

wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:14 PM BST

PDB ID : 4UQ8
EMDB ID: : EMD-2676
Title : Electron cryo-microscopy of bovine Complex I
Authors : Vinothkumar, K.R.; Zhu, J.; Hirst, J.
Deposited on : 2014-06-21
Resolution : 4.95 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

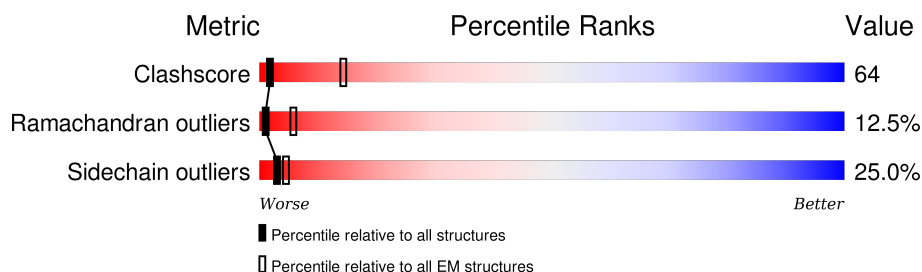
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.95 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.







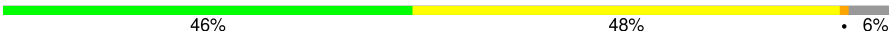

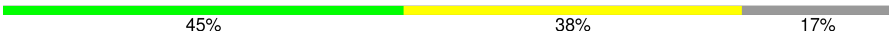

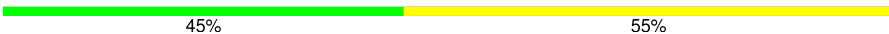



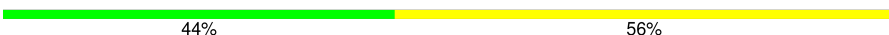




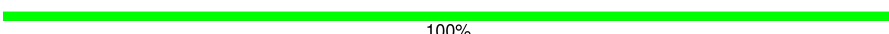
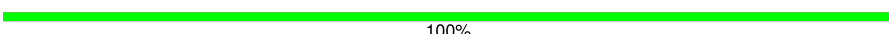
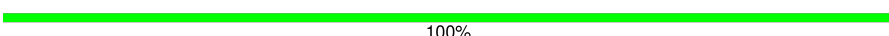
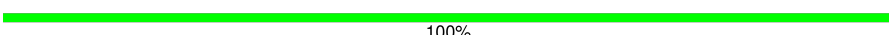
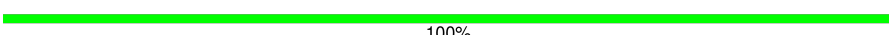
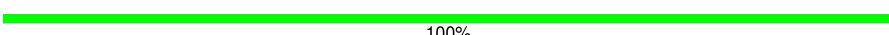
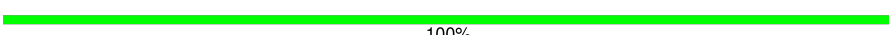
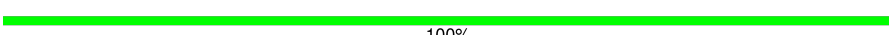
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	A	111	49% 26% 25%
2	B	143	54% 43% ..
3	C	154	63% 36% .
4	D	384	63% 36%
5	E	159	63% 37%
6	F	411	49% 51%
7	G	538	53% 44% ..
8	H	313	57% 34% 9%
9	I	162	55% 43% .

