
31:V:201:CDL:O1	31:V:201:CDL:OA7	2.15	0.61
7:Y:73:PHE:O	7:Y:73:PHE:HD1	1.84	0.61
5:W:39:GLY:O	5:W:42:THR:OG1	2.15	0.60
5:W:111:PHE:HE2	5:W:117:VAL:HG11	1.66	0.60
7:Y:45:ARG:HG3	8:Z:52:ARG:HB2	1.84	0.59
4:V:40:ARG:HA	31:V:201:CDL:OB3	2.02	0.59
8:Z:25:GLU:HA	8:Z:30:GLU:HG3	1.84	0.59
6:X:84:LEU:O	6:X:88:LYS:HG2	2.03	0.58
3:U:67:PRO:HB3	3:U:74:GLN:HB2	1.86	0.57
4:V:40:ARG:HD3	4:V:59:TYR:HE2	1.68	0.57
7:Y:39:HIS:ND1	7:Y:40:ILE:HG13	2.20	0.57
4:V:139:PRO:O	4:V:141:VAL:N	2.38	0.56
32:V:202:PEE:H40	32:V:202:PEE:H57	1.87	0.56
2:S:59:ARG:O	2:S:61:TYR:N	2.36	0.56
4:V:40:ARG:NH2	4:V:55:LYS:HD3	2.20	0.56
8:Z:51:TRP:O	8:Z:53:TYR:N	2.37	0.56
8:Z:22:TRP:CE3	8:Z:51:TRP:HA	2.41	0.56
4:V:62:THR:HG22	4:V:104:ARG:HE	1.69	0.56
4:V:3:PRO:HA	4:V:6:PHE:HB3	1.88	0.56
32:V:202:PEE:C24	32:V:202:PEE:H60	2.36	0.55
4:V:40:ARG:HD3	4:V:59:TYR:CE2	2.41	0.55
3:U:67:PRO:HA	3:U:74:GLN:OE1	2.07	0.55
7:Y:74:TRP:HE3	7:Y:75:HIS:CA	2.19	0.55
6:X:84:LEU:HD11	6:X:100:VAL:HG22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:96:GLU:O	7:Y:97:LEU:CD2	2.54	0.54
7:Y:96:GLU:O	7:Y:97:LEU:CB	2.55	0.54
1:Q:72:PRO:O	1:Q:75:THR:OG1	2.18	0.54
1:Q:69:VAL:HG12	1:Q:72:PRO:HD2	1.90	0.53
8:Z:24:ILE:HG22	8:Z:30:GLU:HB2	1.90	0.53
32:V:202:PEE:C24	32:V:202:PEE:H57	2.39	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	0.53
3:U:69:HIS:ND1	3:U:70:PRO:HA	2.24	0.53
1:Q:39:PRO:HB3	1:Q:43:TRP:CE3	2.45	0.52
5:W:33:TYR:CG	5:W:34:SER:N	2.77	0.52
5:W:35:MET:HA	5:W:38:ILE:HD12	1.91	0.52
2:S:37:ARG:O	5:W:143:TYR:OH	2.27	0.52
4:V:58:GLN:O	4:V:62:THR:HG23	2.10	0.52
3:U:84:LEU:O	5:W:59:ARG:NH1	2.41	0.51
4:V:12:ILE:HG22	4:V:13:PRO:O	2.11	0.51
6:X:77:GLU:HB2	8:Z:13:LYS:HE2	1.93	0.51
7:Y:86:TYR:HB3	7:Y:87:PRO:HB3	1.93	0.51
6:X:85:TYR:HE2	7:Y:45:ARG:NH1	2.09	0.51
7:Y:86:TYR:HB3	7:Y:87:PRO:CB	2.40	0.50
7:Y:74:TRP:CE3	7:Y:74:TRP:C	2.85	0.50
1:Q:65:PRO:HG2	1:Q:69:VAL:HG22	1.94	0.50
4:V:14:ASP:O	4:V:21:LYS:NZ	2.45	0.50
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.50
32:V:202:PEE:H40	32:V:202:PEE:C35	2.42	0.49
