



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2023 – 01:23 pm BST

PDB ID : 8AD0
Title : X-ray structure of Na⁺-NQR from *Vibrio cholerae* in different conformation at 3.1 Å
Authors : Fritz, G.
Deposited on : 2022-07-07
Resolution : 3.11 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

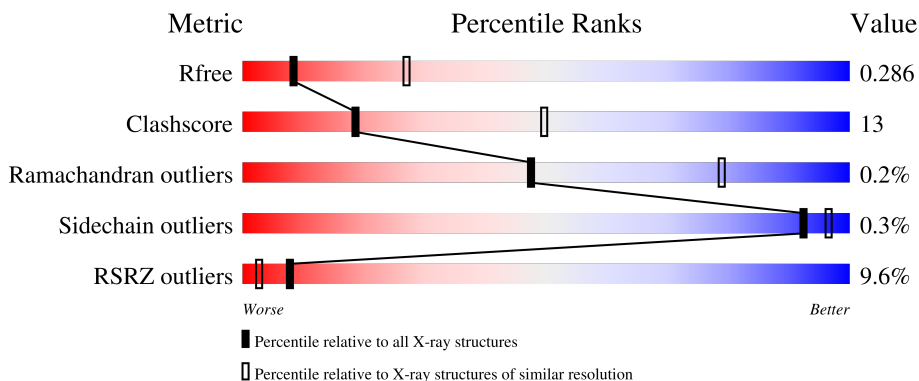
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	468	 4% 73% 13% 14%
2	B	415	 9% 75% 16% 7%
3	C	257	 24% 68% 27% 2%
4	D	210	 7% 59% 36% 2%
5	E	198	 7% 59% 38% 2%

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Mol	Chain	Length	Quality of chain
6	F	408	

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
10	3PE	B	504	-	-	-	X
12	K	B	506	-	-	-	X
9	LMT	B	503	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 28966 atoms, of which 14558 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 Na(+)-translocating NADH-quinone reductase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	403	6192	1946	3122	521	588	15	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A655PZA5
A	-20	GLY	-	expression tag	UNP A0A655PZA5
A	-19	SER	-	expression tag	UNP A0A655PZA5
A	-18	SER	-	expression tag	UNP A0A655PZA5
A	-17	HIS	-	expression tag	UNP A0A655PZA5
A	-16	HIS	-	expression tag	UNP A0A655PZA5
A	-15	HIS	-	expression tag	UNP A0A655PZA5
A	-14	HIS	-	expression tag	UNP A0A655PZA5
A	-13	HIS	-	expression tag	UNP A0A655PZA5
A	-12	HIS	-	expression tag	UNP A0A655PZA5
A	-11	SER	-	expression tag	UNP A0A655PZA5
A	-10	SER	-	expression tag	UNP A0A655PZA5
A	-9	GLY	-	expression tag	UNP A0A655PZA5
A	-8	LEU	-	expression tag	UNP A0A655PZA5
A	-7	GLU	-	expression tag	UNP A0A655PZA5
A	-6	VAL	-	expression tag	UNP A0A655PZA5
A	-5	LEU	-	expression tag	UNP A0A655PZA5
A	-4	PHE	-	expression tag	UNP A0A655PZA5
A	-3	GLN	-	expression tag	UNP A0A655PZA5
A	-2	GLY	-	expression tag	UNP A0A655PZA5
A	-1	PRO	-	expression tag	UNP A0A655PZA5
A	0	HIS	-	expression tag	UNP A0A655PZA5

- Molecule 2 is a protein called Na(+)-translocating NADH-quinone reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	384	5881	1946	2939	479	495	22	0	0	0

- Molecule 3 is a protein called Na(+)-translocating NADH-quinone reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	C	247	3767	1190	1889	323	361	4	0	0	0

- Molecule 4 is a protein called Na(+)-translocating NADH-quinone reductase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	D	202	3176	1026	1631	245	264	10	0	0	0

- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
5	E	197	3078	1008	1574	229	257	10	0	0	0

- Molecule 6 is a protein called Na(+)-translocating NADH-quinone reductase subunit F.

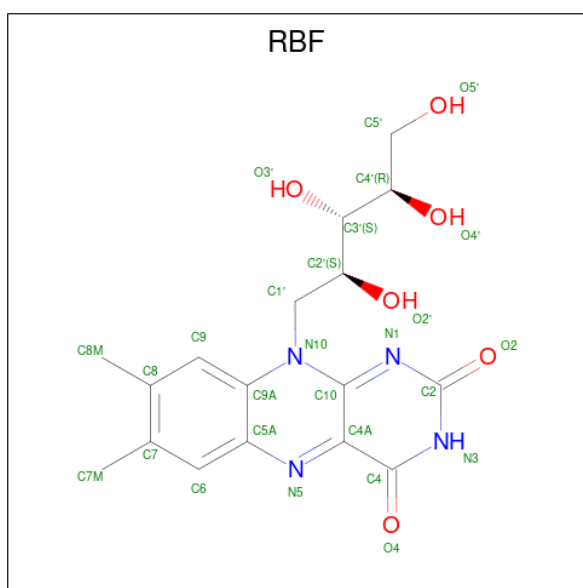
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
6	F	406	6252	2023	3095	517	593	24	0	0	0

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
7	B	1	49	17	19	4	8	1	0	0
7	C	1	49	17	19	4	8	1	0	0

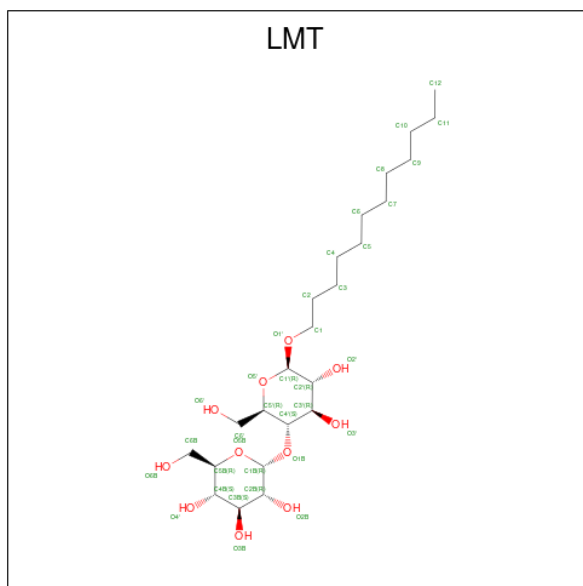
- Molecule 8 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	B	1	46	17	19	4	6	0	0

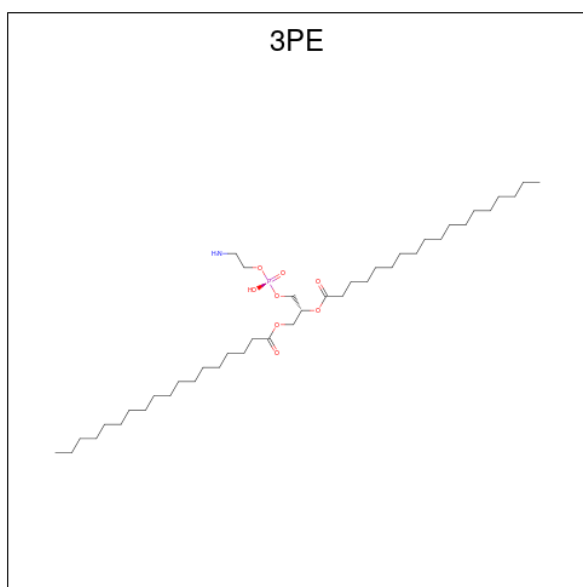
- Molecule 9 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:

C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	B	1	81	24	46	11	0	0
9	D	1	81	24	46	11	0	0
9	E	1	81	24	46	11	0	0

- Molecule 10 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
10	B	1	133	41	82	1	8	1	0	0

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
11	B	1	1	1	0	0

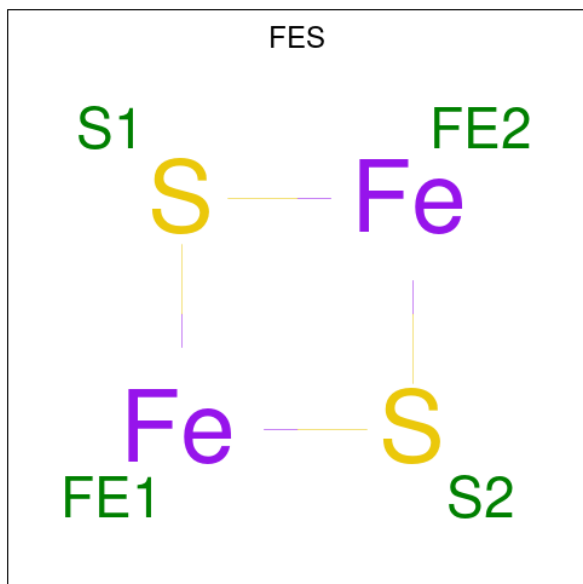
- Molecule 12 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
12	B	1	1	1	0	0

- Molecule 13 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Br		
13	C	1	1	1	0	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



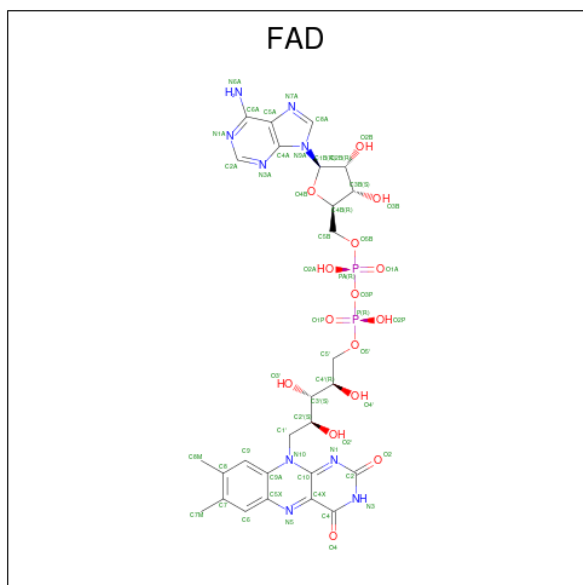
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
14	D	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
14	F	1	4	2	2	0	0

- Molecule 15 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
15	F	1	84	27	31	9	15	2	0	0

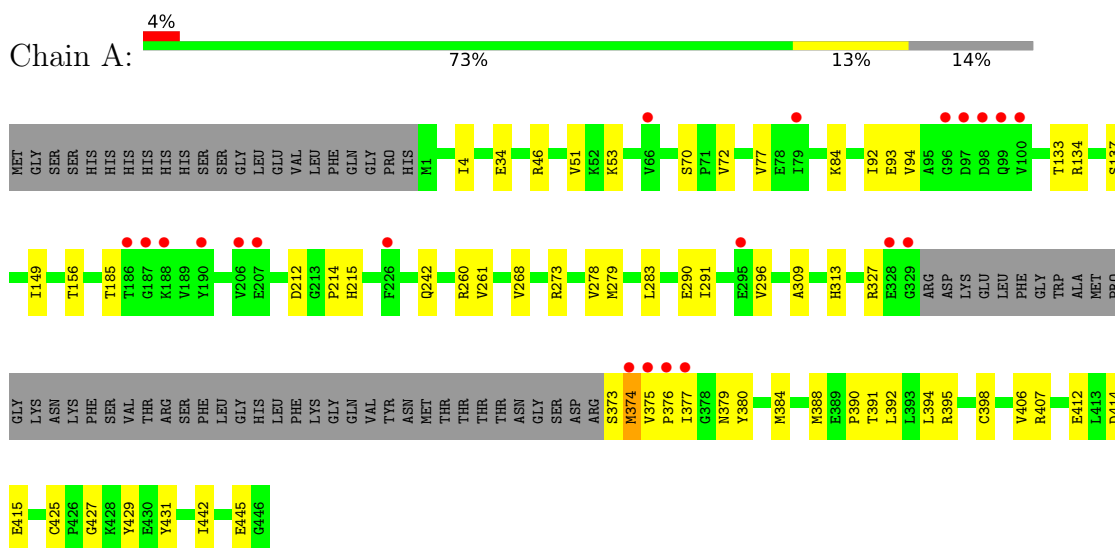
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	A	1	1	1	0	0
16	B	3	3	3	0	0
16	E	1	1	1	0	0

