



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:51 PM UTC

PDB ID : 8AD0 / pdb_00008ad0
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

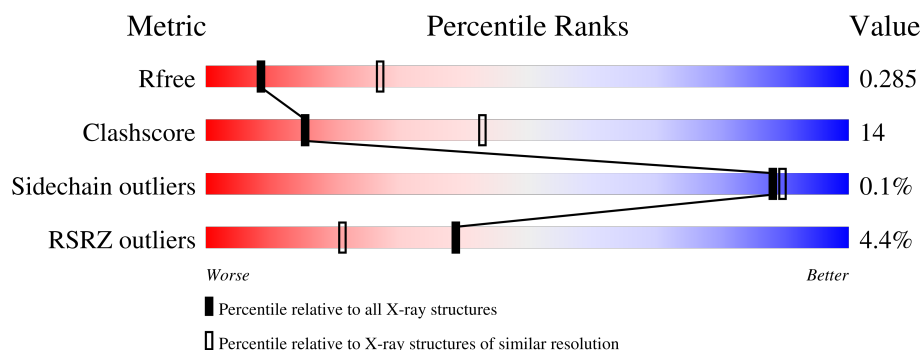
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (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	2% 74%18%7%
3	C	257	10% 68%27%. .
4	D	210	% 60%36%. .
5	E	198	3% 59%39%..
6	F	408	6% 74%24%. .

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
12	K	B	506	-	-	-	X

2 Entry composition

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
2	B	384	Total	C	H	N	O	S	0	0	0
			5881	1946	2939	479	495	22			

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

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

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

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

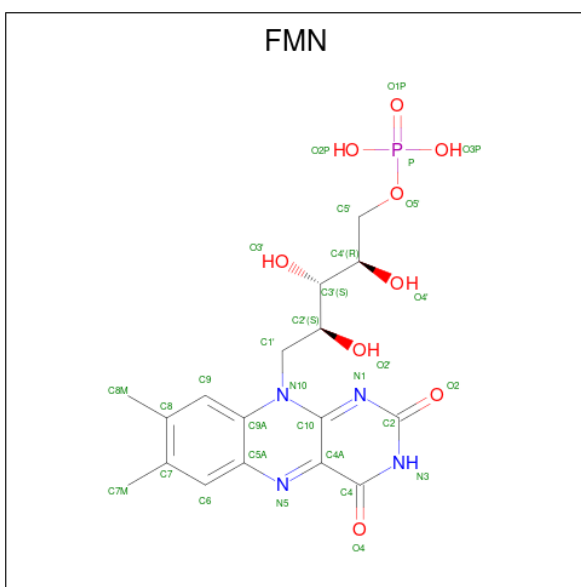
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

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

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

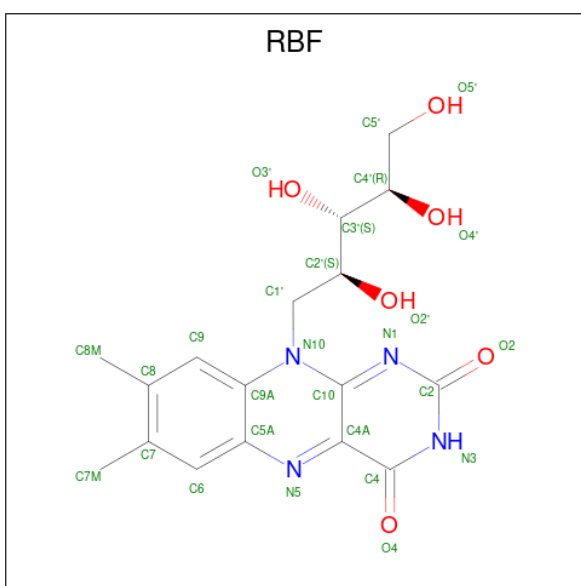
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	406	Total	C	H	N	O	S	0	0	0
			6252	2023	3095	517	593	24			