4:V:62:THR:HG22	4:V:104:ARG:NE	2.27	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	0.49
4:V:39:TYR:HD2	31:V:201:CDL:H721	1.76	0.49
32:V:202:PEE:C37	32:V:202:PEE:H41	2.40	0.49
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	0.49
4:V:62:THR:HG22	4:V:104:ARG:HD3	1.95	0.48
8:Z:28:PRO:O	8:Z:31:THR:OG1	2.22	0.48
2:S:50:ARG:CZ	2:S:54:ILE:HD11	2.43	0.48
4:V:29:ALA:O	4:V:63:ALA:HB1	2.14	0.48
5:W:47:HIS:O	5:W:51:MET:HG3	2.13	0.48
2:S:28:ARG:O	2:S:33:GLY:N	2.47	0.48
4:V:47:GLY:O	4:V:48:THR:OG1	2.25	0.48
5:W:30:LEU:HB2	5:W:32:GLY:H	1.78	0.48
7:Y:71:TRP:C	7:Y:71:TRP:CE3	2.87	0.48
6:X:102:SER:O	6:X:140:CYS:HA	2.14	0.48
32:W:201:PEE:N	32:W:201:PEE:P	2.87	0.47
31:V:201:CDL:H552	31:V:201:CDL:H522	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:40:ARG:HG3	31:V:201:CDL:HB22	1.97	0.47
4:V:37:ALA:HB1	4:V:56:VAL:HG22	1.95	0.47
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	0.47
4:V:96:ALA:HA	4:V:99:LEU:HD12	1.95	0.47
7:Y:50:LEU:O	7:Y:51:THR:OG1	2.27	0.47
32:W:201:PEE:H28	32:W:201:PEE:H22	1.50	0.47
7:Y:73:PHE:C	7:Y:73:PHE:CD1	2.88	0.47
5:W:101:VAL:HG13	5:W:102:PRO:HD2	1.96	0.47
5:W:48:TRP:O	5:W:51:MET:HB2	2.15	0.47
2:S:35:GLU:HG2	2:S:35:GLU:O	2.14	0.47
7:Y:88:ASP:N	7:Y:89:PRO:CD	2.78	0.47
7:Y:74:TRP:CE3	7:Y:75:HIS:CA	2.91	0.46
2:S:4:GLU:O	2:S:7:PRO:HD2	2.15	0.46
5:W:77:ALA:O	5:W:80:ASP:HB3	2.16	0.46
6:X:82:ARG:O	6:X:86:VAL:HG23	2.15	0.46
2:S:47:LEU:HA	2:S:50:ARG:HB3	1.98	0.46
4:V:121:ALA:O	4:V:125:VAL:HG23	2.15	0.46
2:S:43:TYR:CZ	5:W:68:ARG:HD2	2.51	0.46
8:Z:31:THR:O	8:Z:34:LYS:HB3	2.16	0.46
7:Y:42:PRO:HD2	8:Z:14:MET:HG3	1.98	0.46
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.98	0.45
5:W:111:PHE:CD2	5:W:117:VAL:HG21	2.51	0.45
2:S:16:LEU:O	2:S:19:PRO:HD2	2.16	0.45
31:V:201:CDL:H541	31:V:201:CDL:H572	1.46	0.45
4:V:2:ALA:O	4:V:6:PHE:N	2.45	0.45
7:Y:74:TRP:HE3	7:Y:75:HIS:N	2.15	0.45
6:X:138:LEU:CD2	6:X:144:ILE:HG12	2.47	0.45
32:V:202:PEE:H40	32:V:202:PEE:H60	1.99	0.44
2:S:31:ASN:HD21	2:S:36:LYS:HD3	1.83	0.44
4:V:69:VAL:HG21	4:V:100:THR:HG21	1.98	0.44