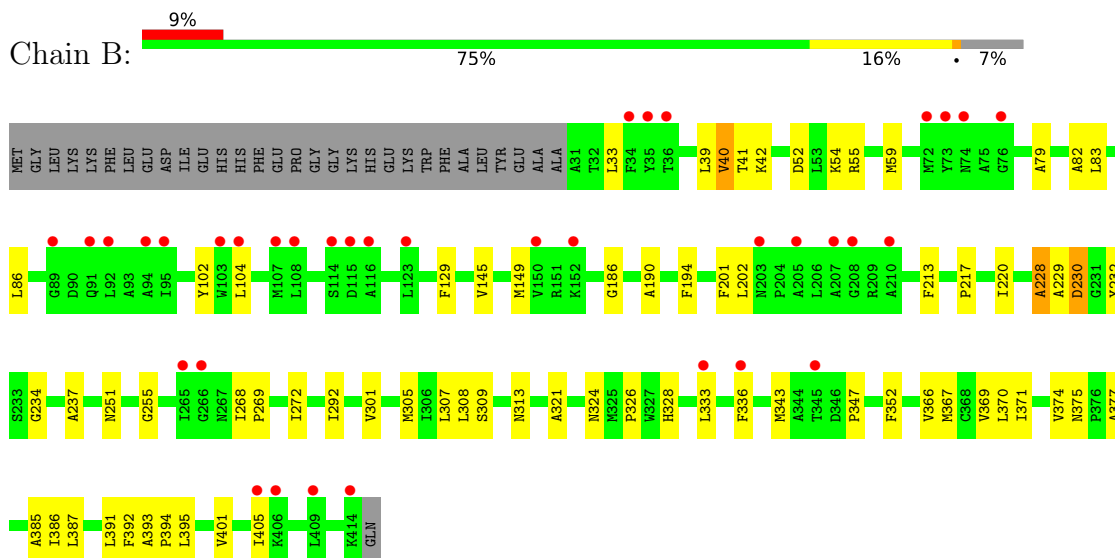
3 Residue-property plots i

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

- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A

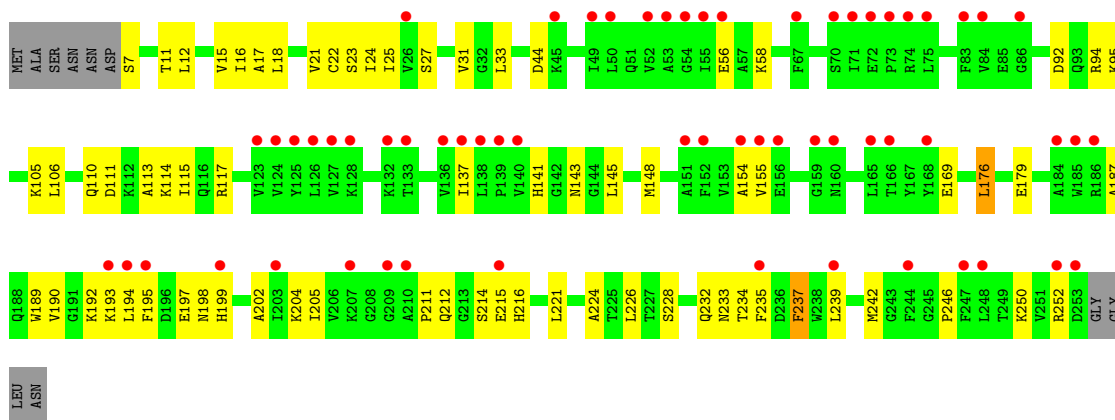


- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B

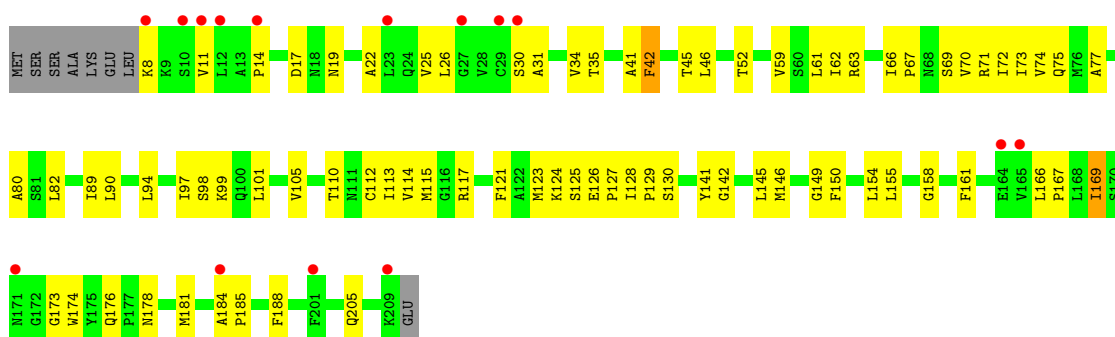


- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C

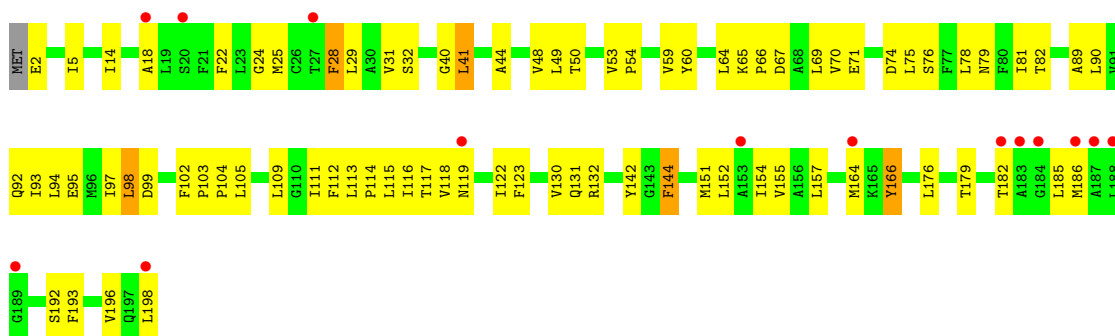




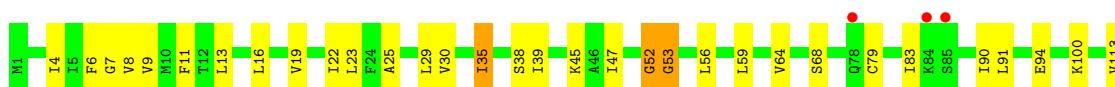
- Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D

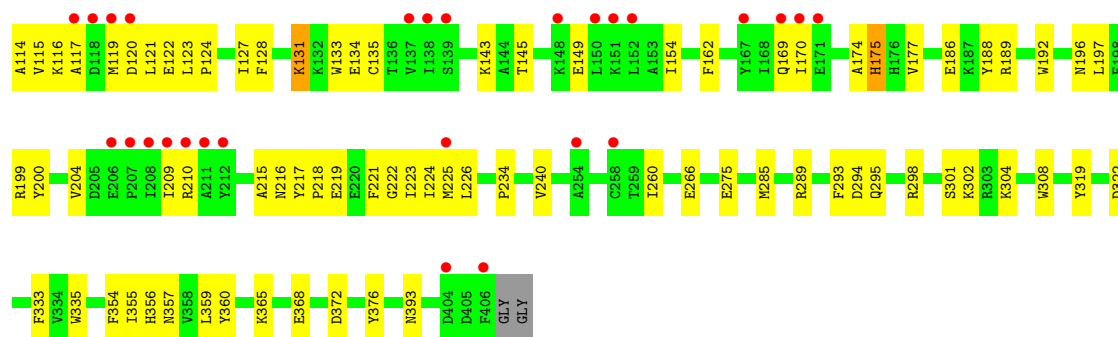


- Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E



- Molecule 6: Na(+)-translocating NADH-quinone reductase subunit F





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.31Å 142.15Å 105.93Å 90.00° 109.83° 90.00°	Depositor
Resolution (Å)	48.12 – 3.11 48.12 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.12-3.11) 99.4 (48.12-3.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.248 , 0.288 0.249 , 0.286	Depositor DCC
R_{free} test set	2233 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	114.8	Xtrriage
Anisotropy	0.248	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	28966	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, FMN, RBF, FES, K, NA, BR, FAD, 3PE

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	0.45	0/3124	0.75	0/4236
2	B	0.44	0/3030	0.80	2/4127 (0.0%)
3	C	0.44	0/1910	0.89	5/2578 (0.2%)
4	D	0.49	0/1577	1.00	8/2141 (0.4%)
5	E	0.50	0/1537	1.03	7/2084 (0.3%)
6	F	0.57	1/3235 (0.0%)	1.09	14/4379 (0.3%)
All	All	0.48	1/14413 (0.0%)	0.92	36/19545 (0.2%)

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
2	B	0	1
6	F	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	335	TRP	CB-CG	-6.83	1.38	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	28	PHE	CB-CG-CD1	-8.10	115.13	120.80
6	F	52	GLY	N-CA-C	-7.92	93.29	113.10
6	F	91	LEU	CB-CG-CD2	7.50	123.75	111.00
6	F	122	GLU	C-N-CA	7.40	140.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	42	PHE	CB-CG-CD1	-7.38	115.63	120.80
6	F	333	PHE	CB-CG-CD1	-7.00	115.90	120.80
5	E	28	PHE	CB-CG-CD2	6.80	125.56	120.80
6	F	333	PHE	CB-CG-CD2	6.54	125.38	120.80
3	C	18	LEU	CB-CG-CD2	6.52	122.08	111.00
4	D	42	PHE	CB-CG-CD2	6.43	125.30	120.80
6	F	53	GLY	C-N-CA	-6.32	105.90	121.70
4	D	150	PHE	CB-CG-CD2	-6.29	116.39	120.80
2	B	307	LEU	CB-CG-CD2	6.18	121.50	111.00
2	B	386	ILE	CG1-CB-CG2	-6.04	98.12	111.40
6	F	354	PHE	CB-CG-CD1	-5.98	116.61	120.80
5	E	144	PHE	CB-CG-CD1	-5.93	116.65	120.80
6	F	131	LYS	CA-CB-CG	5.82	126.20	113.40
6	F	200	TYR	CB-CG-CD2	-5.76	117.55	121.00
6	F	376	TYR	CB-CG-CD1	5.65	124.39	121.00
4	D	82	LEU	CB-CG-CD2	-5.61	101.47	111.00
6	F	11	PHE	CB-CG-CD2	-5.54	116.93	120.80
4	D	150	PHE	CB-CG-CD1	5.53	124.67	120.80
5	E	166	TYR	CB-CG-CD1	-5.48	117.71	121.00
3	C	25	ILE	CG1-CB-CG2	-5.46	99.39	111.40
4	D	169	ILE	CG1-CB-CG2	-5.40	99.53	111.40
4	D	72	ILE	CG1-CB-CG2	-5.33	99.67	111.40
6	F	200	TYR	CB-CG-CD1	5.29	124.17	121.00
6	F	376	TYR	CB-CG-CD2	-5.18	117.89	121.00
5	E	142	TYR	CB-CG-CD1	-5.16	117.91	121.00
6	F	91	LEU	CA-CB-CG	-5.10	103.57	115.30
3	C	176	LEU	CA-CB-CG	5.10	127.02	115.30
5	E	166	TYR	CB-CG-CD2	5.07	124.04	121.00
3	C	237	PHE	CB-CG-CD1	5.07	124.35	120.80
4	D	161	PHE	CB-CG-CD1	-5.04	117.28	120.80
3	C	237	PHE	CB-CG-CD2	-5.03	117.28	120.80
5	E	41	LEU	CB-CG-CD2	-5.00	102.49	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	228	ALA	Mainchain
6	F	175	HIS	Mainchain
6	F	372	ASP	Mainchain

5.2 Too-close contacts [i](#)

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	3070	3122	3123	48	1
2	B	2942	2939	2939	69	0
3	C	1878	1889	1889	66	1
4	D	1545	1631	1631	65	0
5	E	1504	1574	1574	90	0
6	F	3157	3095	3095	89	0
7	B	30	19	19	0	0
7	C	30	19	19	7	0
8	B	27	19	20	2	0
9	B	35	46	44	3	0
9	D	35	46	44	2	0
9	E	35	46	44	3	0
10	B	51	82	82	2	0
11	B	1	0	0	0	0
12	B	1	0	0	0	0
13	C	1	0	0	0	0
14	D	4	0	0	0	0
14	F	4	0	0	0	0
15	F	53	31	31	1	0
16	A	1	0	0	0	0
16	B	3	0	0	0	0
16	E	1	0	0	0	0
All	All	14408	14558	14554	383	1

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 13.