- Molecule 7 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



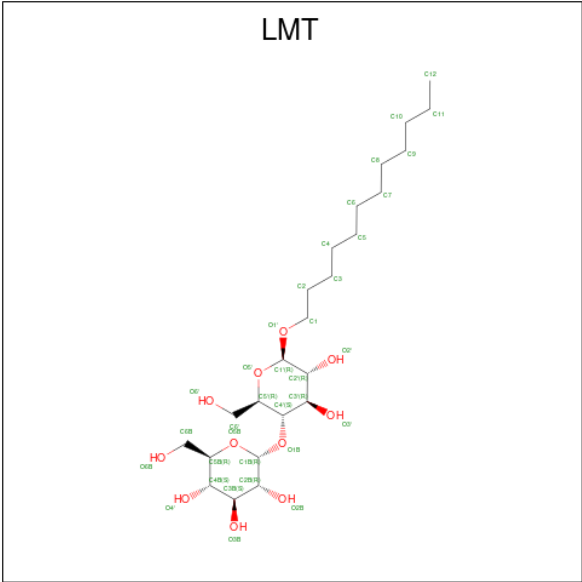
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	B	1	Total	C	H	N	O	P	0	0
			49	17	19	4	8	1		
7	C	1	Total	C	H	N	O	P	0	0
			49	17	19	4	8	1		

- Molecule 8 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$).



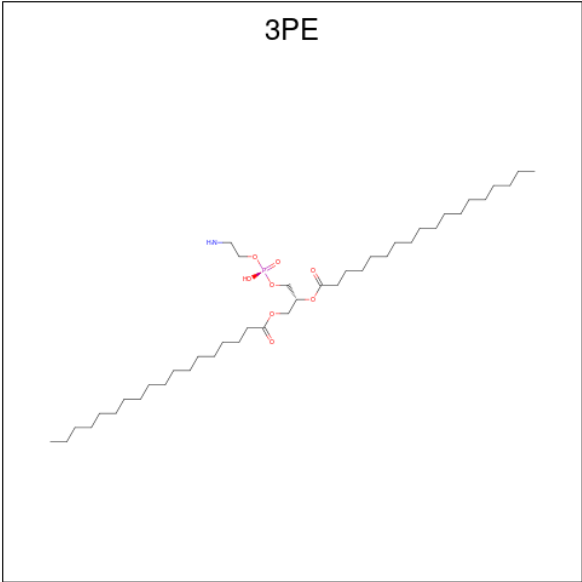
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			46	17	19	4	6		

- Molecule 9 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 10 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



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

- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

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

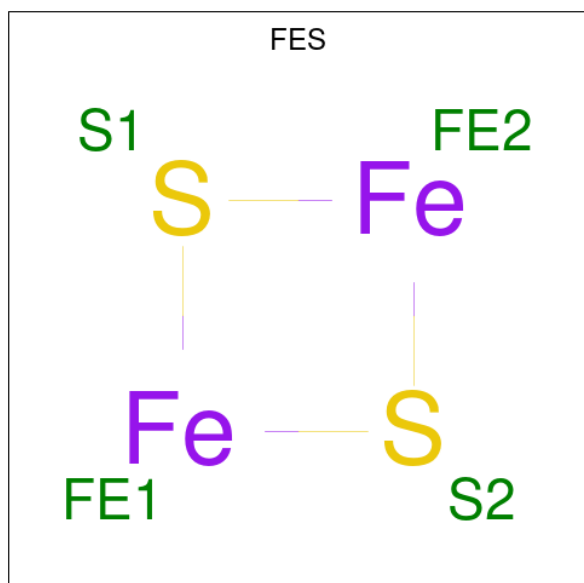
- Molecule 12 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 13 is BROMIDE ION (CCD ID: BR) (formula: Br).