5:W:111:PHE:CE2	5:W:117:VAL:HG11	2.49	0.44
7:Y:85:PRO:O	7:Y:86:TYR:CD1	2.70	0.44
4:V:40:ARG:HE	31:V:201:CDL:CA2	2.30	0.44
32:W:201:PEE:H51	32:W:201:PEE:H56	1.33	0.44
1:Q:55:SER:N	1:Q:58:THR:OG1	2.51	0.44
4:V:51:GLU:HB3	4:V:55:LYS:NZ	2.34	0.43
2:S:43:TYR:CE2	5:W:68:ARG:HD2	2.53	0.43
6:X:123:GLU:HB2	6:X:128:PHE:O	2.18	0.43
8:Z:65:ASP:O	8:Z:69:LYS:HB2	2.19	0.43
30:V:203:PLX:H141	30:V:203:PLX:H332	2.01	0.43
4:V:19:HIS:CD2	4:V:20:ARG:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:69:VAL:HG12	1:Q:72:PRO:CD	2.48	0.43
5:W:33:TYR:O	5:W:34:SER:OG	2.27	0.43
4:V:95:CYS:O	4:V:99:LEU:HG	2.19	0.42
4:V:62:THR:HG22	4:V:104:ARG:CD	2.49	0.42
4:V:133:TRP:CG	32:V:202:PEE:H7	2.54	0.42
8:Z:18:ASP:OD1	8:Z:19:TYR:N	2.52	0.42
2:S:7:PRO:O	2:S:10:SER:OG	2.23	0.42
5:W:72:LEU:HD23	5:W:72:LEU:HA	1.84	0.42
3:U:40:LYS:O	3:U:44:MET:HG2	2.18	0.42
3:U:69:HIS:CE1	3:U:70:PRO:HA	2.54	0.42
6:X:155:TYR:CD2	6:X:155:TYR:O	2.73	0.42
3:U:19:LEU:O	3:U:22:SER:OG	2.29	0.41
4:V:126:LYS:HE3	4:V:130:LEU:HD11	2.02	0.41
4:V:23:TYR:O	4:V:24:SER:HB2	2.20	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	0.41
31:V:201:CDL:H722	31:V:201:CDL:H752	1.75	0.41
5:W:86:MET:HG2	5:W:128:ARG:HH22	1.86	0.41
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.41
4:V:114:ALA:HB1	4:V:118:PHE:CE2	2.56	0.41
2:S:47:LEU:O	2:S:50:ARG:HB3	2.20	0.41
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
6:X:88:LYS:HZ2	6:X:98:LEU:HD13	1.85	0.41
7:Y:62:SER:O	7:Y:65:MET:HB3	2.21	0.41
1:Q:65:PRO:CG	1:Q:69:VAL:HG22	2.51	0.40
30:V:203:PLX:H342	30:V:203:PLX:H371	1.76	0.40
7:Y:45:ARG:HG2	7:Y:45:ARG:O	2.22	0.40
30:U:101:PLX:H1B3	30:U:101:PLX:H22	1.86	0.40
7:Y:43:ARG:HH11	7:Y:49:GLN:HG2	1.86	0.40
7:Y:74:TRP:CZ3	7:Y:75:HIS:HA	2.53	0.40
3:U:50:PRO:HB2	5:W:69:ILE:HD11	2.03	0.40
5:W:111:PHE:CE2	5:W:117:VAL:HG21	2.56	0.40
1:Q:50:ALA:HB2	1:Q:63:PRO:HB3	2.03	0.40
1:Q:69:VAL:O	1:Q:72:PRO:HD2	2.22	0.40
3:U:8:PHE:O	3:U:11:ASN:HB3	2.21	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 PDB entries followed by that with respect to all EM entries.