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Mol	Chain	Length	Quality of chain
10	J	171	
11	K	84	
12	L	601	
13	M	453	
14	N	345	
15	O	220	
16	P	303	
17	Q	85	
18	R	47	
19	S	80	
20	T	75	
21	U	79	
22	V	71	
23	W	72	
24	X	79	
25	Y	106	
26	Z	65	
27	a	29	
28	b	42	
29	c	27	
29	w	27	
30	d	39	
31	e	20	
32	f	30	
32	h	30	

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Mol	Chain	Length	Quality of chain
32	i	30	 100%
33	g	22	 100%
34	j	24	 100%
34	l	24	 100%
35	k	28	 100%
35	p	28	 100%
35	s	28	 100%
36	m	34	 100%
37	n	59	 100%
38	o	21	 100%
39	q	25	 100%
40	r	26	 100%
41	t	57	 100%
42	u	43	 35% 65%
43	v	32	 100%

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
44	SF4	B	201	-	-	X	-
44	SF4	I	222	-	-	X	-
44	SF4	I	223	-	-	X	-
45	FES	G	804	-	-	X	-

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 28647 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 UBIQUINONE OXIDOREDUCTASE CHAIN 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	83	Total	C	N	O	0	0
			415	249	83	83		

- Molecule 2 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	143	Total	C	N	O	S	0	0
			719	429	143	143	4		

- Molecule 3 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	154	Total	C	N	O	0	0
			770	462	154	154		

- Molecule 4 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	384	Total	C	N	O	0	0
			1920	1152	384	384		

- Molecule 5 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	159	Total	C	N	O	S	0	0
			799	477	159	159	4		

- Molecule 6 is a protein called NADH DEHYDROGENASE [UBIQUINONE] FLAVOPROTEIN 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	411	Total	C	N	O	S	0	0
			2059	1233	411	411	4		

- Molecule 7 is a protein called NADH-UBIQUINONE OXIDOREDUCTASE 75 KDA SUB-UNIT, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	527	Total	C	N	O	S	0	0
			2651	1584	529	527	11		

- Molecule 8 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	285	Total	C	N	O	S	0	0
			1425	855	285	285			

- Molecule 9 is a protein called NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			818	486	162	162	8		

- Molecule 10 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	131	Total	C	N	O	S	0	0
			655	393	131	131			

- Molecule 11 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	84	Total	C	N	O	S	0	0
			420	252	84	84			

- Molecule 12 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	558	Total	C	N	O	S	0	0
			2790	1674	558	558			

- Molecule 13 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	439	Total	C	N	O	0	0
			2195	1317	439	439		

- Molecule 14 is a protein called NADH UBIQUINONE OXIDOREDUCTASE CHAIN 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	326	Total	C	N	O	0	0
			1630	978	326	326		

- Molecule 15 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	181	Total	C	N	O	0	0
			905	543	181	181		

- Molecule 16 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	252	Total	C	N	O	0	0
			1260	756	252	252		

- Molecule 17 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	69	Total	C	N	O	0	0
			345	207	69	69		

- Molecule 18 is a protein called NADH DEHYDROGENASE [UBIQUINONE] SUBUNIT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 19 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 20 is a protein called ACYL CARRIER PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 21 is a protein called NADH UBIQUINONE DEHYDROGENASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	75	Total	C	N	O	0	0
			375	225	75	75		

- Molecule 22 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	71	Total	C	N	O	0	0
			355	213	71	71		

- Molecule 23 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 24 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	79	Total	C	N	O	0	0
			395	237	79	79		

- Molecule 25 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT; 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 26 is a protein called NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUBUNIT 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 27 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 28 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	42	Total	C	N	O	0	0
			210	126	42	42		

- Molecule 29 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	c	27	Total	C	N	O	0	0
			135	81	27	27		
29	w	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 30 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	d	39	Total	C	N	O	0	0
			195	117	39	39		

- Molecule 31 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 32 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	f	30	Total	C	N	O	0	0
			150	90	30	30		
32	h	30	Total	C	N	O	0	0
			150	90	30	30		
32	i	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 33 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	g	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 34 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	j	24	Total	C	N	O	0	0
			120	72	24	24		
34	l	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 35 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	k	28	Total	C	N	O	0	0
			140	84	28	28		
35	p	28	Total	C	N	O	0	0
			140	84	28	28		
35	s	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 36 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	m	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 37 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	n	59	Total	C	N	O	0	0
			295	177	59	59		

- Molecule 38 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	21	Total	C	N	O	0	0
			105	63	21	21		

- Molecule 39 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	q	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 40 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	r	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 41 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	t	57	Total	C	N	O	0	0
			285	171	57	57		