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

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



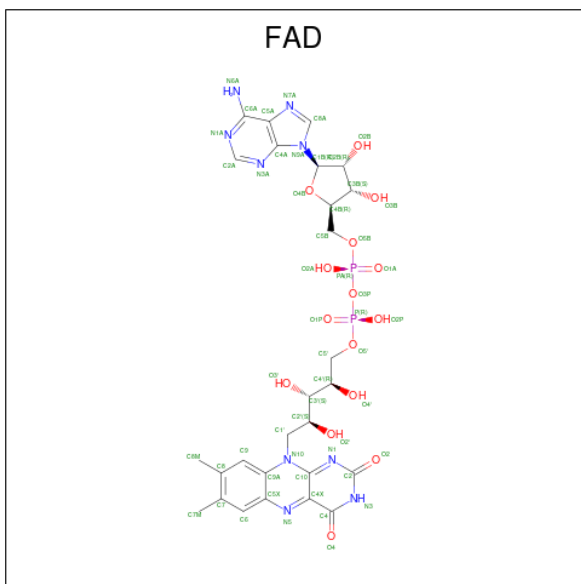
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	Fe	S		
			4	2	2	0	0

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

- Molecule 15 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

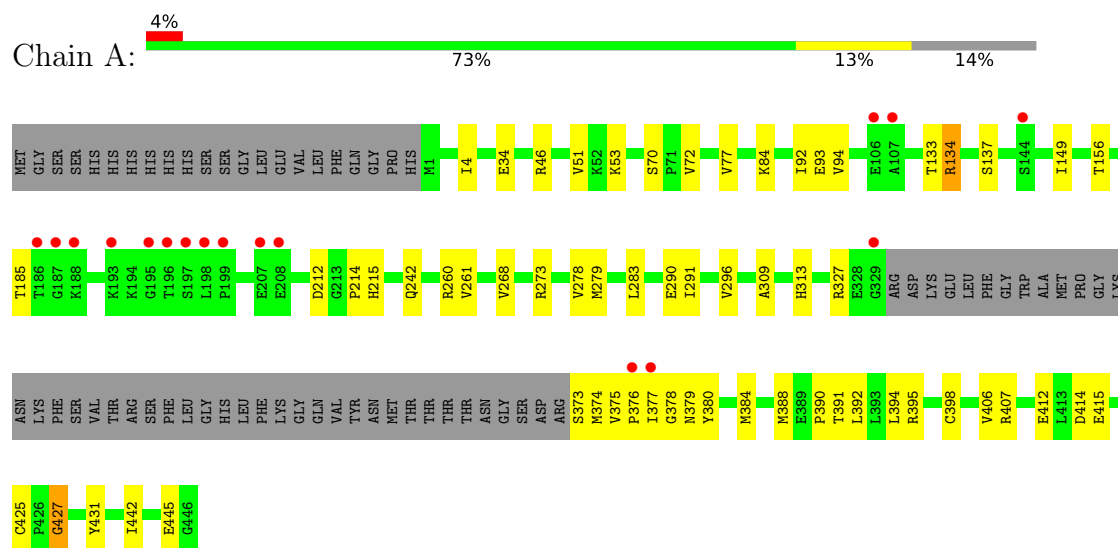
- Molecule 16 is water.

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

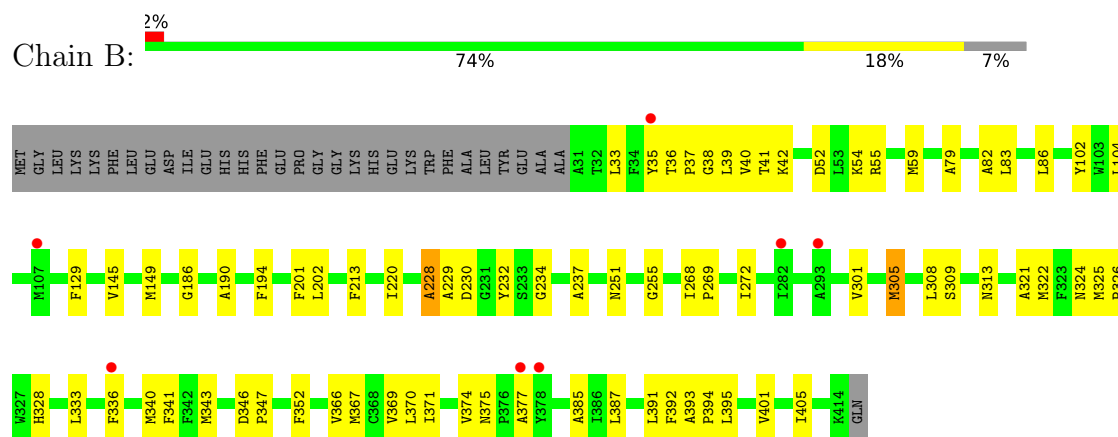
3 Residue-property plots [i](#)