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	Q	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	3	31
2	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	5	42
3	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	15	59
4	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	8	48
5	W	114/116 (98%)	109 (96%)	4 (4%)	1 (1%)	20	64
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	29
7	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	10
8	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
9	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	8	48
10	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	3	33
11	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	3	30
12	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	28	70
13	e	95/97 (98%)	84 (88%)	8 (8%)	3 (3%)	5	40
14	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	8	48
15	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	2	28
16	h	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	2	24
17	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	11	53
18	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	6	43
19	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	5	40
20	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	9	50
21	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	2	24
22	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	4	36
23	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	5	40
24	p	170/172 (99%)	157 (92%)	10 (6%)	3 (2%)	10	52
25	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	9	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	6	43
27	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	5	41
28	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	6	43
29	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	6	43
All	All	4641/4716 (98%)	4217 (91%)	295 (6%)	129 (3%)	9	43

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	60	TYR
3	U	71	GLN
5	W	34	SER
6	X	155	TYR
7	Y	84	PHE
9	a	58	ARG
11	c	115	ASN
11	c	178	PRO
12	d	2	PRO
16	h	20	ILE
17	i	91	ASN
17	i	323	THR
18	j	24	LEU
18	j	26	GLN
19	k	52	HIS
20	l	450	LEU
21	m	115	VAL
21	m	116	VAL
21	m	118	PHE
22	n	55	VAL
25	r	52	CYS
25	r	346	GLN
29	w	57	SER
29	w	264	GLN
29	w	282	PRO
29	w	347	VAL
4	V	135	VAL
4	V	140	LYS
7	Y	44	TYR
7	Y	51	THR
9	a	57	ILE
9	a	185	ALA

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Mol	Chain	Res	Type
10	b	101	LYS
11	c	170	ARG
15	g	9	PRO
16	h	3	PHE
16	h	24	GLU
16	h	43	CYS
18	j	2	ASN
20	l	73	THR
20	l	512	LYS
21	m	122	GLY
22	n	52	SER
25	r	45	ILE
25	r	188	ASN
25	r	250	LEU
25	r	421	HIS
26	s	203	GLY
26	s	213	ILE
26	s	217	ALA
26	s	316	PRO
28	v	56	ARG
29	w	285	LYS
1	Q	36	GLN
6	X	140	CYS
7	Y	85	PRO
10	b	37	PRO
10	b	109	THR
11	c	164	ASN
13	e	61	PRO
13	e	111	ASP
15	g	10	LEU
15	g	12	PHE
15	g	50	ARG
17	i	87	THR
19	k	83	ASN
19	k	96	LEU
20	l	65	ASN
20	l	451	LEU
20	l	511	LEU
20	l	549	PRO
20	l	554	ASP
20	l	563	PRO
21	m	4	ALA

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Mol	Chain	Res	Type
21	m	76	GLU
21	m	110	ASP
23	o	5	LYS
23	o	12	ARG
25	r	139	GLN
26	s	38	ASN
27	u	36	CYS
27	u	101	ARG
27	u	143	HIS
28	v	73	SER
29	w	351	TRP
2	S	36	LYS
6	X	74	LEU
7	Y	42	PRO
7	Y	87	PRO
10	b	115	GLU
11	c	40	PRO
11	c	41	TYR
15	g	49	ARG
15	g	56	GLY
16	h	32	ARG
16	h	45	HIS
17	i	150	ASN
20	l	249	SER
20	l	387	THR
20	l	562	LEU
23	o	59	LEU
23	o	120	LYS
24	p	76	HIS
25	r	251	ASN
26	s	208	VAL
26	s	288	LEU
26	s	289	LEU
27	u	167	PHE
28	v	36	GLU
4	V	48	THR
6	X	153	ASP
11	c	171	GLY
17	i	92	GLN
21	m	113	VAL
24	p	175	ARG
27	u	144	SER

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Mol	Chain	Res	Type
29	w	58	ARG
29	w	121	PRO
29	w	160	GLU
10	b	41	GLY
14	f	39	PRO
21	m	24	SER
24	p	32	VAL
25	r	205	VAL
26	s	241	ILE
21	m	23	PRO
1	Q	69	VAL
17	i	338	PRO
13	e	135	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 PDB entries followed by that with respect to all EM entries.