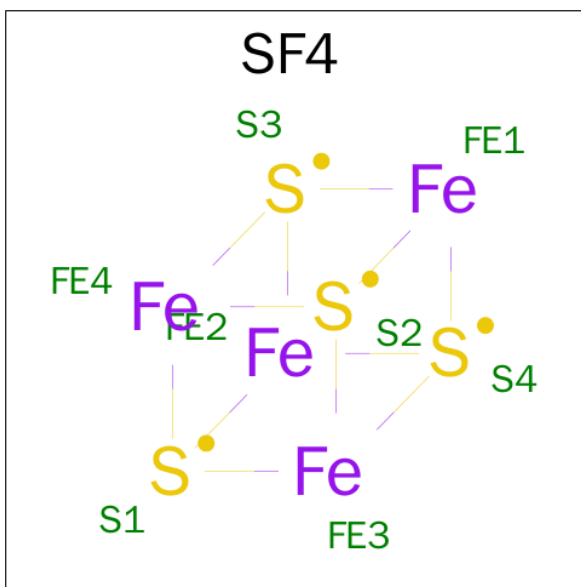
- Molecule 42 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	u	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 43 is a protein called NADH UBIQUINONE OXIDOREDUCTASE.

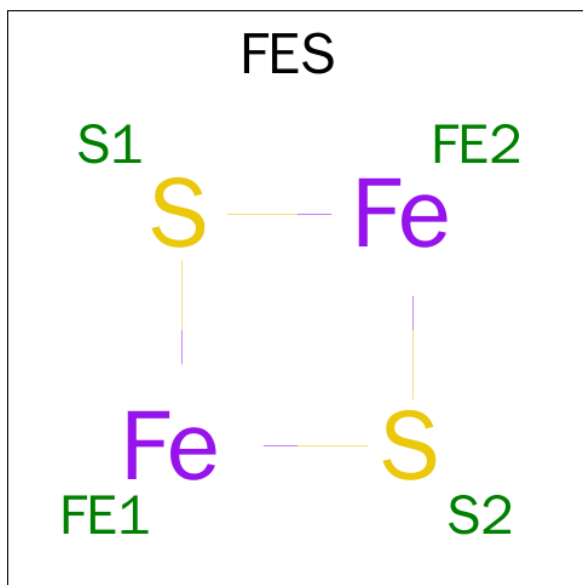
Mol	Chain	Residues	Atoms				AltConf	Trace
43	v	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 44 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
44	B	1	Total	Fe	S	0
			8	4	4	
44	F	1	Total	Fe	S	0
			8	4	4	
44	G	1	Total	Fe	S	0
			16	8	8	
44	G	1	Total	Fe	S	0
			16	8	8	
44	I	1	Total	Fe	S	0
			16	8	8	
44	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