All (383) 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)
3:C:193:LYS:HB2	3:C:216:HIS:CE1	1.92	1.04
2:B:321:ALA:O	2:B:324:ASN:ND2	1.98	0.96
5:E:103:PRO:HD2	5:E:104:PRO:HD2	1.53	0.90
5:E:90:LEU:O	5:E:93:ILE:HG13	1.79	0.82
6:F:52:GLY:O	6:F:115:VAL:CG1	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:PHE:O	3:C:216:HIS:HE1	1.64	0.81
3:C:195:PHE:O	3:C:216:HIS:CE1	2.34	0.81
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.64	0.80
4:D:77:ALA:HA	5:E:81:ILE:HD11	1.63	0.80
6:F:121:LEU:HD13	6:F:123:LEU:HD13	1.61	0.79
1:A:156:THR:OG1	1:A:215:HIS:O	2.01	0.77
6:F:52:GLY:O	6:F:115:VAL:HG12	1.83	0.76
6:F:35:ILE:HG21	6:F:115:VAL:CG2	2.15	0.76
5:E:29:LEU:HD22	5:E:179:THR:HG22	1.68	0.76
6:F:154:ILE:HD11	6:F:224:ILE:HG12	1.66	0.75
6:F:39:ILE:HD12	6:F:121:LEU:HD11	1.68	0.75
6:F:47:ILE:HD11	6:F:59:LEU:HD23	1.67	0.75
6:F:216:ASN:ND2	6:F:223:ILE:O	2.23	0.71
1:A:134:ARG:HD3	1:A:412:GLU:O	1.90	0.71
3:C:33:LEU:HD11	4:D:89:ILE:HD13	1.73	0.71
3:C:11:THR:HG22	4:D:67:PRO:CB	2.21	0.70
3:C:24:ILE:HD13	6:F:8:VAL:HG21	1.72	0.70
4:D:167:PRO:HB2	4:D:173:GLY:HA3	1.74	0.69
6:F:53:GLY:O	6:F:114:ALA:HA	1.91	0.69
3:C:193:LYS:HG3	3:C:215:GLU:HB3	1.72	0.69
3:C:44:ASP:OD2	4:D:99:LYS:NZ	2.20	0.69
1:A:34:GLU:HB2	2:B:39:LEU:HD13	1.75	0.69
3:C:11:THR:HG22	4:D:67:PRO:CG	2.23	0.69
2:B:251:ASN:O	2:B:255:GLY:N	2.27	0.68
3:C:193:LYS:HB2	3:C:216:HIS:ND1	2.07	0.68
6:F:30:VAL:HG12	6:F:30:VAL:O	1.95	0.67
3:C:205:ILE:HG21	3:C:228:SER:HB2	1.76	0.66
3:C:24:ILE:CD1	6:F:8:VAL:HG21	2.26	0.66
3:C:226:LEU:N	7:C:301:FMN:O2	2.29	0.65
5:E:60:TYR:CE2	5:E:130:VAL:HG13	2.32	0.65
5:E:103:PRO:CD	5:E:104:PRO:HD2	2.26	0.65
3:C:193:LYS:CB	3:C:216:HIS:CE1	2.75	0.64
6:F:356:HIS:CD2	6:F:357:ASN:OD1	2.50	0.64
3:C:11:THR:HG22	4:D:67:PRO:HB3	1.78	0.64
6:F:169:GLN:OE1	6:F:209:ILE:HD11	1.97	0.64
6:F:35:ILE:HD11	6:F:117:ALA:HA	1.80	0.64
5:E:119:ASN:HB3	5:E:122:ILE:HG12	1.80	0.64
2:B:377:ALA:O	7:C:301:FMN:O2'	2.16	0.63
4:D:30:SER:O	4:D:34:VAL:HG22	1.98	0.63
2:B:39:LEU:O	2:B:42:LYS:N	2.29	0.63
1:A:384:MET:HG2	1:A:390:PRO:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:ILE:CD1	6:F:121:LEU:HD11	2.29	0.62
1:A:133:THR:O	1:A:137:SER:N	2.33	0.62
2:B:52:ASP:OD1	2:B:54:LYS:N	2.31	0.62
2:B:395:LEU:HD21	5:E:155:VAL:HG12	1.80	0.62
6:F:47:ILE:CD1	6:F:59:LEU:HD23	2.28	0.62
6:F:217:TYR:CE2	6:F:219:GLU:HB2	2.35	0.62
2:B:308:LEU:HD22	2:B:366:VAL:HG13	1.80	0.61
5:E:66:PRO:HA	5:E:74:ASP:HA	1.83	0.61
2:B:102:TYR:OH	2:B:228:ALA:O	2.17	0.61
3:C:11:THR:HA	4:D:67:PRO:HG2	1.82	0.60
4:D:69:SER:O	5:E:92:GLN:NE2	2.35	0.60
1:A:379:ASN:N	1:A:379:ASN:OD1	2.33	0.60
6:F:294:ASP:OD1	6:F:298:ARG:HD3	2.02	0.60
5:E:66:PRO:HB3	5:E:74:ASP:CB	2.32	0.60
5:E:28:PHE:O	5:E:32:SER:OG	2.08	0.59
4:D:155:LEU:HD13	9:D:301:LMT:H51	1.82	0.59
4:D:42:PHE:CZ	4:D:46:LEU:HD11	2.37	0.59
5:E:64:LEU:HD22	5:E:78:LEU:HB2	1.84	0.58
3:C:187:ALA:O	3:C:190:VAL:HG22	2.04	0.58
2:B:82:ALA:HB1	2:B:232:TYR:CD2	2.38	0.58
5:E:28:PHE:HA	5:E:154:ILE:HD13	1.85	0.58
5:E:60:TYR:O	5:E:65:LYS:N	2.34	0.57
2:B:82:ALA:HB3	2:B:229:ALA:HB2	1.85	0.57
5:E:29:LEU:CD2	5:E:179:THR:HG22	2.33	0.57
6:F:56:LEU:O	6:F:56:LEU:HD23	2.04	0.57
6:F:302:LYS:CD	6:F:302:LYS:O	2.52	0.57
4:D:8:LYS:O	4:D:11:VAL:HG12	2.04	0.57
5:E:40:GLY:HA3	5:E:105:LEU:HD21	1.85	0.57
5:E:44:ALA:O	5:E:48:VAL:HG23	2.05	0.57
9:B:503:LMT:O2B	9:B:503:LMT:H4'	2.04	0.57
1:A:273:ARG:NH2	1:A:290:GLU:OE2	2.35	0.57
2:B:202:LEU:HD22	5:E:185:LEU:HB3	1.86	0.57
3:C:155:VAL:HG22	3:C:194:LEU:HD11	1.86	0.57
4:D:77:ALA:HA	5:E:81:ILE:CD1	2.35	0.57
5:E:94:LEU:O	5:E:98:LEU:CD2	2.53	0.57
5:E:102:PHE:CG	5:E:103:PRO:HD3	2.40	0.57
2:B:391:LEU:HD22	5:E:186:MET:HG2	1.86	0.56
5:E:155:VAL:HG11	9:E:201:LMT:H22	1.87	0.56
4:D:63:ARG:O	4:D:66:ILE:HG22	2.06	0.56
5:E:93:ILE:HD12	5:E:94:LEU:N	2.20	0.56
5:E:66:PRO:HB3	5:E:74:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:26:LEU:HD22	4:D:112:CYS:HB3	1.88	0.55
4:D:123:MET:O	4:D:124:LYS:HB2	2.06	0.55
6:F:234:PRO:HD2	6:F:240:VAL:HG21	1.89	0.55
1:A:313:HIS:CE1	2:B:39:LEU:HD12	2.42	0.55
3:C:92:ASP:OD2	3:C:95:LYS:HD3	2.07	0.55
5:E:49:LEU:HD21	5:E:122:ILE:HA	1.89	0.55
5:E:114:PRO:O	5:E:117:THR:HG22	2.07	0.55
6:F:215:ALA:O	6:F:289:ARG:NH1	2.40	0.55
6:F:79:CYS:SG	6:F:79:CYS:O	2.65	0.55
2:B:217:PRO:HB3	7:C:301:FMN:HM83	1.89	0.54
4:D:25:VAL:O	4:D:26:LEU:HD23	2.08	0.54
6:F:186:GLU:HA	6:F:189:ARG:HG2	1.87	0.54
6:F:302:LYS:O	6:F:302:LYS:HD2	2.08	0.54
1:A:429:TYR:HH	5:E:166:TYR:HH	1.50	0.54
3:C:155:VAL:CG2	3:C:194:LEU:HD11	2.38	0.54
3:C:205:ILE:HD12	3:C:205:ILE:N	2.23	0.54
1:A:149:ILE:HD12	1:A:185:THR:HB	1.89	0.54
1:A:377:ILE:HG13	1:A:379:ASN:HB3	1.90	0.54
2:B:40:VAL:HG23	2:B:41:THR:N	2.23	0.54
5:E:53:VAL:HB	5:E:54:PRO:HD3	1.89	0.54
6:F:289:ARG:HD2	6:F:319:TYR:CD2	2.43	0.54
1:A:291:ILE:HG21	1:A:296:VAL:HG21	1.90	0.53
4:D:73:ILE:HD11	5:E:89:ALA:HA	1.90	0.53
6:F:219:GLU:O	6:F:221:PHE:CD2	2.62	0.53
1:A:429:TYR:OH	5:E:166:TYR:OH	2.22	0.53
3:C:211:PRO:HG2	3:C:214:SER:HB3	1.91	0.53
1:A:445:GLU:HG3	6:F:100:LYS:HD3	1.90	0.53
3:C:115:ILE:HD11	3:C:237:PHE:CE1	2.44	0.53
4:D:41:ALA:O	4:D:45:THR:HG23	2.09	0.53
5:E:113:LEU:O	5:E:116:ILE:HG12	2.09	0.53
10:B:504:3PE:H3I3	10:B:504:3PE:C2I	2.39	0.53
3:C:12:LEU:HD11	6:F:16:LEU:HD11	1.90	0.53
4:D:45:THR:HG21	4:D:142:GLY:HA2	1.90	0.52
1:A:414:ASP:OD1	1:A:415:GLU:N	2.42	0.52
3:C:106:LEU:HD22	3:C:242:MET:CE	2.39	0.52
3:C:106:LEU:HD13	3:C:237:PHE:CE2	2.45	0.52
3:C:23:SER:O	3:C:27:SER:HB2	2.09	0.52
3:C:113:ALA:O	3:C:114:LYS:HB2	2.10	0.52
6:F:35:ILE:HG21	6:F:115:VAL:HG22	1.89	0.52
6:F:39:ILE:HB	6:F:45:LYS:HB3	1.90	0.52
6:F:133:TRP:HE3	6:F:260:ILE:HG13	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:VAL:HG23	2:B:41:THR:H	1.76	0.51
5:E:32:SER:OG	5:E:157:LEU:HD23	2.10	0.51
6:F:135:CYS:SG	6:F:154:ILE:HD13	2.51	0.51
6:F:196:ASN:O	6:F:199:ARG:HG2	2.10	0.51
2:B:39:LEU:O	2:B:40:VAL:C	2.49	0.51
4:D:154:LEU:O	4:D:158:GLY:HA2	2.10	0.51
5:E:31:VAL:HG12	5:E:31:VAL:O	2.10	0.51
6:F:293:PHE:HZ	6:F:322:ASP:HB3	1.75	0.51
4:D:42:PHE:N	4:D:146:MET:HE1	2.24	0.51
6:F:124:PRO:O	6:F:127:ILE:HG12	2.10	0.51
2:B:371:ILE:HD11	5:E:192:SER:HB2	1.93	0.51
3:C:114:LYS:HB2	3:C:143:ASN:HB3	1.93	0.51
3:C:145:LEU:HD22	3:C:226:LEU:HD12	1.92	0.51
4:D:67:PRO:HB2	4:D:70:VAL:HG22	1.92	0.51
6:F:45:LYS:HD3	6:F:128:PHE:CZ	2.46	0.51
1:A:313:HIS:ND1	2:B:42:LYS:HE3	2.26	0.51
2:B:377:ALA:HA	3:C:226:LEU:HD11	1.91	0.51
6:F:308:TRP:HB3	6:F:355:ILE:HD11	1.92	0.51
1:A:53:LYS:O	1:A:70:SER:O	2.29	0.50
2:B:305:MET:CE	2:B:336:PHE:CZ	2.94	0.50
6:F:302:LYS:O	6:F:302:LYS:CG	2.58	0.50
1:A:406:VAL:CG2	1:A:442:ILE:HD13	2.42	0.50
2:B:308:LEU:HD23	2:B:369:VAL:HB	1.94	0.50
4:D:110:THR:HG21	5:E:123:PHE:HB3	1.93	0.50
5:E:28:PHE:HA	5:E:154:ILE:CD1	2.41	0.50
5:E:66:PRO:HB3	5:E:74:ASP:HB2	1.93	0.50
5:E:89:ALA:HA	6:F:22:ILE:HD11	1.94	0.50
6:F:266:GLU:N	6:F:266:GLU:OE1	2.44	0.50
2:B:86:LEU:HD11	2:B:232:TYR:HB2	1.93	0.50
3:C:106:LEU:HD22	3:C:242:MET:HE1	1.92	0.50
6:F:225:MET:O	6:F:226:LEU:HD23	2.12	0.50
3:C:31:VAL:HG21	6:F:4:ILE:HG12	1.94	0.50
6:F:154:ILE:HG12	6:F:222:GLY:O	2.12	0.50
1:A:77:VAL:HG11	1:A:93:GLU:HB2	1.94	0.50
4:D:188:PHE:CE1	5:E:25:MET:HE2	2.46	0.49
5:E:24:GLY:CA	5:E:119:ASN:OD1	2.60	0.49
3:C:27:SER:HB3	6:F:4:ILE:HG23	1.94	0.49
1:A:373:SER:O	1:A:375:VAL:N	2.42	0.49
6:F:25:ALA:HA	6:F:29:LEU:HD13	1.94	0.49
4:D:123:MET:O	4:D:124:LYS:CB	2.60	0.49
3:C:145:LEU:HD23	7:C:301:FMN:C4	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:192:TRP:HA	6:F:197:LEU:HD12	1.93	0.49
3:C:115:ILE:O	3:C:115:ILE:HG13	2.11	0.49
2:B:375:ASN:ND2	5:E:192:SER:O	2.45	0.49
1:A:260:ARG:HD2	1:A:279:MET:HG3	1.94	0.49
1:A:380:TYR:HH	1:A:425:CYS:HG	1.58	0.49
3:C:11:THR:O	3:C:15:VAL:HG22	2.13	0.49
4:D:141:TYR:O	4:D:145:LEU:HD13	2.13	0.49
5:E:102:PHE:N	5:E:103:PRO:CD	2.75	0.49
3:C:141:HIS:C	3:C:234:THR:HG23	2.33	0.49
4:D:22:ALA:O	5:E:176:LEU:HD23	2.12	0.48
1:A:374:MET:HE1	1:A:398:CYS:SG	2.53	0.48
1:A:392:LEU:HD13	2:B:401:VAL:HG21	1.94	0.48
6:F:162:PHE:CZ	6:F:218:PRO:HA	2.48	0.48
5:E:75:LEU:HD13	6:F:7:GLY:HA2	1.94	0.48
1:A:374:MET:CE	1:A:398:CYS:SG	3.02	0.48
4:D:141:TYR:CE2	4:D:145:LEU:HD22	2.49	0.48
1:A:278:VAL:HG22	1:A:279:MET:N	2.28	0.48
6:F:175:HIS:CE1	6:F:204:VAL:HG21	2.49	0.48
3:C:235:PHE:O	3:C:239:LEU:HB2	2.13	0.48
5:E:98:LEU:O	5:E:102:PHE:HB3	2.14	0.48
3:C:110:GLN:HB3	3:C:242:MET:CE	2.44	0.48
2:B:213:PHE:HA	2:B:220:ILE:HG21	1.96	0.48
2:B:292:ILE:HG22	8:B:502:RBF:HC71	1.96	0.48
2:B:326:PRO:HB2	2:B:328:HIS:CD2	2.48	0.48
3:C:246:PRO:O	3:C:250:LYS:HE2	2.13	0.48
4:D:113:ILE:O	4:D:117:ARG:HG2	2.14	0.48
5:E:67:ASP:HA	5:E:70:VAL:O	2.14	0.48
6:F:127:ILE:HG13	6:F:128:PHE:N	2.28	0.48