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	Q	41/41 (100%)	41 (100%)	0	100	100
2	S	59/59 (100%)	59 (100%)	0	100	100
3	U	72/72 (100%)	72 (100%)	0	100	100
4	V	102/102 (100%)	102 (100%)	0	100	100
5	W	100/100 (100%)	100 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	Y	57/57 (100%)	49 (86%)	8 (14%)	4	27
8	Z	62/63 (98%)	62 (100%)	0	100	100
9	a	124/124 (100%)	122 (98%)	2 (2%)	68	88
10	b	118/122 (97%)	114 (97%)	4 (3%)	42	75
11	c	124/137 (90%)	124 (100%)	0	100	100
12	d	145/154 (94%)	137 (94%)	8 (6%)	25	64
13	e	90/90 (100%)	90 (100%)	0	100	100
14	f	43/43 (100%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	g	105/105 (100%)	105 (100%)	0	100	100
16	h	90/90 (100%)	90 (100%)	0	100	100
17	i	314/314 (100%)	314 (100%)	0	100	100
18	j	102/103 (99%)	102 (100%)	0	100	100
19	k	85/85 (100%)	82 (96%)	3 (4%)	41	75
20	l	531/532 (100%)	511 (96%)	20 (4%)	38	73
21	m	137/137 (100%)	137 (100%)	0	100	100
22	n	53/53 (100%)	53 (100%)	0	100	100
23	o	114/114 (100%)	114 (100%)	0	100	100
24	p	157/157 (100%)	157 (100%)	0	100	100
25	r	416/416 (100%)	416 (100%)	0	100	100
26	s	278/278 (100%)	278 (100%)	0	100	100
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	89/111 (80%)	89 (100%)	0	100	100
29	w	249/288 (86%)	249 (100%)	0	100	100
All	All	4088/4179 (98%)	4043 (99%)	45 (1%)	79	90

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Y	73	PHE
7	Y	75	HIS
7	Y	78	GLU
7	Y	80	VAL
7	Y	81	LEU
7	Y	83	HIS
7	Y	87	PRO
7	Y	97	LEU
9	a	53	ARG
9	a	55	PHE
10	b	21	ARG
10	b	38	GLN
10	b	111	LEU
10	b	112	GLU
12	d	54	ARG
12	d	55	TYR
12	d	57	TYR

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Mol	Chain	Res	Type
12	d	60	ARG
12	d	61	GLN
12	d	113	GLN
12	d	115	TYR
12	d	117	GLN
19	k	1	MET
19	k	3	LEU
19	k	8	ILE
20	l	25	ASN
20	l	59	GLN
20	l	87	MET
20	l	88	MET
20	l	94	LEU
20	l	95	PHE
20	l	97	THR
20	l	99	SER
20	l	191	LEU
20	l	193	SER
20	l	195	SER
20	l	196	TRP
20	l	197	ASP
20	l	217	LEU
20	l	218	LEU
20	l	223	LYS
20	l	226	GLN
20	l	447	ASN
20	l	450	LEU
20	l	452	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	38	GLN
2	S	44	HIS
2	S	68	ASN
5	W	61	GLN
5	W	112	HIS
5	W	135	HIS
7	Y	75	HIS
9	a	90	ASN
9	a	189	ASN
10	b	14	GLN

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Mol	Chain	Res	Type
10	b	83	HIS
10	b	89	HIS
10	b	126	GLN
11	c	56	ASN
11	c	84	HIS
11	c	154	GLN
12	d	59	HIS
12	d	61	GLN
12	d	85	GLN
12	d	113	GLN
12	d	117	GLN