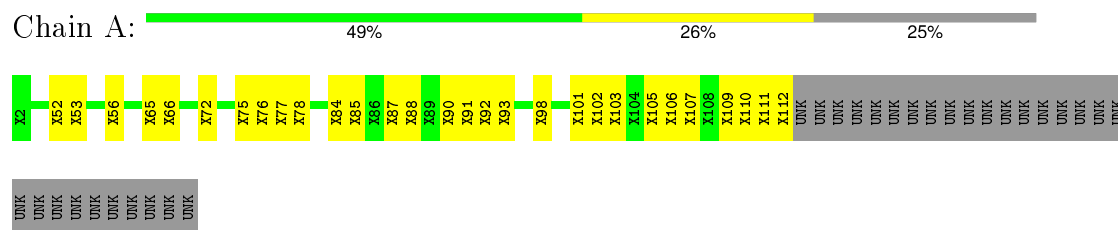


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	E	1	4	2	2	0
45	G	1	4	2	2	0

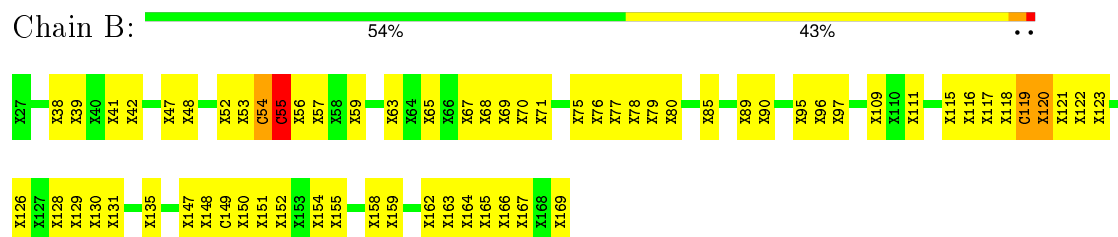
3 Residue-property plots

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. 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.

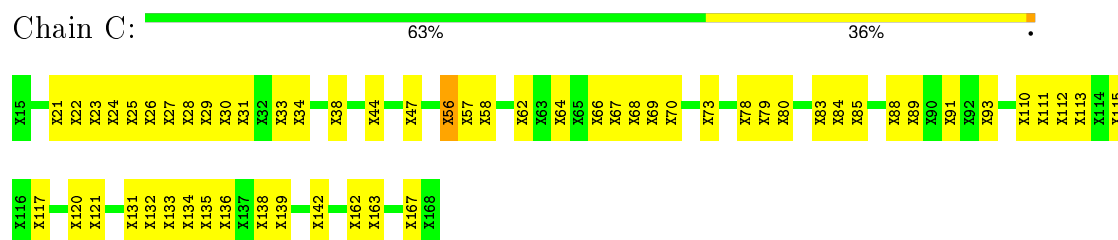
- Molecule 1: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 3



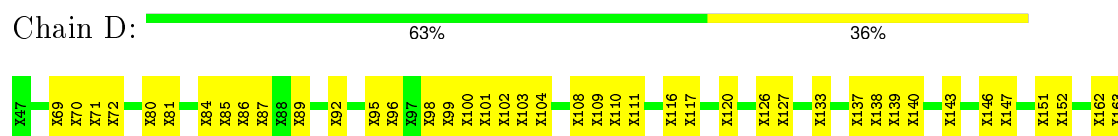
- Molecule 2: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 7, MITOCHONDRIAL

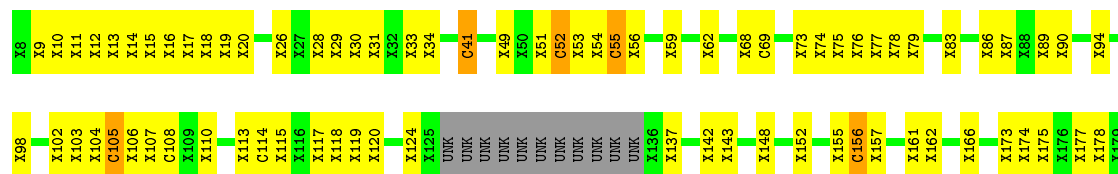


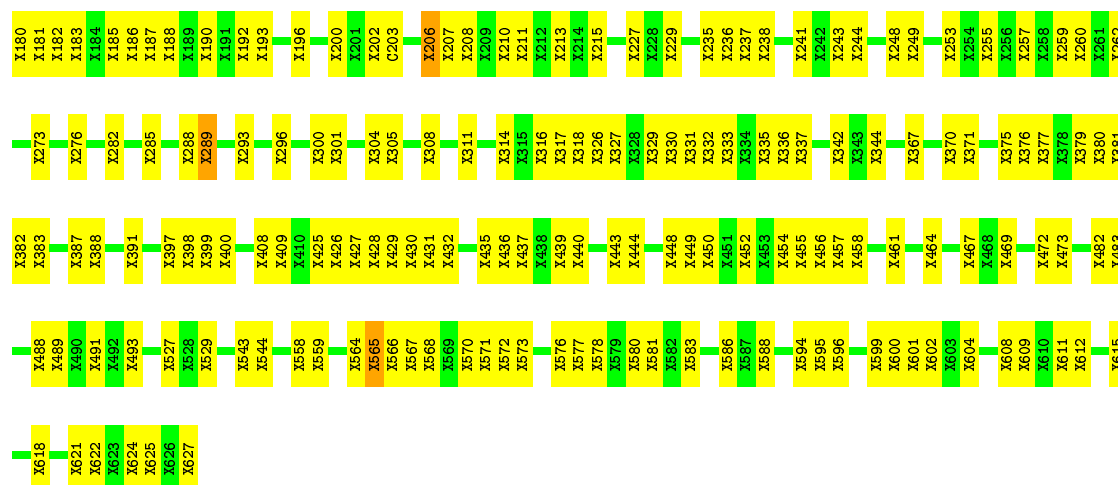
- Molecule 3: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 3, MITOCHONDRIAL