2:B:370:LEU:O	2:B:374:VAL:HG22	2.14	0.47
10:B:504:3PE:H3I3	10:B:504:3PE:H2I1	1.95	0.47
3:C:221:LEU:CB	3:C:224:ALA:HB3	2.44	0.47
4:D:80:ALA:HB3	5:E:81:ILE:HD13	1.96	0.47
6:F:9:VAL:O	6:F:13:LEU:HD13	2.13	0.47
4:D:52:THR:CG2	4:D:114:VAL:HG22	2.44	0.47
2:B:387:LEU:O	2:B:391:LEU:HG	2.13	0.47
3:C:113:ALA:HA	3:C:233:ASN:HB3	1.95	0.47
6:F:234:PRO:HD2	6:F:240:VAL:CG2	2.43	0.47
3:C:114:LYS:HD2	3:C:114:LYS:N	2.30	0.47
5:E:97:ILE:C	5:E:99:ASP:H	2.17	0.47
6:F:308:TRP:CE2	6:F:359:LEU:HD13	2.50	0.47
3:C:179:GLU:HB2	3:C:221:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ASN:HB3	4:D:22:ALA:HB3	1.97	0.47
4:D:35:THR:O	4:D:149:GLY:HA2	2.15	0.47
4:D:121:PHE:CE1	4:D:130:SER:HA	2.50	0.47
4:D:155:LEU:HB2	4:D:181:MET:HG3	1.97	0.47
6:F:114:ALA:HB1	6:F:116:LYS:HD3	1.97	0.47
4:D:128:ILE:HB	4:D:129:PRO:HD3	1.97	0.47
1:A:374:MET:SD	1:A:395:ARG:HD2	2.55	0.46
5:E:14:ILE:HA	5:E:193:PHE:HB3	1.97	0.46
1:A:51:VAL:HG21	1:A:92:ILE:HD13	1.95	0.46
2:B:393:ALA:HB3	2:B:394:PRO:HD3	1.97	0.46
4:D:52:THR:HG22	4:D:114:VAL:HG22	1.96	0.46
2:B:232:TYR:HE1	2:B:234:GLY:HA3	1.79	0.46
2:B:301:VAL:HG12	2:B:336:PHE:CZ	2.50	0.46
5:E:31:VAL:HG11	5:E:109:LEU:HD23	1.97	0.46
6:F:223:ILE:O	6:F:223:ILE:HG13	2.15	0.46
1:A:374:MET:SD	1:A:395:ARG:HA	2.56	0.46
2:B:82:ALA:HB3	2:B:229:ALA:CB	2.45	0.46
2:B:392:PHE:CE1	5:E:152:LEU:HG	2.51	0.46
3:C:106:LEU:HB2	3:C:111:ASP:HB2	1.96	0.46
6:F:217:TYR:CD1	6:F:293:PHE:HB3	2.51	0.46
2:B:230:ASP:N	2:B:230:ASP:OD2	2.49	0.46
3:C:176:LEU:O	3:C:224:ALA:HB2	2.16	0.46
3:C:202:ALA:O	3:C:204:LYS:HG2	2.16	0.45
4:D:184:ALA:N	4:D:185:PRO:CD	2.78	0.45
1:A:425:CYS:SG	1:A:427:GLY:O	2.74	0.45
6:F:59:LEU:HD22	6:F:64:VAL:HG21	1.98	0.45
4:D:94:LEU:HB3	4:D:97:ILE:HD12	1.99	0.45
5:E:59:VAL:HG11	5:E:82:THR:HG21	1.98	0.45
5:E:18:ALA:O	5:E:22:PHE:HA	2.16	0.45
2:B:40:VAL:HG23	2:B:41:THR:HG23	1.99	0.45
2:B:194:PHE:HD1	5:E:164:MET:CE	2.29	0.45
4:D:11:VAL:O	4:D:14:PRO:HD2	2.17	0.45
6:F:275:GLU:CD	6:F:304:LYS:HD3	2.37	0.45
2:B:33:LEU:C	2:B:33:LEU:HD12	2.37	0.45
3:C:111:ASP:CG	3:C:115:ILE:O	2.55	0.45
3:C:221:LEU:HB2	3:C:224:ALA:HB3	1.98	0.45
5:E:24:GLY:HA3	5:E:119:ASN:OD1	2.17	0.45
5:E:50:THR:HG22	5:E:144:PHE:CA	2.47	0.45
5:E:95:GLU:HA	5:E:98:LEU:HD23	1.98	0.45
5:E:103:PRO:HD2	5:E:104:PRO:CD	2.36	0.45
2:B:83:LEU:HD11	2:B:102:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:ILE:HD12	4:D:62:ILE:C	2.37	0.45
2:B:343:MET:HA	8:B:502:RBF:O4	2.17	0.45
5:E:102:PHE:CD1	5:E:103:PRO:HD3	2.52	0.45
5:E:157:LEU:HB2	5:E:186:MET:HE1	1.99	0.45
1:A:84:LYS:HA	6:F:393:ASN:O	2.17	0.45
2:B:268:ILE:HB	2:B:269:PRO:HD2	1.98	0.45
3:C:199:HIS:NE2	3:C:252:ARG:HD3	2.32	0.45
6:F:47:ILE:CD1	6:F:59:LEU:HA	2.47	0.45
6:F:210:ARG:NE	15:F:1501:FAD:O1P	2.50	0.44
2:B:392:PHE:HE1	5:E:152:LEU:HG	1.82	0.44
6:F:19:VAL:O	6:F:23:LEU:HD13	2.18	0.44
6:F:170:ILE:HG12	6:F:260:ILE:HG22	1.99	0.44
2:B:232:TYR:CD1	2:B:232:TYR:C	2.91	0.44
3:C:110:GLN:HB3	3:C:242:MET:HE2	2.00	0.44
1:A:313:HIS:CD2	2:B:39:LEU:HD11	2.53	0.44
4:D:184:ALA:CB	5:E:22:PHE:CE2	3.01	0.44
4:D:31:ALA:O	4:D:35:THR:HG23	2.17	0.44
7:C:301:FMN:H9	7:C:301:FMN:H1'1	1.84	0.44
4:D:188:PHE:CE1	5:E:25:MET:CE	3.01	0.44
1:A:313:HIS:NE2	2:B:39:LEU:HD12	2.33	0.44
4:D:59:VAL:CG1	4:D:123:MET:HG2	2.48	0.44
4:D:184:ALA:HB3	5:E:22:PHE:CE2	2.53	0.44
5:E:2:GLU:HB2	5:E:5:ILE:HD12	2.00	0.44
5:E:198:LEU:C	5:E:198:LEU:HD23	2.38	0.44
6:F:90:ILE:HG23	6:F:94:GLU:OE1	2.18	0.44
2:B:86:LEU:CD1	2:B:232:TYR:HB2	2.48	0.44
2:B:305:MET:HE2	2:B:336:PHE:CZ	2.52	0.44
3:C:56:GLU:OE1	3:C:56:GLU:N	2.46	0.44
4:D:126:GLU:HB2	4:D:129:PRO:HD2	2.00	0.44
6:F:302:LYS:O	6:F:302:LYS:HG3	2.17	0.44
9:B:503:LMT:O2B	9:B:503:LMT:H5B	2.18	0.43
3:C:94:ARG:NH2	3:C:169:GLU:OE1	2.50	0.43
4:D:61:LEU:CD1	4:D:127:PRO:HB3	2.47	0.43
5:E:70:VAL:HG12	5:E:71:GLU:N	2.32	0.43
6:F:52:GLY:O	6:F:115:VAL:HG13	2.15	0.43
1:A:388:MET:O	1:A:390:PRO:HD3	2.18	0.43
5:E:131:GLN:HG3	5:E:132:ARG:N	2.33	0.43
4:D:121:PHE:O	4:D:125:SER:HB3	2.19	0.43
1:A:46:ARG:NE	6:F:368:GLU:OE2	2.41	0.43
2:B:39:LEU:HA	2:B:42:LYS:HG3	2.00	0.43
3:C:137:ILE:HG12	3:C:154:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:175:HIS:H	6:F:204:VAL:CG2	2.31	0.43
1:A:376:PRO:HG2	2:B:352:PHE:CD1	2.53	0.43
2:B:309:SER:O	2:B:313:ASN:ND2	2.51	0.43
6:F:143:LYS:HD2	6:F:149:GLU:OE1	2.18	0.43
4:D:71:ARG:O	4:D:75:GLN:HG3	2.19	0.43
2:B:104:LEU:O	2:B:104:LEU:HD13	2.18	0.43
3:C:197:GLU:HG3	3:C:198:ASN:N	2.34	0.43
3:C:224:ALA:HA	7:C:301:FMN:C2	2.49	0.43
6:F:38:SER:HB3	6:F:120:ASP:OD1	2.18	0.43
2:B:328:HIS:CD2	2:B:328:HIS:H	2.37	0.43
2:B:367:MET:HB3	2:B:385:ALA:HB1	2.01	0.42
3:C:7:SER:O	3:C:11:THR:HG23	2.19	0.42
3:C:17:ALA:O	3:C:21:VAL:HG22	2.19	0.42
4:D:188:PHE:CZ	5:E:25:MET:CE	3.03	0.42
5:E:14:ILE:HG12	5:E:196:VAL:CG1	2.50	0.42
4:D:42:PHE:N	4:D:146:MET:CE	2.82	0.42
3:C:143:ASN:HB2	3:C:148:MET:SD	2.59	0.42
4:D:178:ASN:HB3	4:D:181:MET:HG2	2.01	0.42
6:F:174:ALA:HA	6:F:204:VAL:HG23	2.02	0.42
4:D:101:LEU:HB3	4:D:105:VAL:HG23	2.02	0.42
6:F:4:ILE:O	6:F:8:VAL:HG23	2.19	0.42
6:F:83:ILE:HD11	6:F:113:VAL:HG11	2.01	0.42
6:F:134:GLU:O	6:F:134:GLU:OE1	2.38	0.42
2:B:395:LEU:HD13	9:E:201:LMT:H41	2.00	0.42
6:F:360:TYR:O	6:F:365:LYS:HB2	2.20	0.42
1:A:268:VAL:HG11	1:A:327:ARG:HG2	2.01	0.42
2:B:393:ALA:N	2:B:394:PRO:CD	2.83	0.42
3:C:204:LYS:HD3	3:C:232:GLN:HE21	1.84	0.42
5:E:98:LEU:HD22	5:E:98:LEU:N	2.35	0.42
6:F:175:HIS:HD2	6:F:177:VAL:HG13	1.85	0.42
1:A:4:ILE:O	1:A:214:PRO:HD2	2.19	0.42
5:E:151:MET:O	5:E:155:VAL:HG23	2.20	0.42
6:F:35:ILE:HD12	6:F:35:ILE:HA	1.66	0.42
1:A:391:THR:O	1:A:395:ARG:HG3	2.20	0.42
2:B:201:PHE:CZ	5:E:182:THR:HG23	2.54	0.42
3:C:105:LYS:HD3	3:C:117:ARG:HD3	2.01	0.42
3:C:224:ALA:C	7:C:301:FMN:O2	2.58	0.42
5:E:97:ILE:C	5:E:99:ASP:N	2.73	0.42
5:E:154:ILE:CG2	5:E:155:VAL:N	2.82	0.42
1:A:133:THR:O	1:A:137:SER:HA	2.20	0.42
1:A:242:GLN:NE2	1:A:261:VAL:O	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:HIS:NE2	2:B:39:LEU:CD1	2.83	0.42
6:F:131:LYS:HB2	6:F:133:TRP:CZ2	2.54	0.42
6:F:39:ILE:HG21	6:F:128:PHE:HZ	1.84	0.41
4:D:52:THR:HG22	4:D:114:VAL:HA	2.02	0.41
6:F:175:HIS:CD2	6:F:177:VAL:HG13	2.55	0.41
5:E:69:LEU:HG	5:E:70:VAL:HG23	2.02	0.41
1:A:283:LEU:HD12	1:A:309:ALA:CB	2.50	0.41
2:B:129:PHE:CD1	2:B:272:ILE:HD13	2.56	0.41
2:B:145:VAL:HG22	2:B:149:MET:HG3	2.03	0.41
5:E:111:ILE:HD11	5:E:112:PHE:CE1	2.55	0.41
6:F:285:MET:HG3	6:F:285:MET:O	2.20	0.41
1:A:406:VAL:CG2	1:A:442:ILE:CD1	2.98	0.41
2:B:79:ALA:HB2	2:B:228:ALA:HB3	2.02	0.41
9:E:201:LMT:O3'	9:E:201:LMT:C1B	2.68	0.41
6:F:56:LEU:HD11	6:F:68:SER:HB3	2.02	0.41
2:B:308:LEU:HD21	2:B:370:LEU:HG	2.02	0.41
9:B:503:LMT:O5B	9:B:503:LMT:O3'	2.38	0.41
3:C:58:LYS:HE3	3:C:58:LYS:HB2	1.97	0.41
5:E:60:TYR:HA	5:E:64:LEU:HB2	2.02	0.41
2:B:237:ALA:HB3	2:B:333:LEU:HD22	2.02	0.41
5:E:117:THR:HG23	5:E:118:VAL:HG13	2.03	0.41
6:F:145:THR:HA	6:F:188:TYR:HB3	2.03	0.41
1:A:407:ARG:CZ	2:B:405:ILE:HD13	2.50	0.41
5:E:50:THR:HG22	5:E:144:PHE:HB2	2.02	0.41
6:F:293:PHE:CZ	6:F:322:ASP:HB3	2.53	0.41
2:B:55:ARG:O	2:B:59:MET:HG2	2.21	0.41
2:B:186:GLY:O	2:B:190:ALA:HB3	2.19	0.41
4:D:70:VAL:O	4:D:74:VAL:HG23	2.21	0.41
4:D:188:PHE:CZ	5:E:25:MET:HE1	2.56	0.41
6:F:295:GLN:O	6:F:301:SER:HB3	2.21	0.41
1:A:375:VAL:HG13	2:B:347:PRO:HB2	2.02	0.41
1:A:394:LEU:HD22	1:A:431:TYR:CD1	2.56	0.41
3:C:189:TRP:O	3:C:192:LYS:HG2	2.20	0.41
4:D:17:ASP:O	4:D:205:GLN:NE2	2.54	0.41
4:D:126:GLU:HB2	4:D:129:PRO:HG2	2.03	0.41
4:D:169:ILE:HD12	4:D:176:GLN:HB2	2.02	0.41
5:E:14:ILE:HD12	5:E:14:ILE:N	2.36	0.40
4:D:90:LEU:HB3	4:D:98:SER:HB2	2.02	0.40
5:E:76:SER:O	5:E:79:ASN:CG	2.60	0.40
6:F:127:ILE:CG1	6:F:128:PHE:N	2.83	0.40
3:C:15:VAL:HG23	3:C:16:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:ILE:HG13	5:E:193:PHE:HB3	2.03	0.40
2:B:40:VAL:CG2	2:B:41:THR:H	2.34	0.40
9:D:301:LMT:O1B	9:D:301:LMT:O6'	2.39	0.40
5:E:41:LEU:HD11	5:E:116:ILE:HD12	2.02	0.40
5:E:44:ALA:HB1	5:E:94:LEU:HD21	2.04	0.40
6:F:219:GLU:HA	6:F:221:PHE:CZ	2.57	0.40
4:D:115:MET:HE3	5:E:115:LEU:HD23	2.03	0.40
4:D:166:LEU:CD2	4:D:174:TRP:CZ2	3.04	0.40
5:E:151:MET:HA	5:E:154:ILE:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:OD2	3:C:212:GLN:H[2_646]	1.59	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/468 (85%)	391 (98%)	7 (2%)	1 (0%)	41	73
2	B	382/415 (92%)	375 (98%)	6 (2%)	1 (0%)	41	73
3	C	245/257 (95%)	241 (98%)	4 (2%)	0	100	100
4	D	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
5	E	195/198 (98%)	187 (96%)	7 (4%)	1 (0%)	29	63
6	F	404/408 (99%)	389 (96%)	15 (4%)	0	100	100
All	All	1825/1956 (93%)	1778 (97%)	44 (2%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	MET
5	E	98	LEU
2	B	40	VAL