12	d	138	GLN
15	g	60	GLN
15	g	96	HIS
17	i	83	GLN
17	i	112	HIS
17	i	150	ASN
17	i	186	HIS
17	i	222	ASN
18	j	10	ASN
19	k	7	ASN
19	k	94	ASN
20	l	4	HIS
20	l	59	GLN
20	l	139	GLN
20	l	192	HIS
20	l	199	GLN
20	l	205	ASN
20	l	226	GLN
20	l	248	HIS
20	l	274	GLN
20	l	296	ASN
20	l	320	ASN
20	l	332	HIS
20	l	348	HIS
20	l	394	HIS
20	l	400	ASN
20	l	442	ASN
20	l	446	ASN
20	l	534	HIS
20	l	569	HIS
20	l	580	GLN

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Mol	Chain	Res	Type
21	m	45	ASN
21	m	117	ASN
22	n	40	ASN
23	o	62	ASN
23	o	126	HIS
24	p	75	GLN
25	r	48	ASN
25	r	168	HIS
25	r	390	ASN
25	r	415	GLN
25	r	425	ASN
26	s	93	ASN
26	s	169	GLN
26	s	235	ASN
27	u	30	HIS
27	u	31	HIS
27	u	64	ASN
27	u	77	HIS
27	u	99	HIS
27	u	104	GLN
27	u	143	HIS
28	v	43	GLN
28	v	61	HIS
28	v	85	HIS
28	v	92	HIS
29	w	85	HIS
29	w	111	ASN
29	w	132	GLN
29	w	149	HIS
29	w	257	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

19 ligands 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	$\# Z  > 2$
30	PLX	U	101	-	51,51,51	0.73	1 (1%)	54,59,59	0.74	2 (3%)
31	CDL	V	201	-	61,61,99	1.24	5 (8%)	60,71,111	0.99	3 (5%)
32	PEE	V	202	-	50,50,50	0.88	4 (8%)	52,55,55	0.84	2 (3%)
30	PLX	V	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.61	1 (1%)
32	PEE	W	201	-	50,50,50	0.86	4 (8%)	52,55,55	0.92	2 (3%)
30	PLX	b	201	-	51,51,51	0.60	0	54,59,59	0.64	0
30	PLX	g	201	-	51,51,51	0.81	1 (1%)	54,59,59	0.69	1 (1%)
30	PLX	g	202	-	51,51,51	0.74	1 (1%)	54,59,59	0.62	1 (1%)
30	PLX	g	203	-	51,51,51	0.77	1 (1%)	54,59,59	0.59	1 (1%)
31	CDL	i	401	-	63,63,99	1.20	5 (7%)	65,75,111	1.10	5 (7%)
32	PEE	l	701	-	48,48,50	1.02	2 (4%)	50,53,55	0.89	2 (4%)
32	PEE	l	702	-	50,50,50	0.88	4 (8%)	52,55,55	0.93	2 (3%)
31	CDL	l	703	-	63,63,99	1.19	5 (7%)	65,75,111	1.12	4 (6%)
31	CDL	l	704	-	63,63,99	1.24	5 (7%)	65,75,111	1.06	4 (6%)
31	CDL	n	101	-	63,63,99	1.22	5 (7%)	65,75,111	1.12	4 (6%)
33	8Q1	p	201	-	32,34,34	1.67	5 (15%)	39,43,43	1.80	5 (12%)
30	PLX	r	501	-	51,51,51	0.74	1 (1%)	54,59,59	0.66	1 (1%)
30	PLX	r	502	-	51,51,51	0.67	0	54,59,59	0.67	1 (1%)
30	PLX	s	401	-	51,51,51	0.75	1 (1%)	54,59,59	0.69	1 (1%)

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
30	PLX	U	101	-	-	0/54/55/55	0/0/0/0
31	CDL	V	201	-	-	0/69/69/110	0/0/0/0
32	PEE	V	202	-	-	0/54/54/54	0/0/0/0
30	PLX	V	203	-	-	0/54/55/55	0/0/0/0
32	PEE	W	201	-	-	0/54/54/54	0/0/0/0
30	PLX	b	201	-	-	0/54/55/55	0/0/0/0