- Molecule 4: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 2, MITOCHONDRIAL







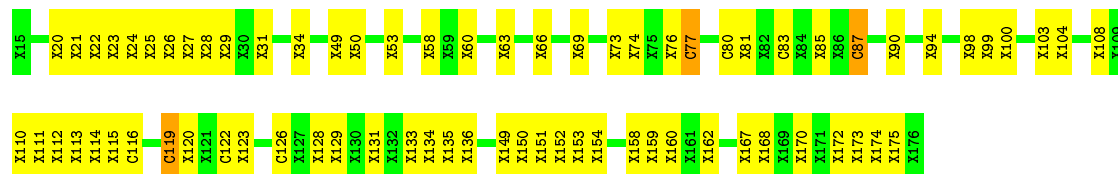
• Molecule 8: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 1

Chain H: 57% 34% 9%



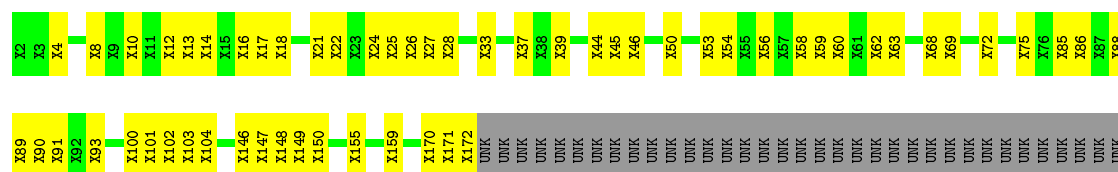
• Molecule 9: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTEIN 8, MITOCHONDRIAL

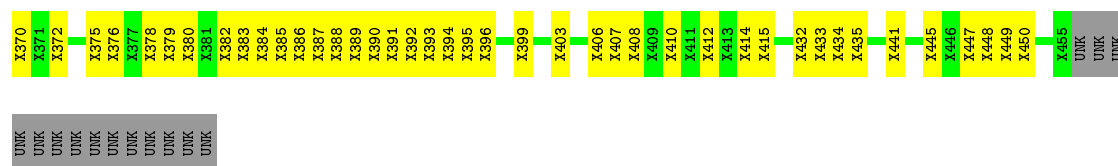
Chain I: 55% 43% 2%



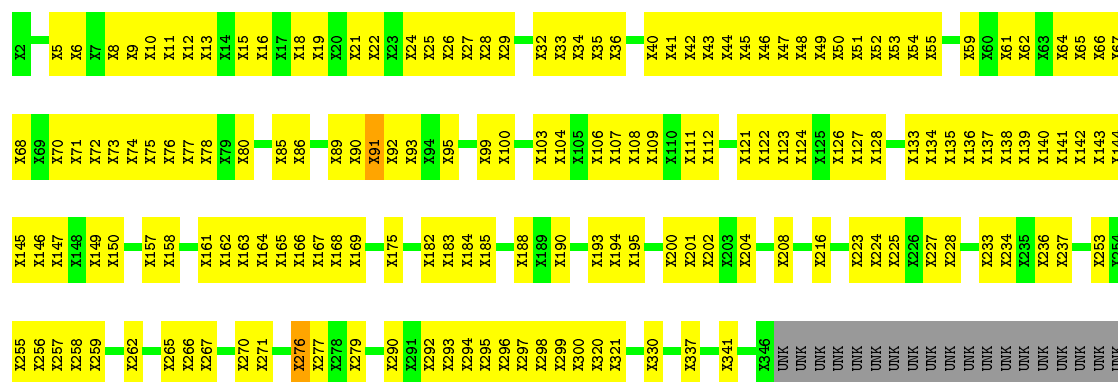
• Molecule 10: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 6