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.

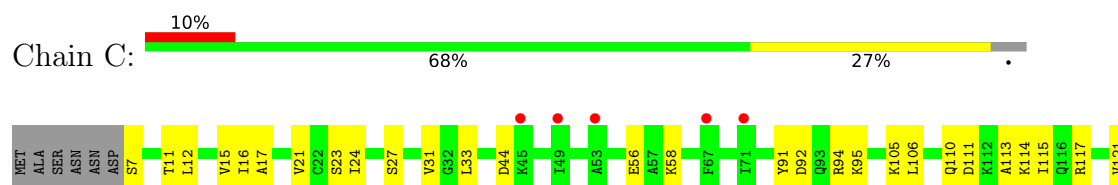
- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A

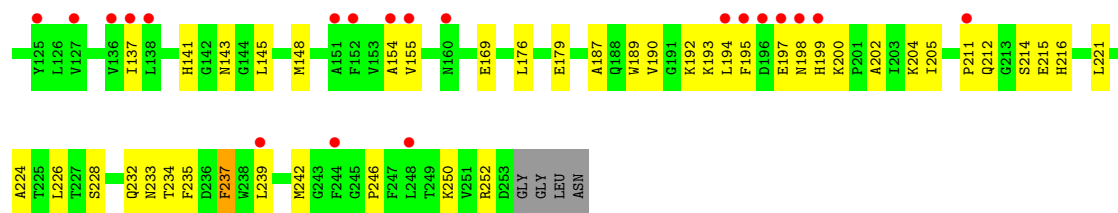


- Molecule 2: Na(+)-translocating NADH-quinone reductase subunit B

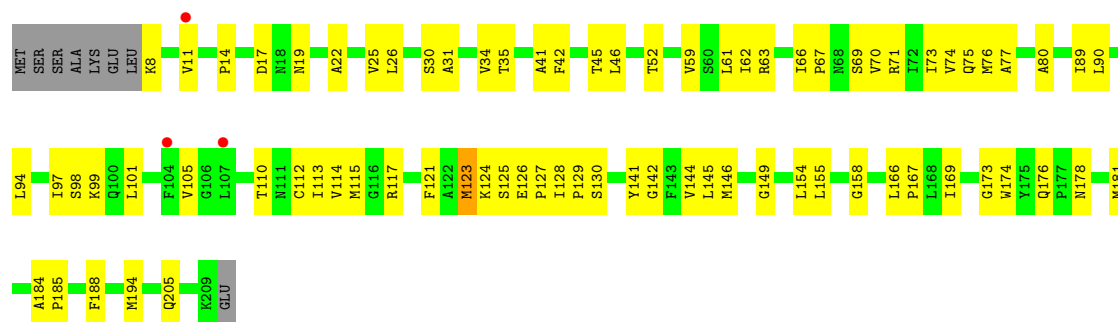


- Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C

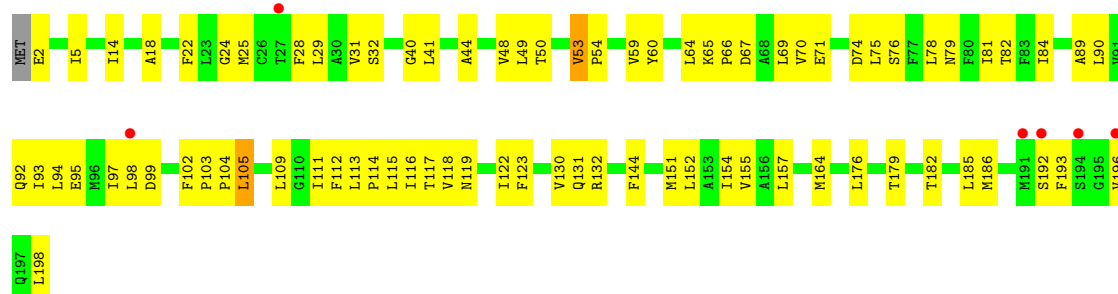




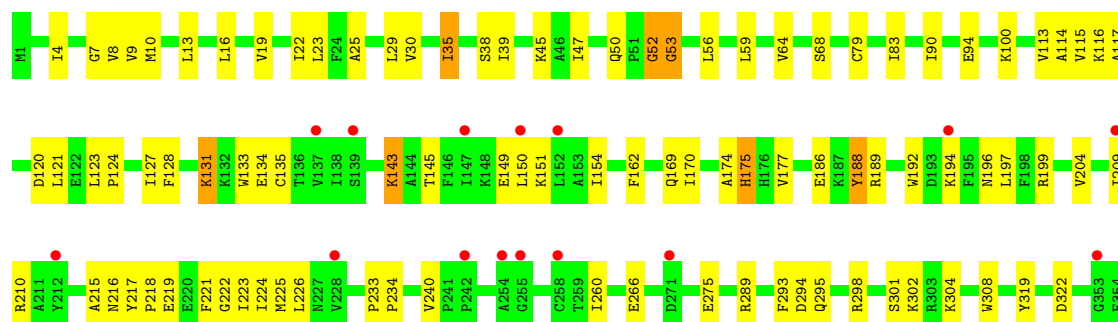
• Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D

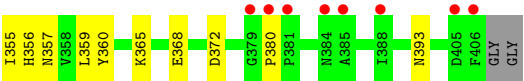


• Molecule 5: Na(+)-translocating NADH-quinone reductase subunit E



• 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) 99.6 (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)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.248 , 0.288 (Not available) , 0.285	Depositor DCC
R_{free} test set	2233 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	114.8	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	0.39	0/3124	0.74	3/4236 (0.1%)
2	B	0.40	0/3030	0.81	6/4127 (0.1%)
3	C	0.40	0/1910	0.92	2/2578 (0.1%)
4	D	0.46	0/1577	1.01	1/2141 (0.0%)
5	E	0.49	1/1537 (0.1%)	1.01	1/2084 (0.0%)
6	F	0.54	2/3235 (0.1%)	1.20	12/4379 (0.3%)