5.3.2 Protein sidechains [i](#)

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	339/395 (86%)	339 (100%)	0	100	100
2	B	295/320 (92%)	294 (100%)	1 (0%)	92	96
3	C	198/205 (97%)	197 (100%)	1 (0%)	88	94
4	D	169/176 (96%)	169 (100%)	0	100	100
5	E	164/165 (99%)	164 (100%)	0	100	100
6	F	337/337 (100%)	334 (99%)	3 (1%)	78	91
All	All	1502/1598 (94%)	1497 (100%)	5 (0%)	92	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	230	ASP
3	C	22	CYS
6	F	6	PHE
6	F	35	ILE
6	F	119	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	324	ASN
3	C	90	ASN
3	C	143	ASN
3	C	232	GLN
6	F	295	GLN
6	F	356	HIS

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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
9	LMT	B	503	-	36,36,36	1.32	5 (13%)	47,47,47	1.64	5 (10%)
9	LMT	D	301	-	36,36,36	1.31	5 (13%)	47,47,47	1.03	1 (2%)
9	LMT	E	201	-	36,36,36	1.34	5 (13%)	47,47,47	1.01	4 (8%)
14	FES	F	1502	6	0,4,4	-	-	-	-	-
7	FMN	C	301	3	29,32,33	1.09	2 (6%)	40,47,50	1.39	8 (20%)
10	3PE	B	504	-	50,50,50	0.50	0	53,55,55	0.73	1 (1%)
8	RBF	B	502	-	29,29,29	0.57	0	41,43,43	0.71	2 (4%)
15	FAD	F	1501	-	53,58,58	0.49	0	68,89,89	0.69	2 (2%)
7	FMN	B	501	2	29,32,33	1.11	2 (6%)	40,47,50	1.47	9 (22%)
14	FES	D	302	5,4	0,4,4	-	-	-	-	-

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
9	LMT	B	503	-	-	8/21/61/61	0/2/2/2
9	LMT	D	301	-	-	8/21/61/61	0/2/2/2
9	LMT	E	201	-	-	10/21/61/61	0/2/2/2
14	FES	F	1502	6	-	-	0/1/1/1
7	FMN	C	301	3	-	0/15/17/18	0/3/3/3
10	3PE	B	504	-	-	23/54/54/54	-
8	RBF	B	502	-	-	0/14/14/14	0/3/3/3
15	FAD	F	1501	-	-	4/30/50/50	0/6/6/6
7	FMN	B	501	2	-	1/15/17/18	0/3/3/3
14	FES	D	302	5,4	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	201	LMT	O3'-C3'	-3.84	1.33	1.43
9	D	301	LMT	O2'-C2'	-3.72	1.34	1.43
7	B	501	FMN	C4A-N5	3.72	1.38	1.30
7	C	301	FMN	C4A-N5	3.67	1.37	1.30
9	B	503	LMT	O3'-C3'	-3.22	1.35	1.43
9	E	201	LMT	O2'-C2'	-3.09	1.35	1.43
9	D	301	LMT	O3'-C3'	-3.06	1.35	1.43
9	B	503	LMT	C3'-C2'	2.93	1.59	1.52
9	B	503	LMT	O2'-C2'	-2.89	1.36	1.43
7	C	301	FMN	C10-N1	2.58	1.38	1.33
9	D	301	LMT	O2B-C2B	-2.55	1.37	1.43
9	E	201	LMT	O2B-C2B	-2.51	1.37	1.43
7	B	501	FMN	C10-N1	2.50	1.38	1.33
9	B	503	LMT	O5'-C5'	-2.50	1.38	1.44
9	B	503	LMT	O2B-C2B	-2.47	1.37	1.43
9	E	201	LMT	O3B-C3B	-2.37	1.37	1.43
9	E	201	LMT	C4B-C3B	2.30	1.58	1.52
9	D	301	LMT	O3B-C3B	-2.28	1.37	1.43
9	D	301	LMT	C3'-C2'	2.02	1.57	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	LMT	O1'-C1'-C2'	7.51	120.03	108.30
7	B	501	FMN	C4-N3-C2	-3.40	119.35	125.64
9	B	503	LMT	O5'-C1'-O1'	-3.24	102.30	109.97
7	C	301	FMN	C4-N3-C2	-3.17	119.79	125.64
15	F	1501	FAD	P-O3P-PA	-3.13	122.10	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	301	FMN	C4A-C10-N10	3.10	121.02	116.48
9	B	503	LMT	C3'-C4'-C5'	-3.03	103.97	110.93
7	B	501	FMN	C4A-C10-N10	2.92	120.75	116.48
7	B	501	FMN	C4A-C4-N3	2.72	120.11	113.19
7	C	301	FMN	C4-C4A-C10	2.68	121.30	116.79
7	C	301	FMN	C4A-C10-N1	-2.63	118.62	124.73
7	B	501	FMN	C10-C4A-N5	-2.62	119.29	124.86
7	B	501	FMN	C4'-C3'-C2'	-2.61	107.94	113.36
7	B	501	FMN	C4A-C10-N1	-2.51	118.91	124.73
9	E	201	LMT	C3'-C4'-C5'	-2.46	105.28	110.93
7	C	301	FMN	O4-C4-C4A	-2.45	120.10	126.60
9	E	201	LMT	O1B-C1B-C2B	2.39	114.29	108.10
9	B	503	LMT	O5B-C5B-C4B	2.38	114.02	109.69
7	B	501	FMN	O4-C4-C4A	-2.38	120.30	126.60
9	D	301	LMT	O1'-C1'-C2'	2.37	112.01	108.30
7	C	301	FMN	C4A-C4-N3	2.35	119.16	113.19
10	B	504	3PE	O12-P-O14	2.32	123.69	112.24
15	F	1501	FAD	C5A-C6A-N6A	2.23	123.74	120.35
9	B	503	LMT	O2'-C2'-C3'	-2.18	105.31	110.35
7	B	501	FMN	C4-C4A-C10	2.17	120.44	116.79
7	B	501	FMN	C9A-C5A-N5	-2.13	120.11	122.43
9	E	201	LMT	C1B-C2B-C3B	-2.12	105.59	110.00
8	B	502	RBF	C4-N3-C2	-2.10	121.76	125.64
8	B	502	RBF	C4A-C4-N3	2.05	118.40	113.19
7	C	301	FMN	C10-C4A-N5	-2.03	120.55	124.86
7	C	301	FMN	C5A-C9A-N10	2.03	120.05	117.95
9	E	201	LMT	O5'-C5'-C6'	2.01	111.42	106.44

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	503	LMT	C2B-C1B-O1B-C4'
9	B	503	LMT	C2'-C1'-O1'-C1
9	B	503	LMT	O5'-C1'-O1'-C1
9	D	301	LMT	C2'-C1'-O1'-C1
9	D	301	LMT	O5'-C1'-O1'-C1
9	E	201	LMT	C2'-C1'-O1'-C1
9	E	201	LMT	O5'-C1'-O1'-C1
10	B	504	3PE	C1-O11-P-O14
10	B	504	3PE	C11-O13-P-O11
10	B	504	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
10	B	504	3PE	O13-C11-C12-N
15	F	1501	FAD	C5'-O5'-P-O1P
15	F	1501	FAD	C5'-O5'-P-O2P
15	F	1501	FAD	C5'-O5'-P-O3P
10	B	504	3PE	O32-C31-O31-C3
9	E	201	LMT	O5B-C1B-O1B-C4'
10	B	504	3PE	C32-C31-O31-C3
10	B	504	3PE	C22-C21-O21-C2
9	D	301	LMT	C3-C4-C5-C6
10	B	504	3PE	O22-C21-O21-C2
9	E	201	LMT	C5'-C4'-O1B-C1B
10	B	504	3PE	C1-O11-P-O13
9	B	503	LMT	C5-C6-C7-C8
10	B	504	3PE	C2A-C2B-C2C-C2D
10	B	504	3PE	C22-C23-C24-C25
9	E	201	LMT	C7-C8-C9-C10
9	D	301	LMT	C6-C7-C8-C9
9	E	201	LMT	C3'-C4'-O1B-C1B
9	B	503	LMT	C5'-C4'-O1B-C1B
10	B	504	3PE	C3D-C3E-C3F-C3G
10	B	504	3PE	C1-C2-C3-O31
9	D	301	LMT	O5'-C5'-C6'-O6'
10	B	504	3PE	O11-C1-C2-O21
9	E	201	LMT	O1'-C1-C2-C3
10	B	504	3PE	O11-C1-C2-C3
9	D	301	LMT	C2-C1-O1'-C1'
9	E	201	LMT	C9-C10-C11-C12
9	B	503	LMT	C11-C10-C9-C8
9	D	301	LMT	C4B-C5B-C6B-O6B
10	B	504	3PE	C2-C1-O11-P
10	B	504	3PE	C1-O11-P-O12
9	B	503	LMT	C3'-C4'-O1B-C1B
7	B	501	FMN	C4'-C5'-O5'-P
10	B	504	3PE	O21-C2-C3-O31
9	E	201	LMT	C3-C4-C5-C6
10	B	504	3PE	C32-C33-C34-C35
10	B	504	3PE	C21-C22-C23-C24
9	D	301	LMT	C7-C8-C9-C10
10	B	504	3PE	C31-C32-C33-C34
10	B	504	3PE	C3C-C3D-C3E-C3F
15	F	1501	FAD	O2'-C2'-C3'-C4'
10	B	504	3PE	C3E-C3F-C3G-C3H

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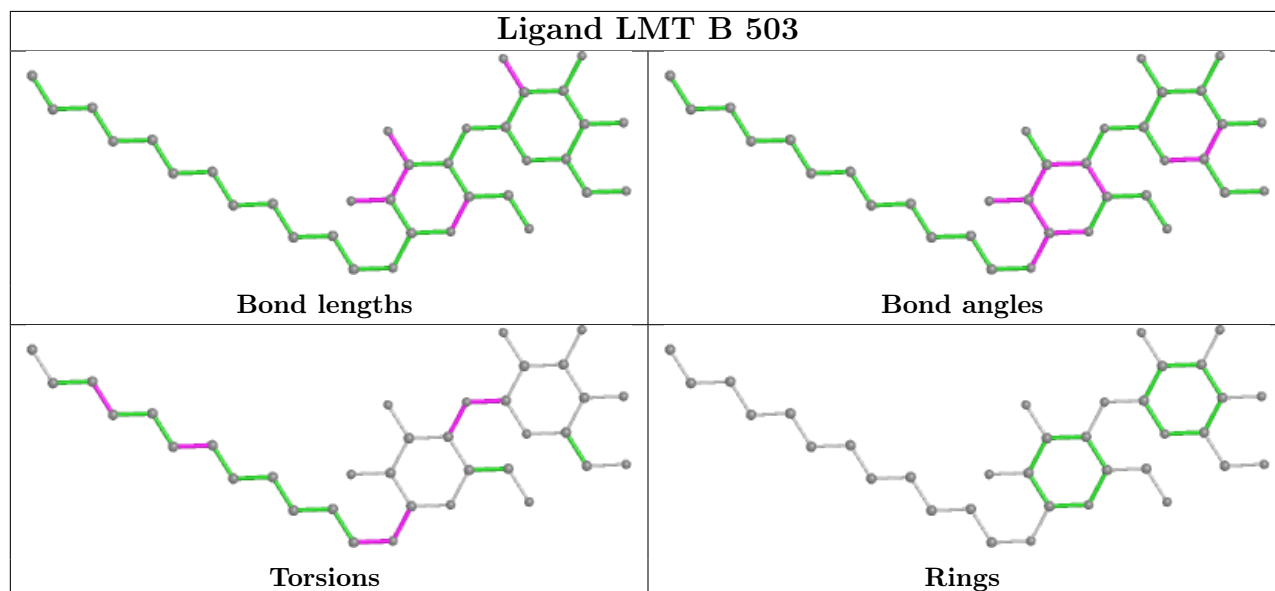
Mol	Chain	Res	Type	Atoms
9	E	201	LMT	C1-C2-C3-C4
9	B	503	LMT	C2-C1-O1'-C1'

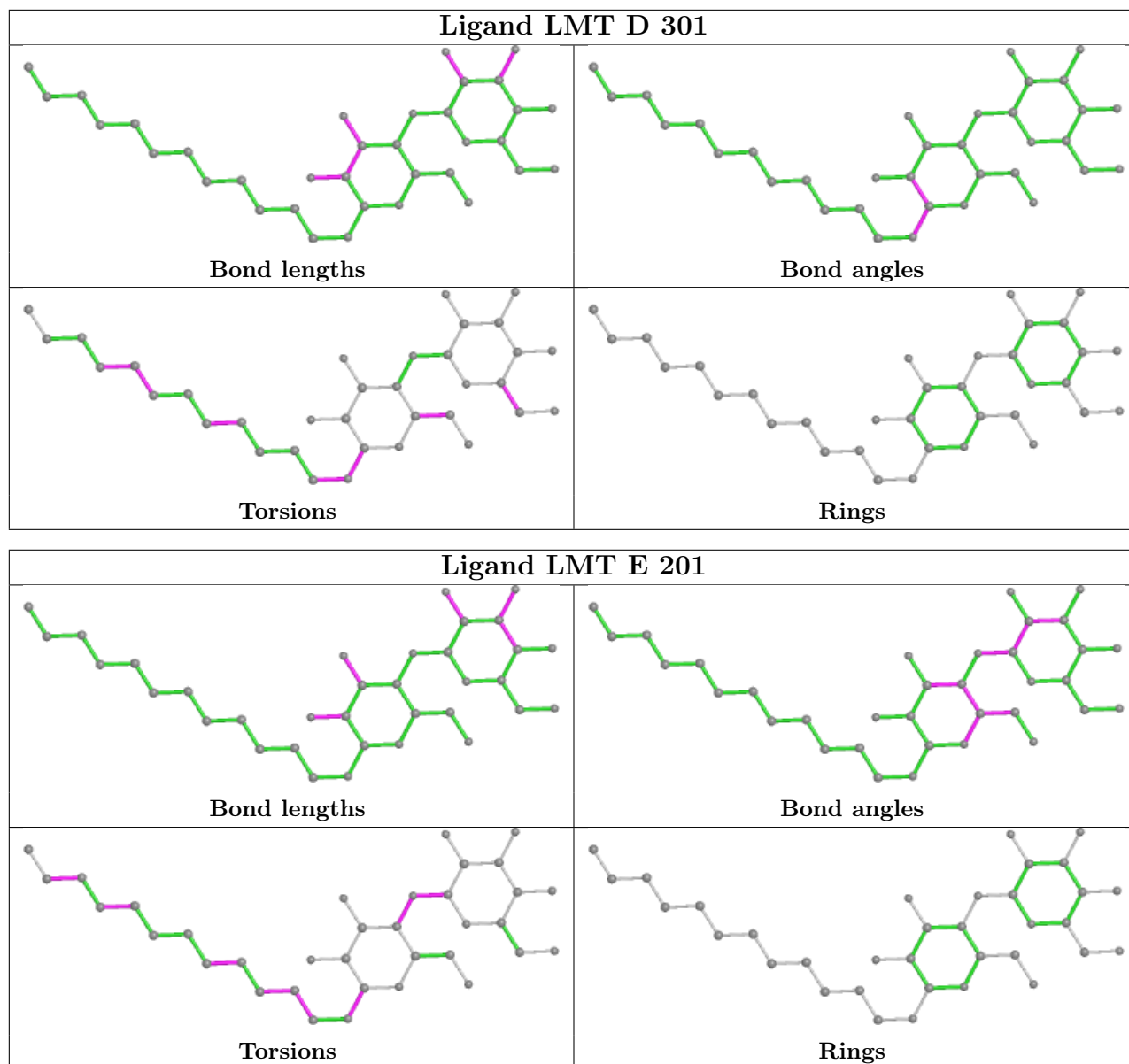
There are no ring outliers.