Chain J: 43% 33% 23%

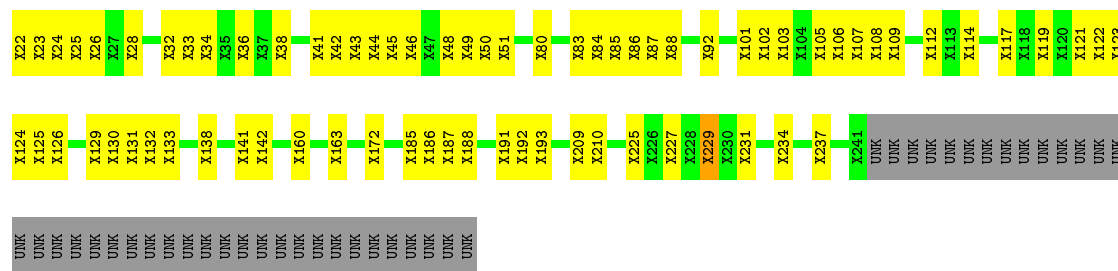




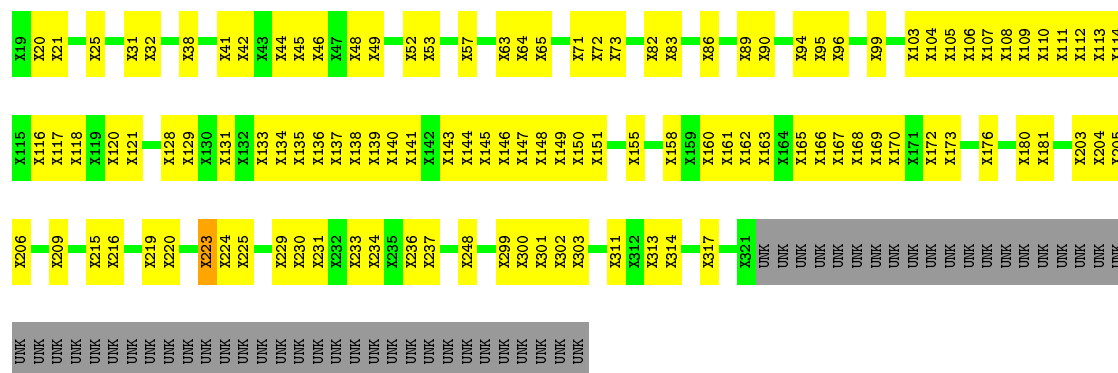
- Molecule 14: NADH UBIQUINONE OXIDOREDUCTASE CHAIN 2



● Molecule 15: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 10



- Molecule 16: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 9, MITOCHONDRIAL



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|--|-----|--|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|--|-----|--|-----|-----|
| X1 | X2 | X3 | X4 | X5 | X6 | | X16 | | X20 | | X24 | X25 | X26 | X27 | | X39 | X40 | X41 | X42 | X43 | X44 | | X47 | X48 | X49 | X50 | X51 | X52 | X53 | | X56 | X57 | X58 | X59 | | X68 | | X71 | X72 |
|----|----|----|----|----|----|--|-----|--|-----|--|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|--|-----|--|-----|-----|

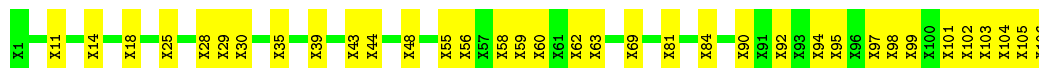
- Molecule 24: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 8

Chain X:  66% 34%



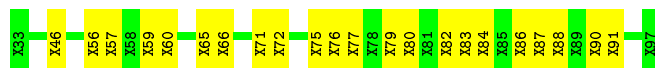
- Molecule 25: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT; 11