All	All	0.45	3/14413 (0.0%)	0.95	25/19545 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
6	F	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	380	PRO	CA-C	-6.85	1.48	1.51
5	E	53	VAL	CA-CB	5.71	1.57	1.54
6	F	233	PRO	CA-C	5.11	1.54	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	52	GLY	N-CA-C	-11.42	93.29	110.87
2	B	36	THR	N-CA-C	8.62	123.15	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	53	GLY	CA-C-N	-8.04	105.90	122.07
6	F	53	GLY	C-N-CA	-8.04	105.90	122.07
6	F	50	GLN	N-CA-C	-7.57	99.63	110.08
1	A	378	GLY	N-CA-C	-7.57	104.76	115.43
1	A	427	GLY	N-CA-C	-7.55	102.40	112.82
4	D	123	MET	N-CA-C	-7.16	101.09	110.53
6	F	53	GLY	N-CA-C	7.14	121.30	112.73
2	B	37	PRO	N-CA-C	6.50	121.15	111.41
2	B	35	TYR	N-CA-C	6.05	120.76	112.04
6	F	131	LYS	CA-CB-CG	6.05	126.20	114.10
6	F	188	TYR	N-CA-C	5.93	120.24	112.89
3	C	237	PHE	N-CA-C	-5.92	102.50	111.56
6	F	150	LEU	N-CA-C	-5.68	99.26	108.52
2	B	36	THR	CA-C-N	5.43	125.41	120.03
2	B	36	THR	C-N-CA	5.43	125.41	120.03
6	F	194	LYS	N-CA-C	5.23	117.06	111.36
2	B	305	MET	CB-CA-C	-5.20	102.69	110.90
1	A	134	ARG	N-CA-C	-5.20	99.08	108.85
3	C	200	LYS	N-CA-C	-5.10	101.27	109.58
5	E	105	LEU	N-CA-C	5.10	120.36	114.04
6	F	50	GLN	CA-C-N	-5.03	114.58	119.76
6	F	50	GLN	C-N-CA	-5.03	114.58	119.76
6	F	143	LYS	CB-CG-CD	5.03	122.86	111.30