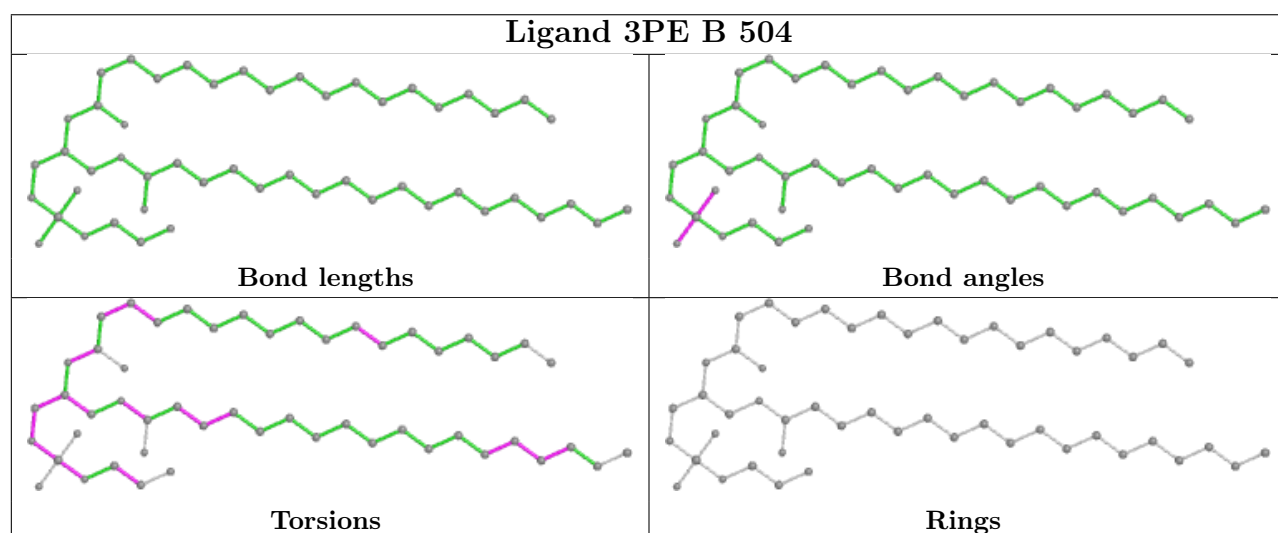
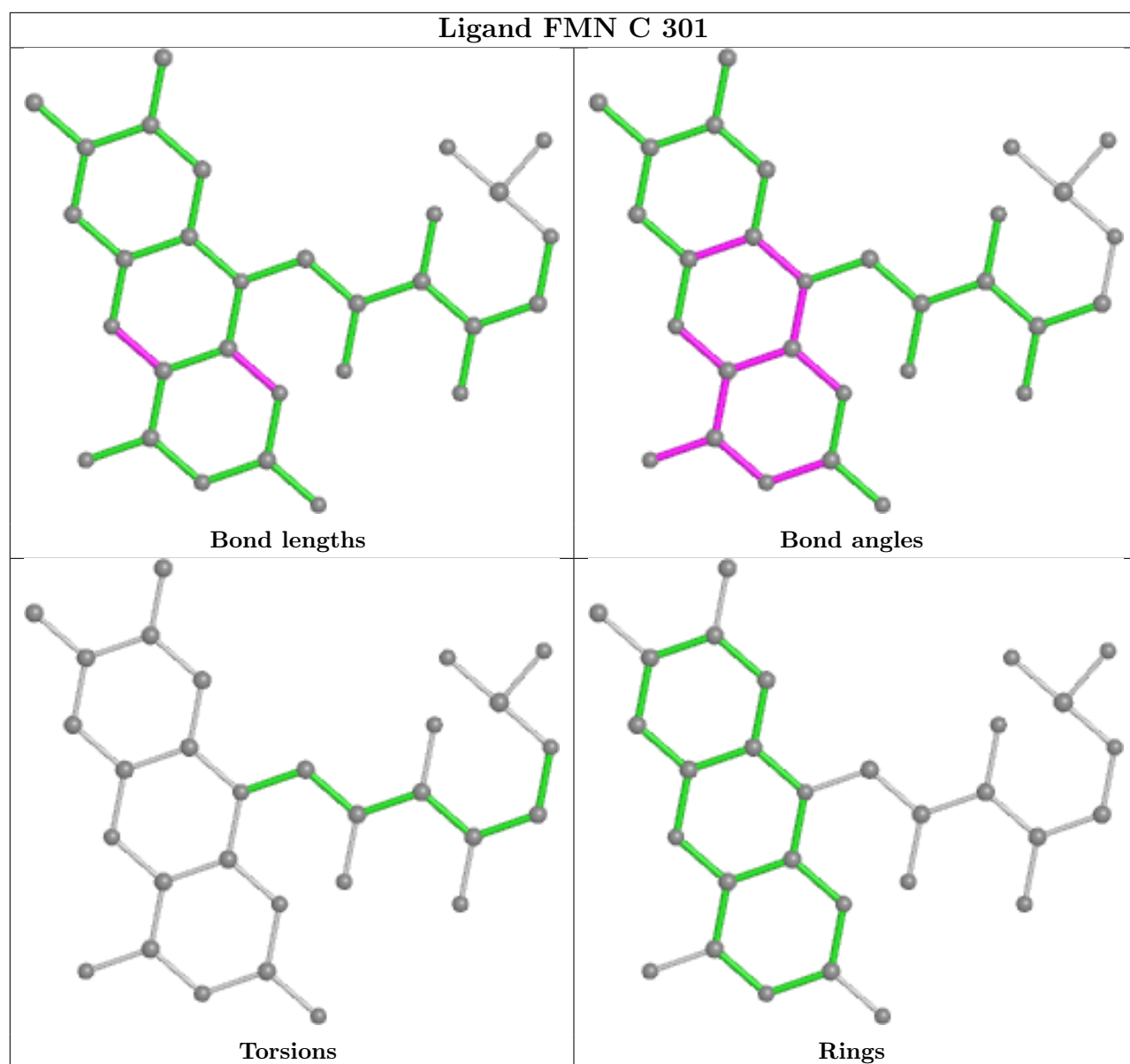
7 monomers are involved in 20 short contacts:

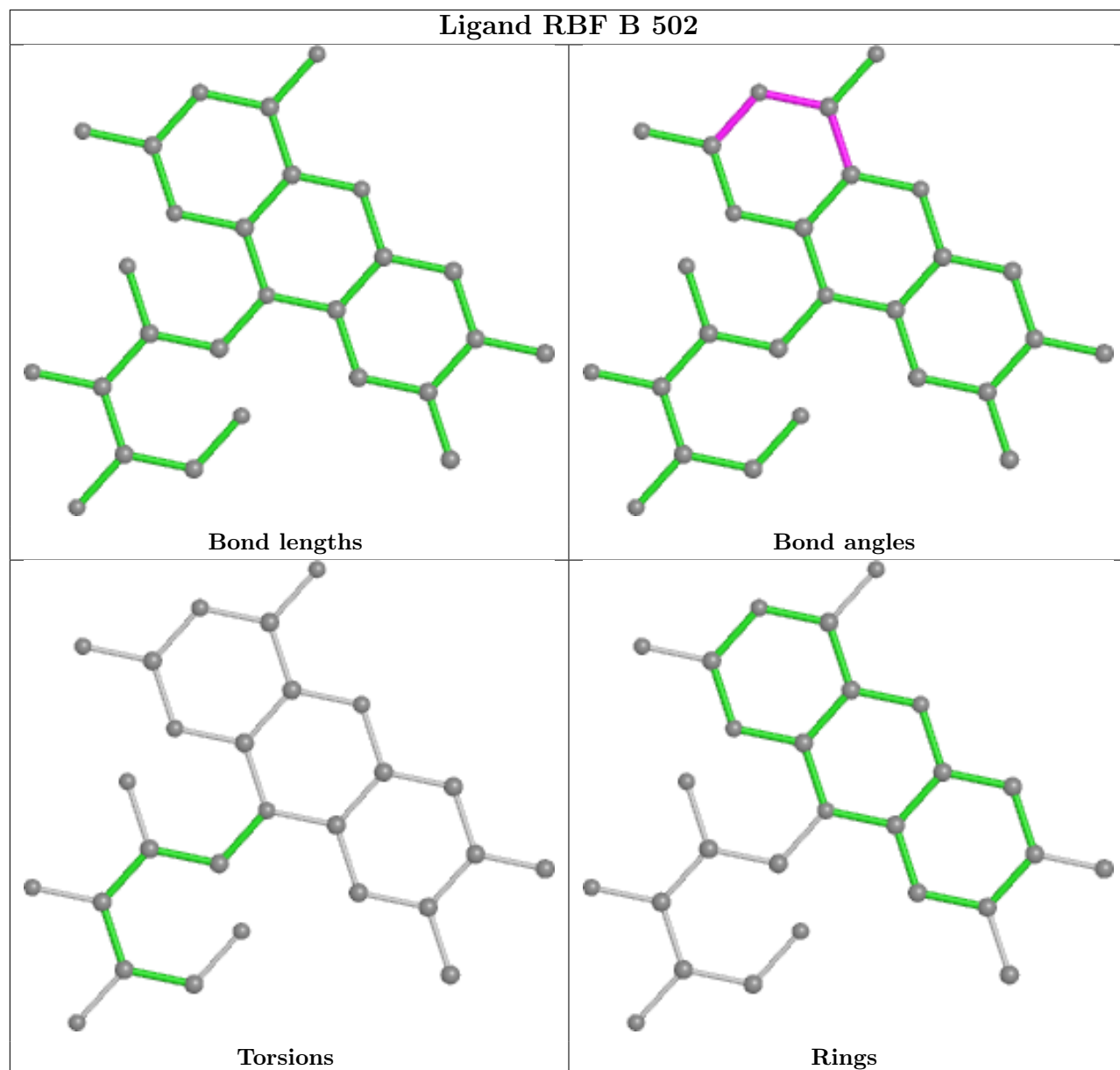
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	LMT	3	0
9	D	301	LMT	2	0
9	E	201	LMT	3	0
7	C	301	FMN	7	0
10	B	504	3PE	2	0
8	B	502	RBF	2	0
15	F	1501	FAD	1	0

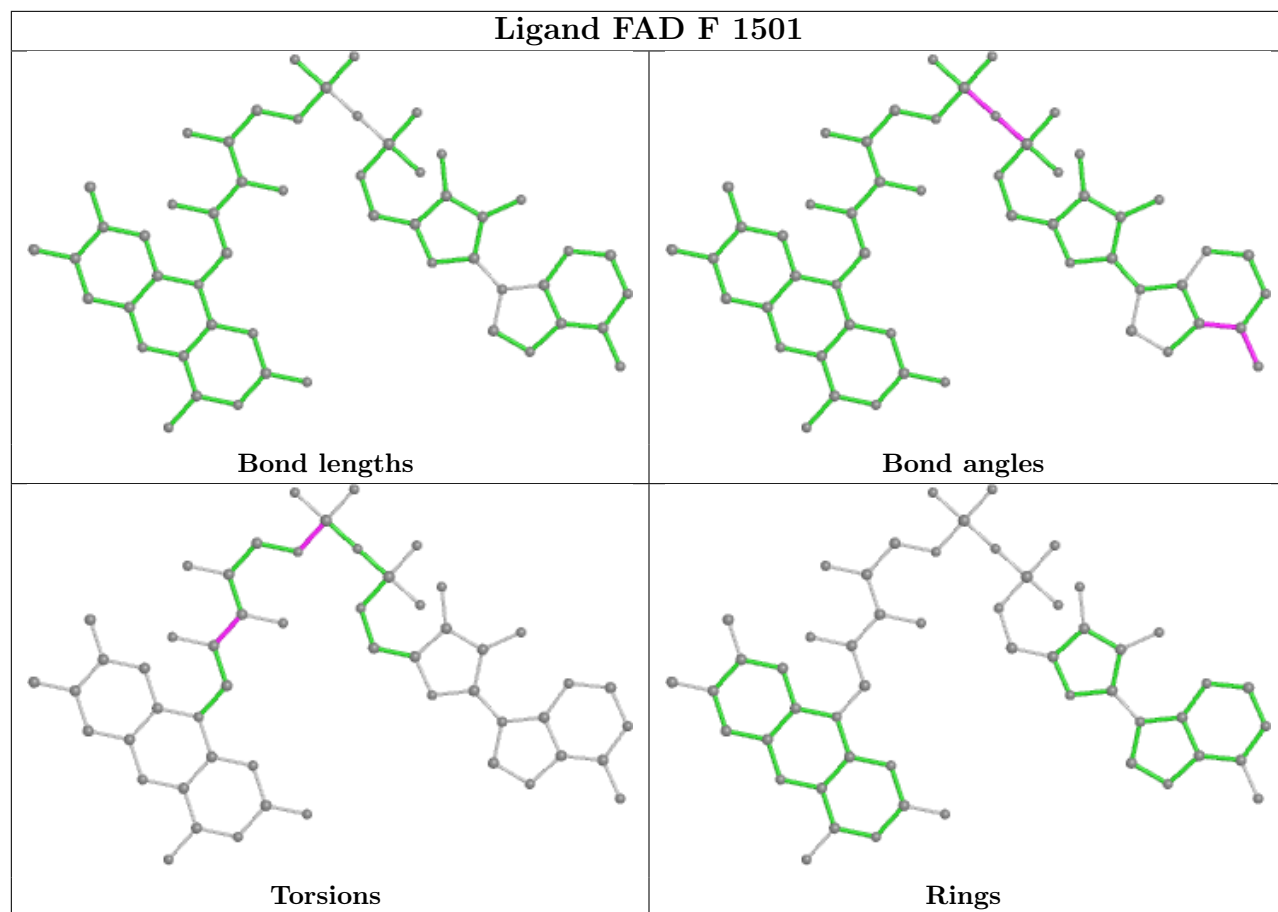
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