Chain Y:  67% 33%



- Molecule 26: NADH DEHYDROGENASE [UBIQUINONE] 1 ALPHA SUBCOMPLEX SUB-UNIT 13

Chain Z:  66% 34%



- Molecule 27: NADH UBIQUINONE OXIDOREDUCTASE

Chain a:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: NADH UBIQUINONE OXIDOREDUCTASE

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: NADH UBIQUINONE OXIDOREDUCTASE

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: NADH UBIQUINONE OXIDOREDUCTASE

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: NADH UBIQUINONE OXIDOREDUCTASE

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: NADH UBIQUINONE OXIDOREDUCTASE

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: NADH UBIQUINONE OXIDOREDUCTASE

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: NADH UBIQUINONE OXIDOREDUCTASE

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: NADH UBIQUINONE OXIDOREDUCTASE

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: NADH UBIQUINONE OXIDOREDUCTASE

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: NADH UBIQUINONE OXIDOREDUCTASE

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: NADH UBIQUINONE OXIDOREDUCTASE

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: NADH UBIQUINONE OXIDOREDUCTASE

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: NADH UBIQUINONE OXIDOREDUCTASE

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: NADH UBIQUINONE OXIDOREDUCTASE

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: NADH UBIQUINONE OXIDOREDUCTASE

Chain r:  100%

There are no outlier residues recorded for this chain.

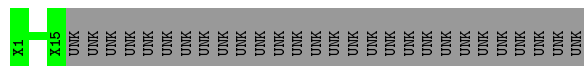
- Molecule 41: NADH UBIQUINONE OXIDOREDUCTASE

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: NADH UBIQUINONE OXIDOREDUCTASE

Chain u:  35% 65%



- Molecule 43: NADH UBIQUINONE OXIDOREDUCTASE

Chain v:  100%

There are no outlier residues recorded for this chain.

4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (4K X 4K)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES

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
2	B	1.57	1/21 (4.8%)	2.68	2/23 (8.7%)
21	U	0.08	0/4	0.20	0/4
5	E	0.77	0/20	1.59	0/20
6	F	2.57	1/20 (5.0%)	2.24	0/20
7	G	1.04	0/65	1.60	0/67
9	I	2.32	2/40 (5.0%)	1.47	0/40
All	All	1.68	4/170 (2.4%)	1.82	2/174 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	4
14	N	0	2
15	O	0	2
16	P	0	3
17	Q	0	1
19	S	0	1
2	B	0	2
23	W	0	1
24	X	0	1
3	C	0	1
4	D	0	1
6	F	0	2
7	G	0	6
9	I	0	1
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	405	CYS	CA-CB	-8.99	1.34	1.53
9	I	87	CYS	CA-CB	7.91	1.71	1.53
9	I	77	CYS	CA-CB	6.99	1.69	1.53
2	B	55	CYS	CA-CB	5.36	1.65	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	CYS	CA-CB-SG	-9.60	96.72	114.00
2	B	55	CYS	CB-CA-C	-5.16	100.09	110.40

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	120	UNK	Peptide
2	B	130	UNK	Peptide
3	C	56	UNK	Peptide
4	D	195	UNK	Peptide
6	F	96	UNK	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	415	0	88	26	0
2	B	719	0	161	89	0
3	C	770	0	163	66	0
4	D	1920	0	402	128	0
5	E	799	0	176	55	0
6	F	2059	0	444	258	0
7	G	2651	0	606	230	0
8	H	1425	0	295	105	0
9	I	818	0	195	77	0
10	J	655	0	138	51	0
11	K	420	0	89	18	0
12	L	2790	0	583	260	0
13	M	2195	0	455	212	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1630	0	340	171	0
15	O	905	0	197	68	0
16	P	1260	0	271	142	0
17	Q	345	0	80	13	0
18	R	235	0	54	21	0
19	S	400	0	86	51	0
20	T	355	0	76	26	0
21	U	375	0	84	17	0
22	V	355	0	77	35	0
23	W	360	0	75	21	0
24	X	395	0	83	19	0
25	Y	530	0	111	29	0
26	Z	325	0	67	24	0
27	a	145	0	31	0	0
28	b	210	0	44	0	0
29	c	135	0	30	0	0
29	w	135	0	29	0	0
30	d	195	0	41	0	0
31	e	100	0	22	0	0
32	f	150	0	33	0	0
32	h	150	0	32	0	0
32	i	150	0	33	0	0
33	g	110	0	24	0	0
34	j	120	0	27	0	0
34	l	120	0	26	0	0
35	k	140	0	30	0	0
35	p	140	0	30	0	0
35	s	140	0	31	0	0
36	m	170	0	36	0	0
37	n	295	0	61	0	0
38	o	105	0	23	0	0
39	q	125	0	27	0	0
40	r	130	0	28	0	0
41	t	285	0	61	0	0
42	u	75	0	17	0	0
43	v	160	0	34	0	0
44	B	8	0	0	4	0
44	F	8	0	0	1	0
44	G	16	0	0	0	0
44	I	16	0	0	5	0
45	E	4	0	0	0	0
45	G	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28647	0	6146	2173	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 64.