30	PLX	g	201	-	-	0/54/55/55	0/0/0/0
30	PLX	g	202	-	-	0/54/55/55	0/0/0/0
30	PLX	g	203	-	-	0/54/55/55	0/0/0/0
31	CDL	i	401	-	-	0/74/74/110	0/0/0/0
32	PEE	l	701	-	-	0/52/52/54	0/0/0/0
32	PEE	l	702	-	-	0/54/54/54	0/0/0/0
31	CDL	l	703	-	-	0/74/74/110	0/0/0/0
31	CDL	l	704	-	-	0/74/74/110	0/0/0/0
31	CDL	n	101	-	-	2/74/74/110	0/0/0/0
33	8Q1	p	201	-	-	2/41/41/41	0/0/0/0
30	PLX	r	501	-	-	0/54/55/55	0/0/0/0
30	PLX	r	502	-	-	0/54/55/55	0/0/0/0
30	PLX	s	401	-	-	0/54/55/55	0/0/0/0

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	s	401	PLX	O6-C4	-2.86	1.40	1.44
30	g	203	PLX	O6-C4	-2.83	1.40	1.44
30	g	201	PLX	O6-C4	-2.72	1.40	1.44
30	V	203	PLX	O6-C4	-2.70	1.40	1.44
31	n	101	CDL	OB6-CB4	-2.63	1.39	1.46
31	V	201	CDL	OB6-CB4	-2.50	1.40	1.46
33	p	201	8Q1	O35-C34	-2.47	1.18	1.23
30	U	101	PLX	O6-C4	-2.45	1.41	1.44
31	i	401	CDL	OB6-CB4	-2.44	1.40	1.46
30	g	202	PLX	O6-C4	-2.40	1.41	1.44
30	r	501	PLX	O6-C4	-2.32	1.41	1.44
32	V	202	PEE	O3-C3	-2.31	1.40	1.45
31	l	703	CDL	OB6-CB4	-2.27	1.40	1.46
33	p	201	8Q1	O40-C39	-2.27	1.18	1.23
31	l	704	CDL	OB6-CB4	-2.26	1.40	1.46
32	l	702	PEE	O3-C3	-2.24	1.40	1.45
32	W	201	PEE	O3-C3	-2.19	1.40	1.45
32	l	702	PEE	O2-C2	-2.18	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	V	202	PEE	O2-C2	-2.16	1.41	1.46
32	W	201	PEE	O2-C2	-2.11	1.41	1.46
32	W	201	PEE	O2-C10	2.20	1.40	1.34
32	W	201	PEE	O3-C30	2.22	1.39	1.33
32	V	202	PEE	O3-C30	2.24	1.39	1.33
32	V	202	PEE	O2-C10	2.33	1.41	1.34
32	l	702	PEE	O2-C10	2.33	1.41	1.34
32	l	702	PEE	O3-C30	2.35	1.40	1.33
33	p	201	8Q1	C1-S44	2.49	1.81	1.76
31	V	201	CDL	OB6-CB5	3.04	1.43	1.34
31	i	401	CDL	OB6-CB5	3.05	1.43	1.34
31	l	703	CDL	OB6-CB5	3.16	1.43	1.34
31	n	101	CDL	OB6-CB5	3.19	1.43	1.34
32	l	701	PEE	O2-C10	3.22	1.43	1.34
31	l	704	CDL	OB6-CB5	3.22	1.43	1.34
31	i	401	CDL	OA8-CA7	3.71	1.44	1.33
31	l	703	CDL	OA8-CA7	3.78	1.44	1.33
31	n	101	CDL	OA8-CA7	3.89	1.44	1.33
31	i	401	CDL	OA6-CA5	3.90	1.45	1.34
31	l	704	CDL	OA6-CA5	4.02	1.46	1.34
31	i	401	CDL	OB8-CB7	4.04	1.45	1.33
31	n	101	CDL	OB8-CB7	4.09	1.45	1.33
32	l	701	PEE	O3-C30	4.10	1.45	1.33
31	V	201	CDL	OA8-CA7	4.10	1.45	1.32
31	l	704	CDL	OA8-CA7	4.10	1.45	1.33
31	V	201	CDL	OB8-CB7	4.13	1.45	1.33
31	V	201	CDL	OA6-CA5	4.15	1.46	1.34
31	l	703	CDL	OA6-CA5	4.18	1.46	1.34
31	n	101	CDL	OA6-CA5	4.19	1.46	1.34
31	l	703	CDL	OB8-CB7	4.20	1.45	1.33
31	l	704	CDL	OB8-CB7	4.32	1.46	1.33