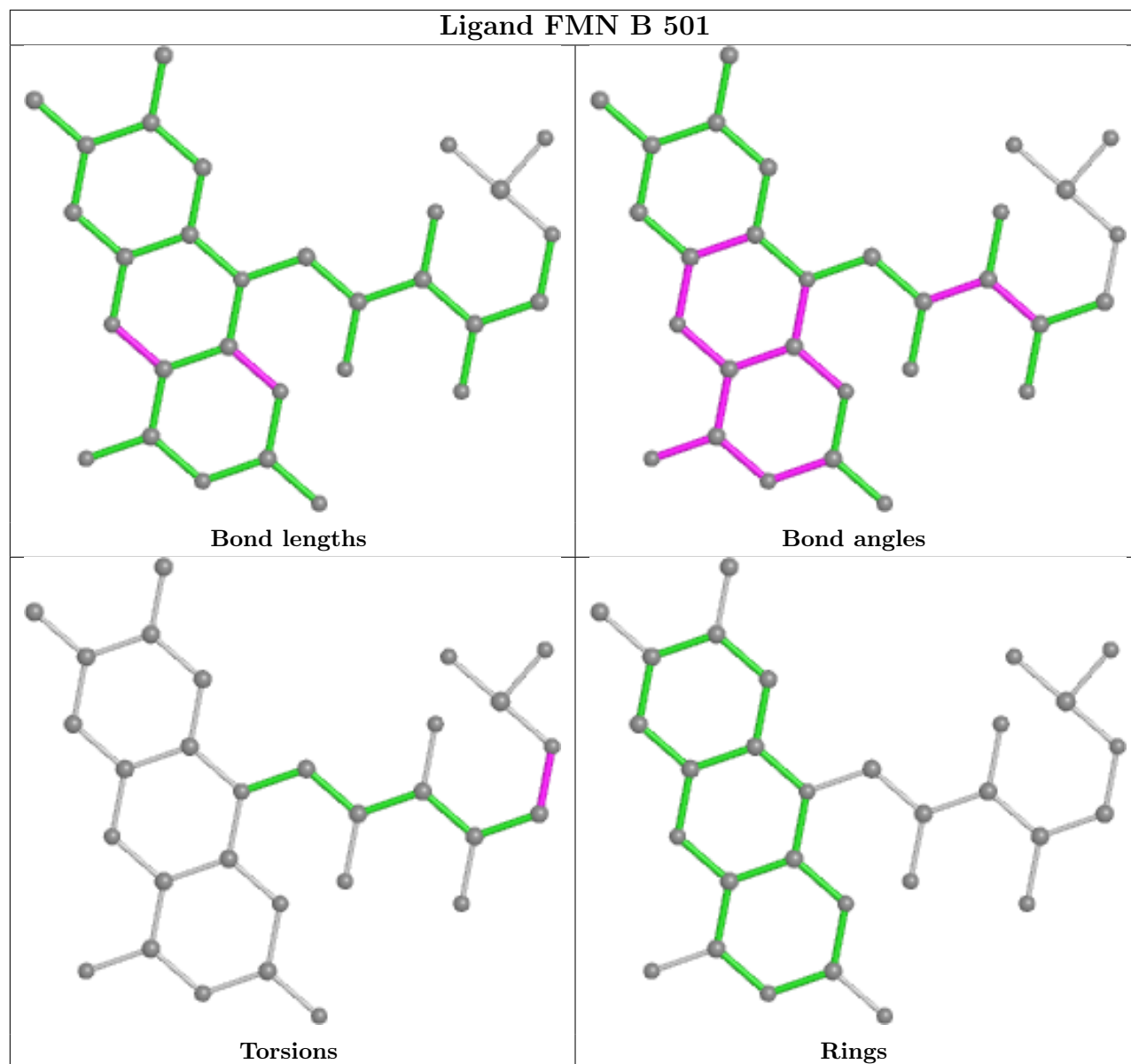












5.7 Other polymers [i](#)

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	403/468 (86%)	0.46	21 (5%) 27 12	93, 113, 143, 271	0
2	B	384/415 (92%)	0.65	36 (9%) 8 3	94, 131, 182, 229	0
3	C	247/257 (96%)	1.13	61 (24%) 0 0	135, 170, 213, 231	0
4	D	202/210 (96%)	0.52	15 (7%) 14 5	101, 139, 187, 234	0
5	E	197/198 (99%)	0.57	14 (7%) 16 6	94, 125, 159, 220	0
6	F	406/408 (99%)	0.30	30 (7%) 14 5	93, 137, 173, 206	0
All	All	1839/1956 (94%)	0.57	177 (9%) 8 3	93, 131, 187, 271	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	127	VAL	8.2
3	C	253	ASP	7.5
3	C	74	ARG	7.4
4	D	10	SER	7.2
1	A	377	ILE	7.1
1	A	329	GLY	6.8
1	A	187	GLY	6.7
3	C	199	HIS	6.1
3	C	71	ILE	6.1
3	C	194	LEU	5.9
1	A	295	GLU	5.9
3	C	133	THR	5.8
6	F	212	TYR	5.1
3	C	193	LYS	5.1
1	A	98	ASP	5.1
1	A	376	PRO	5.1
3	C	53	ALA	5.0
2	B	108	LEU	5.0
3	C	125	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
6	F	152	LEU	4.7
3	C	184	ALA	4.6
3	C	195	PHE	4.6
3	C	155	VAL	4.5
3	C	126	LEU	4.4
2	B	34	PHE	4.4
3	C	55	ILE	4.3
3	C	83	PHE	4.3
3	C	244	PHE	4.2
1	A	186	THR	4.1
6	F	258	CYS	4.1
3	C	54	GLY	4.1
3	C	73	PRO	4.1
3	C	165	LEU	4.0
6	F	254	ALA	3.9
3	C	139	PRO	3.8
6	F	208	ILE	3.8
2	B	116	ALA	3.8
1	A	207	GLU	3.8
4	D	209	LYS	3.7
2	B	414	LYS	3.7
3	C	128	LYS	3.7
4	D	11	VAL	3.7
3	C	137	ILE	3.6
3	C	160	ASN	3.6
2	B	152	LYS	3.6
3	C	136	VAL	3.6
3	C	159	GLY	3.6
3	C	252	ARG	3.5
3	C	166	THR	3.5
6	F	209	ILE	3.5
1	A	188	LYS	3.4
3	C	138	LEU	3.4
2	B	150	VAL	3.4
6	F	150	LEU	3.4
6	F	207	PRO	3.4
3	C	154	ALA	3.3
6	F	171	GLU	3.3
6	F	170	ILE	3.3
3	C	209	GLY	3.3
3	C	151	ALA	3.3
3	C	156	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
6	F	84	LYS	3.3
3	C	50	LEU	3.2
1	A	328	GLU	3.2
6	F	406	PHE	3.2
2	B	115	ASP	3.2
2	B	107	MET	3.2
3	C	72	GLU	3.2
3	C	168	TYR	3.2
2	B	103	TRP	3.1
2	B	405	ILE	3.1
2	B	95	ILE	3.1
3	C	123	VAL	3.1
3	C	215	GLU	3.1
3	C	75	LEU	3.1
2	B	35	TYR	3.1
2	B	114	SER	3.0
6	F	139	SER	3.0
4	D	171	ASN	3.0
5	E	187	ALA	3.0
5	E	189	GLY	3.0
2	B	207	ALA	3.0
6	F	206	GLU	3.0
3	C	185	TRP	3.0
3	C	210	ALA	2.9
4	D	165	VAL	2.9
1	A	99	GLN	2.9
2	B	203	ASN	2.9
6	F	137	VAL	2.9
3	C	152	PHE	2.9
6	F	169	GLN	2.9
3	C	49	ILE	2.8
2	B	210	ALA	2.8
6	F	118	ASP	2.8
4	D	201	PHE	2.8
3	C	239	LEU	2.8
4	D	30	SER	2.8
6	F	85	SER	2.8
5	E	18	ALA	2.8
6	F	117	ALA	2.8
3	C	56	GLU	2.8
2	B	91	GLN	2.7
3	C	235	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	148	LYS	2.7
3	C	132	LYS	2.7
1	A	226	PHE	2.7
6	F	225	MET	2.7
6	F	151	LYS	2.7
2	B	73	TYR	2.7
2	B	74	ASN	2.7
6	F	138	ILE	2.6
3	C	248	LEU	2.6
3	C	140	VAL	2.6
2	B	76	GLY	2.6
4	D	29	CYS	2.6
1	A	66	VAL	2.6
2	B	89	GLY	2.6
2	B	72	MET	2.6
1	A	375	VAL	2.6
4	D	14	PRO	2.6
3	C	186	ARG	2.5
6	F	210	ARG	2.5
3	C	247	PHE	2.5
5	E	27	THR	2.5
3	C	67	PHE	2.5
1	A	97	ASP	2.4
5	E	186	MET	2.4
4	D	23	LEU	2.4
1	A	100	VAL	2.3
4	D	184	ALA	2.3
4	D	12	LEU	2.3
5	E	184	GLY	2.3
3	C	86	GLY	2.3
2	B	205	ALA	2.3
4	D	8	LYS	2.3
2	B	266	GLY	2.3
2	B	345	THR	2.3
3	C	70	SER	2.3
2	B	265	ILE	2.3
3	C	52	VAL	2.2
2	B	104	LEU	2.2
2	B	409	LEU	2.2
5	E	153	ALA	2.2
2	B	92	LEU	2.2
6	F	167	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	2.2
3	C	207	LYS	2.2
6	F	78	GLN	2.2
5	E	164	MET	2.2
6	F	119	MET	2.2
5	E	183	ALA	2.2
6	F	211	ALA	2.2
3	C	26	VAL	2.2
4	D	27	GLY	2.2
6	F	404	ASP	2.2
2	B	336	PHE	2.1
2	B	208	GLY	2.1
3	C	84	VAL	2.1
5	E	119	ASN	2.1
5	E	182	THR	2.1
6	F	120	ASP	2.1
2	B	36	THR	2.1
2	B	123	LEU	2.1
5	E	188	LEU	2.1
1	A	190	TYR	2.1
1	A	79	ILE	2.1
3	C	124	VAL	2.1
2	B	333	LEU	2.1
5	E	20	SER	2.1
3	C	45	LYS	2.0
2	B	406	LYS	2.0
3	C	203	ILE	2.0
5	E	198	LEU	2.0
1	A	374	MET	2.0
1	A	206	VAL	2.0
2	B	94	ALA	2.0
4	D	164	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

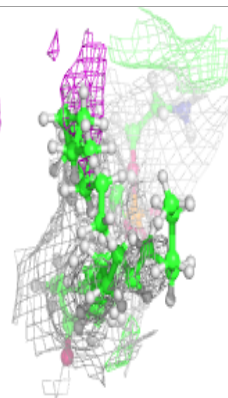
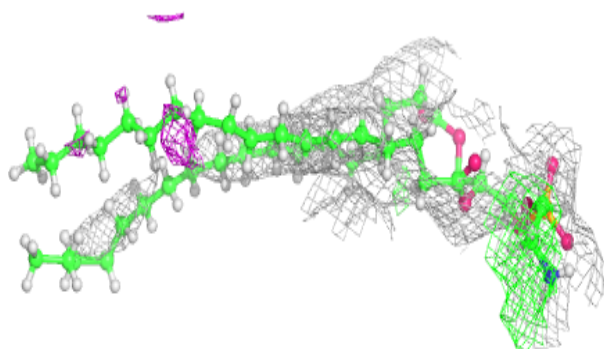
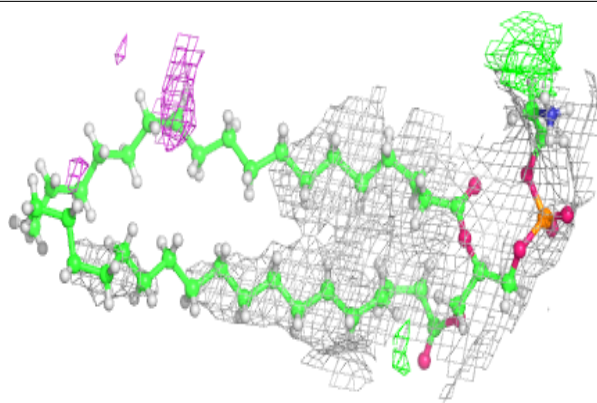
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	K	B	506	1/1	0.23	1.06	133,133,133,133	0
10	3PE	B	504	51/51	0.55	0.52	109,144,197,224	0
9	LMT	B	503	35/35	0.61	0.56	112,143,171,190	0
9	LMT	D	301	35/35	0.74	0.30	102,140,169,170	0
8	RBF	B	502	27/27	0.81	0.43	118,135,166,172	0
7	FMN	C	301	30/31	0.82	0.32	133,164,196,205	0
9	LMT	E	201	35/35	0.86	0.30	96,134,168,179	0
15	FAD	F	1501	53/53	0.87	0.30	107,133,163,179	0
13	BR	C	302	1/1	0.89	0.21	165,165,165,165	0
7	FMN	B	501	30/31	0.91	0.29	109,121,147,151	0
11	NA	B	505	1/1	0.92	0.32	127,127,127,127	0
14	FES	F	1502	4/4	0.96	0.15	161,162,162,193	0
14	FES	D	302	4/4	0.99	0.32	115,115,117,118	0