The worst 5 of 2173 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:UNK:CB	2:B:151:UNK:CA	1.77	1.57
6:F:405:CYS:CB	6:F:406:UNK:CB	1.78	1.54
6:F:405:CYS:HB2	6:F:406:UNK:CB	1.04	1.50
12:L:321:UNK:CB	12:L:324:UNK:CB	1.92	1.46
5:E:148:CYS:SG	6:F:103:UNK:CB	2.04	1.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
2	B	4/143 (3%)	3 (75%)	0	1 (25%)	0	1
5	E	4/159 (2%)	3 (75%)	1 (25%)	0	100	100
6	F	4/411 (1%)	4 (100%)	0	0	100	100
7	G	12/538 (2%)	9 (75%)	1 (8%)	2 (17%)	0	5
9	I	8/162 (5%)	7 (88%)	0	1 (12%)	0	8
All	All	32/1413 (2%)	26 (81%)	2 (6%)	4 (12%)	1	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	119	CYS
7	G	105	CYS
9	I	116	CYS
7	G	156	CYS

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	
2	B	4/4 (100%)	2 (50%)	2 (50%)	0	0
5	E	4/4 (100%)	4 (100%)	0	100	100
6	F	4/4 (100%)	3 (75%)	1 (25%)	1	6
7	G	12/12 (100%)	8 (67%)	4 (33%)	0	2
9	I	8/8 (100%)	7 (88%)	1 (12%)	6	31
All	All	32/32 (100%)	24 (75%)	8 (25%)	3	6

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	41	CYS
9	I	119	CYS
7	G	55	CYS
6	F	405	CYS
7	G	52	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
44	SF4	B	201	2	0,12,12	0.00	-	0,24,24	0.00	-
45	FES	E	201	5	0,4,4	0.00	-	0,4,4	0.00	-
44	SF4	F	508	6	0,12,12	0.00	-	0,24,24	0.00	-
44	SF4	G	801	7	0,12,12	0.00	-	0,24,24	0.00	-
44	SF4	G	802	7	0,12,12	0.00	-	0,24,24	0.00	-
45	FES	G	804	7	0,4,4	0.00	-	0,4,4	0.00	-
44	SF4	I	222	9	0,12,12	0.00	-	0,24,24	0.00	-
44	SF4	I	223	9	0,12,12	0.00	-	0,24,24	0.00	-

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
44	SF4	B	201	2	-	0/0/48/48	0/6/5/5
45	FES	E	201	5	-	0/0/4/4	0/1/1/1
44	SF4	F	508	6	-	0/0/48/48	0/6/5/5
44	SF4	G	801	7	-	0/0/48/48	0/6/5/5
44	SF4	G	802	7	-	0/0/48/48	0/6/5/5
45	FES	G	804	7	-	0/0/4/4	0/1/1/1
44	SF4	I	222	9	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	SF4	I	223	9	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	B	201	SF4	4	0
44	F	508	SF4	1	0
45	G	804	FES	2	0
44	I	222	SF4	2	0
44	I	223	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.