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2942	2939	2939	73	0
3	C	1878	1889	1889	67	1
4	D	1545	1631	1631	67	0
5	E	1504	1574	1574	91	0
6	F	3157	3095	3095	92	0
7	B	30	19	19	0	0
7	C	30	19	19	6	0
8	B	27	19	20	1	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	392	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 14.

All (392) 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
1:A:374:MET:HE1	1:A:398:CYS:SG	2.11	0.91
5:E:103:PRO:HD2	5:E:104:PRO:HD2	1.53	0.90
4:D:188:PHE:CZ	5:E:25:MET:HE2	2.13	0.83
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:THR:OG1	1:A:215:HIS:O	2.01	0.77
3:C:110:GLN:HB3	3:C:242:MET:HE2	1.65	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:151:LYS:HE2	6:F:225:MET:HE2	1.68	0.75
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
4:D:188:PHE:CE1	5:E:25:MET:HE2	2.25	0.70
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
3:C:106:LEU:HD22	3:C:242:MET:HE1	1.74	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
4:D:188:PHE:HZ	5:E:25:MET:HE2	1.60	0.66
3:C:226:LEU:N	7:C:301:FMN:O2	2.29	0.65
5:E:28:PHE:O	5:E:32:SER:OG	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:76:MET:HE2	5:E:84:ILE:HG12	1.81	0.63
1:A:384:MET:HG2	1:A:390:PRO:HG3	1.81	0.62
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
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
1:A:379:ASN:N	1:A:379:ASN:OD1	2.33	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
2:B:39:LEU:O	2:B:40:VAL:C	2.49	0.56
4:D:63:ARG:O	4:D:66:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:ILE:HD12	5:E:94:LEU:N	2.20	0.56
2:B:305:MET:HE3	2:B:336:PHE:CZ	2.41	0.56
5:E:66:PRO:HB3	5:E:74:ASP:HB3	1.88	0.55
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
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
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:322:MET:HE1	2:B:325:MET:CE	2.37	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
3:C:141:HIS:C	3:C:234:THR:HG23	2.33	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
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
5:E:97:ILE:C	5:E:99:ASP:H	2.17	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:HD13	3:C:237:PHE:CE2	2.45	0.52
3:C:23:SER:O	3:C:27:SER:HB2	2.09	0.52
5:E:69:LEU:CD2	6:F:10:MET:HE3	2.39	0.52
6:F:35:ILE:HG21	6:F:115:VAL:HG22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:91:TYR:OH	3:C:121:VAL:O	2.25	0.52
1:A:380:TYR:HH	1:A:425:CYS:HG	1.56	0.51
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
3:C:106:LEU:HD22	3:C:242:MET:CE	2.39	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
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
3:C:113:ALA:O	3:C:114:LYS:HB2	2.10	0.51
4:D:144:VAL:HA	4:D:194:MET:HE1	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
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
6:F:275:GLU:CD	6:F:304:LYS:HD3	2.37	0.50
1:A:77:VAL:HG11	1:A:93:GLU:HB2	1.94	0.50
2:B:33:LEU:C	2:B:33:LEU:HD12	2.37	0.50
3:C:111:ASP:CG	3:C:115:ILE:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:62:ILE:HD12	4:D:62:ILE:C	2.37	0.49
4:D:115:MET:HE1	5:E:115:LEU:HA	1.94	0.49
1:A:373:SER:O	1:A:375:VAL:N	2.42	0.49
2:B:340:MET:HE3	2:B:341:PHE:CZ	2.47	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
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
4:D:42:PHE:N	4:D:146:MET:HE1	2.26	0.49
1:A:260:ARG:HD2	1:A:279:MET:HG3	1.94	0.49