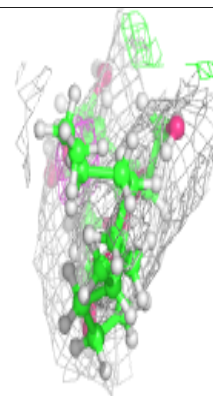
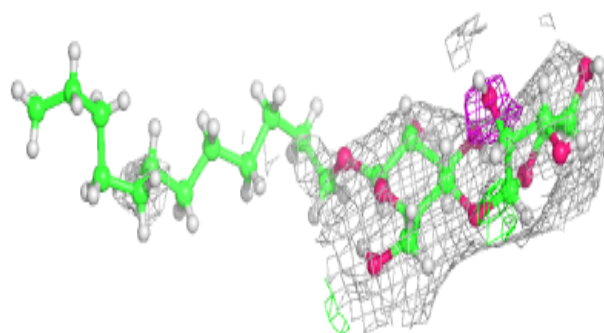
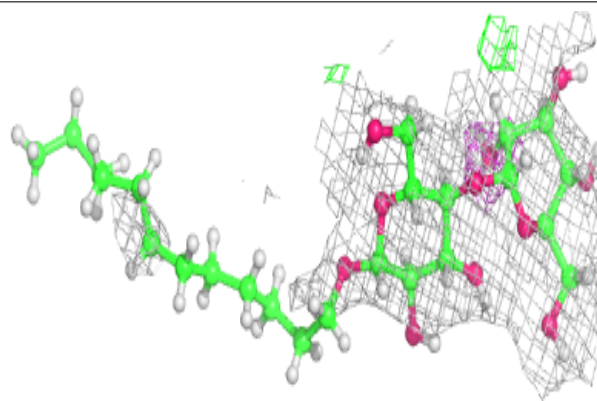
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3PE B 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

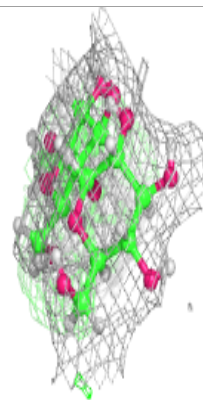
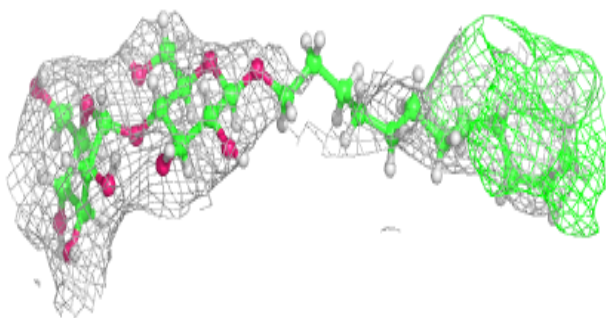
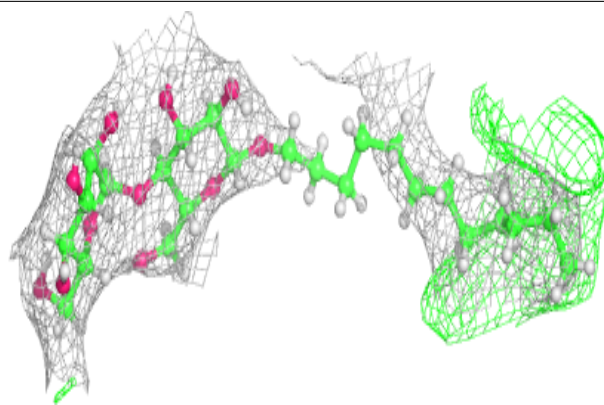
**Electron density around LMT B 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



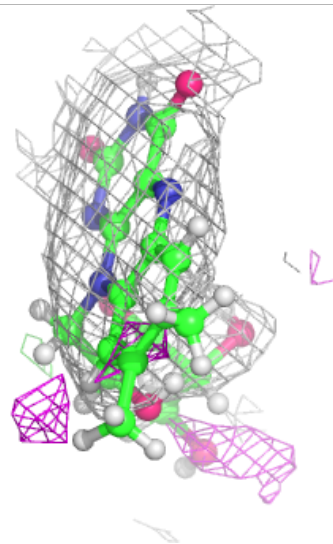
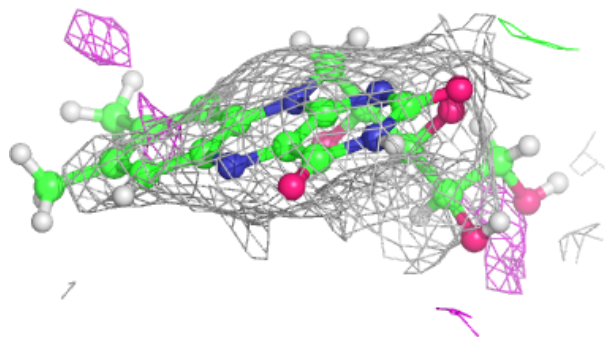
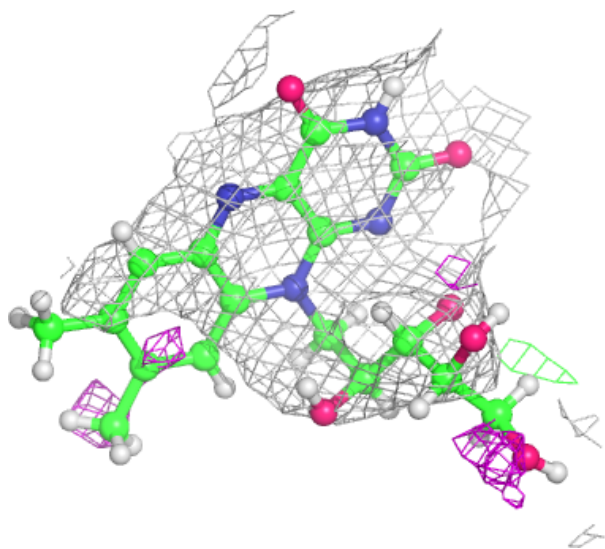
Electron density around LMT D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



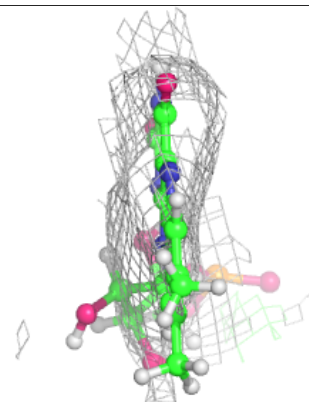
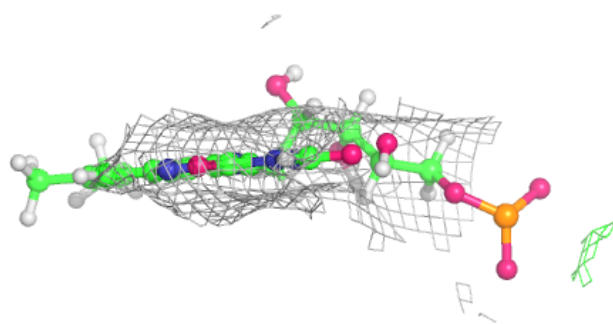
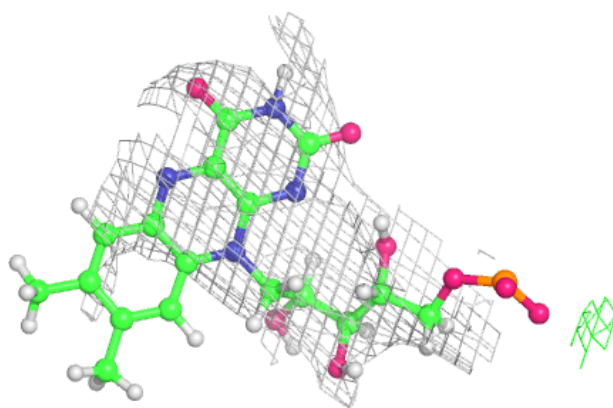
Electron density around RBF B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

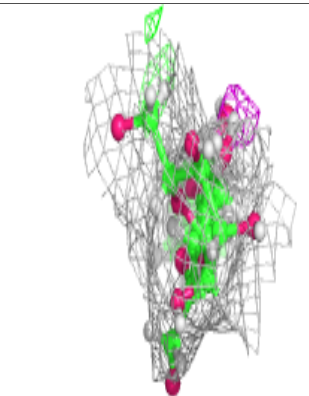
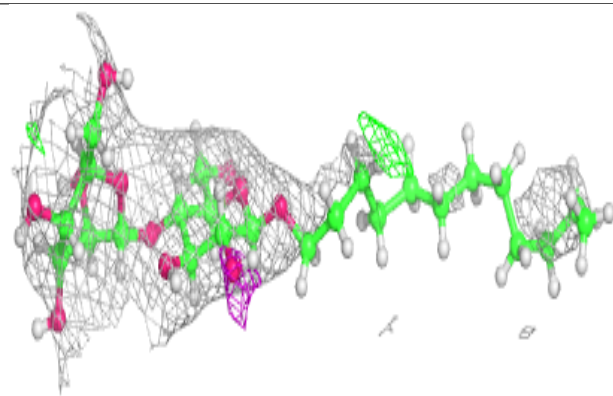
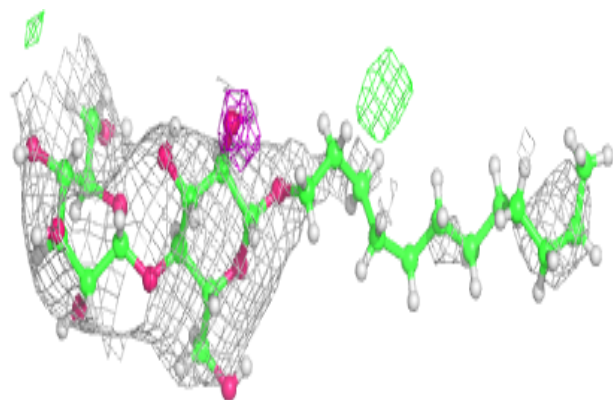


Electron density around FMN C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

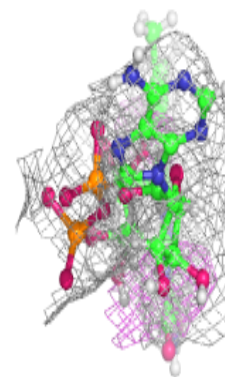
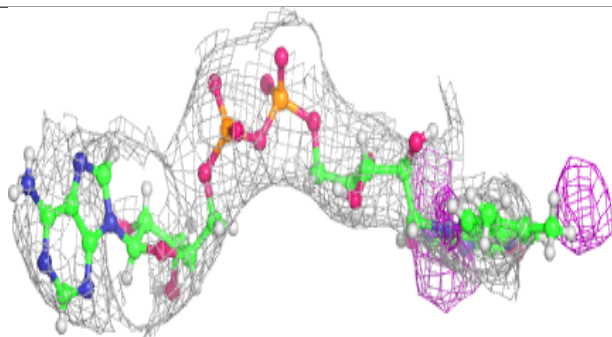
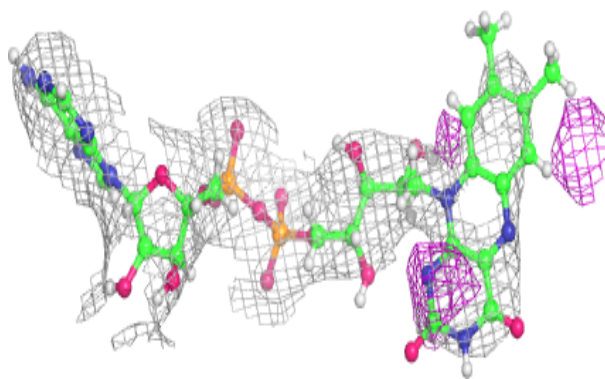
**Electron density around LMT E 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

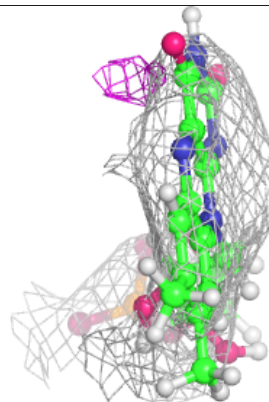
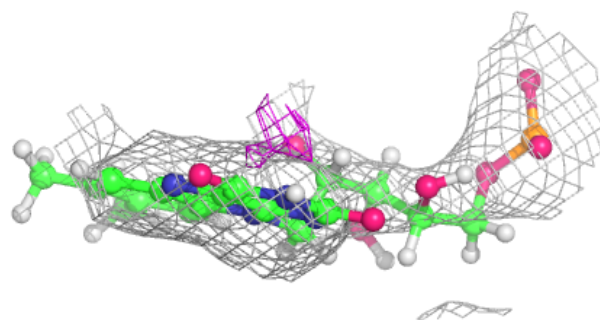
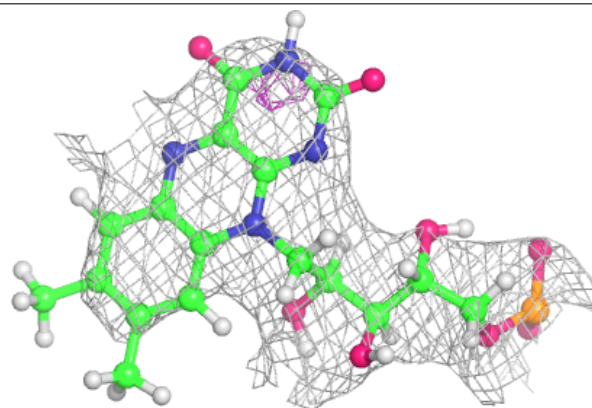


Electron density around FAD F 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FMN B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.