33	p	201	8Q1	C39-N41	5.09	1.45	1.33
33	p	201	8Q1	C34-N36	5.67	1.45	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	p	201	8Q1	O4-C1-C6	-4.84	119.71	123.95
33	p	201	8Q1	O4-C1-S44	-2.88	119.82	122.84
30	U	101	PLX	C5-C4-C3	-2.19	106.91	111.86
30	r	502	PLX	C2-C1-N1	-2.09	108.76	115.86
31	i	401	CDL	CA4-OA6-CA5	-2.01	113.12	117.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	r	501	PLX	C1C-N1-C1	2.20	118.36	109.93
30	g	202	PLX	C1C-N1-C1	2.34	118.91	109.93
30	g	201	PLX	C1C-N1-C1	2.34	118.92	109.93
30	g	203	PLX	C1C-N1-C1	2.40	119.15	109.93
33	p	201	8Q1	C38-C39-N41	2.44	120.71	116.49
30	U	101	PLX	C1C-N1-C1	2.44	119.31	109.93
30	V	203	PLX	C1C-N1-C1	2.47	119.41	109.93
32	l	701	PEE	O3-C30-C31	2.49	119.14	111.90
30	s	401	PLX	C1C-N1-C1	2.52	119.59	109.93
33	p	201	8Q1	C43-S44-C1	2.54	110.30	101.90
31	i	401	CDL	OA8-CA7-C31	2.58	119.40	111.90
31	V	201	CDL	OB8-CB7-C71	2.73	119.83	111.90
31	l	704	CDL	OB8-CB7-C71	2.87	120.26	111.90
31	l	703	CDL	OB8-CB7-C71	2.90	120.35	111.90
31	n	101	CDL	OB8-CB7-C71	2.92	120.39	111.90
32	W	201	PEE	O3-C30-C31	2.92	120.41	111.90
31	l	704	CDL	OA8-CA7-C31	2.94	120.46	111.90
31	n	101	CDL	OA8-CA7-C31	2.95	120.50	111.90
31	i	401	CDL	OB8-CB7-C71	2.97	120.54	111.90
32	l	702	PEE	O3-C30-C31	3.07	120.83	111.90
32	V	202	PEE	O3-C30-C31	3.08	120.86	111.90
31	l	703	CDL	OA8-CA7-C31	3.22	121.28	111.90
31	V	201	CDL	OA6-CA5-C11	3.54	118.89	111.55
31	i	401	CDL	OB6-CB5-C51	3.63	119.09	111.55
32	V	202	PEE	O2-C10-C11	3.68	119.20	111.55
32	W	201	PEE	O2-C10-C11	3.79	119.43	111.55
31	n	101	CDL	OA6-CA5-C11	4.02	119.91	111.55
31	l	704	CDL	OB6-CB5-C51	4.05	119.96	111.55
31	l	703	CDL	OB6-CB5-C51	4.07	120.00	111.55
32	l	701	PEE	O2-C10-C11	4.13	120.14	111.55
31	n	101	CDL	OB6-CB5-C51	4.21	120.29	111.55
31	V	201	CDL	OB6-CB5-C51	4.22	120.31	111.55
31	l	704	CDL	OA6-CA5-C11	4.24	120.36	111.55
31	i	401	CDL	OA6-CA5-C11	4.27	120.42	111.55
31	l	703	CDL	OA6-CA5-C11	4.31	120.51	111.55
32	l	702	PEE	O2-C10-C11	4.53	120.96	111.55
33	p	201	8Q1	C6-C1-S44	7.14	120.47	113.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	n	101	CDL	CA4-OA6-CA5-OA7
31	n	101	CDL	CA4-OA6-CA5-C11
33	p	201	8Q1	C6-C1-S44-C43
33	p	201	8Q1	O4-C1-S44-C43

There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	U	101	PLX	1	0
31	V	201	CDL	8	0
32	V	202	PEE	12	0
30	V	203	PLX	2	0
32	W	201	PEE	5	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.