2:B:232:TYR:CD1	2:B:232:TYR:C	2.91	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
4:D:22:ALA:O	5:E:176:LEU:HD23	2.12	0.48
5:E:198:LEU:C	5:E:198:LEU:HD23	2.38	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
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
2:B:213:PHE:HA	2:B:220:ILE:HG21	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
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:38:GLY:O	2:B:41:THR:OG1	2.32	0.47
2:B:387:LEU:O	2:B:391:LEU:HG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ALA:HA	3:C:233:ASN:HB3	1.95	0.47
5:E:69:LEU:HD22	6:F:10:MET:HE3	1.95	0.47
6:F:127:ILE:HG13	6:F:128:PHE:N	2.28	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
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
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
3:C:224:ALA:C	7:C:301:FMN:O2	2.58	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
2:B:322:MET:HE1	2:B:325:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:LEU:HB2	3:C:224:ALA:HB3	1.98	0.45
5:E:76:SER:O	5:E:79:ASN:CG	2.60	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
2:B:322:MET:HE1	2:B:325:MET:HE1	1.99	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
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
1:A:46:ARG:HE	6:F:368:GLU:CD	2.23	0.44
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
1:A:313:HIS:CD2	2:B:39:LEU:HD11	2.53	0.44
2:B:346:ASP:OD1	2:B:346:ASP:C	2.61	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
1:A:384:MET:HE2	1:A:384:MET:HB2	1.91	0.44
7:C:301:FMN:H9	7:C:301:FMN:H1'1	1.84	0.44
5:E:97:ILE:C	5:E:99:ASP:N	2.73	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:D:115:MET:HE2	5:E:117:THR:CG2	2.49	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
5:E:157:LEU:HB2	5:E:186:MET:HE1	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:LYS:HD3	3:C:117:ARG:HD3	2.01	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
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
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
3:C:110:GLN:HB3	3:C:242:MET:CE	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:VAL:HG23	3:C:16:ILE:N	2.36	0.40
5:E:14:ILE:HG13	5:E:193:PHE:HB3	2.03	0.40
6:F:127:ILE:CG1	6:F:128:PHE:N	2.83	0.40
1:A:374:MET:HE2	1:A:374:MET:HB3	1.84	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: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](#)

There are no protein backbone outliers to report in this entry.

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%)	295 (100%)	0	100	100
3	C	198/205 (97%)	198 (100%)	0	100	100
4	D	169/176 (96%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	164/165 (99%)	164 (100%)	0	100	100
6	F	337/337 (100%)	336 (100%)	1 (0%)	86	86
All	All	1502/1598 (94%)	1501 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	35	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	88	GLN
2	B	243	GLN
3	C	51	GLN
3	C	143	ASN
3	C	232	GLN
4	D	205	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 oligosaccharides 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$
14	FES	F	1502	6	0,4,4	-	-	-		
15	FAD	F	1501	-	58,58,58	0.34	0	85,89,89	0.45	0
7	FMN	C	301	3	29,32,33	1.04	2 (6%)	41,47,50	1.41	8 (19%)
7	FMN	B	501	2	29,32,33	1.07	2 (6%)	41,47,50	1.49	9 (21%)
10	3PE	B	504	-	50,50,50	0.50	0	53,55,55	0.73	1 (1%)
9	LMT	E	201	-	36,36,36	1.30	5 (13%)	47,47,47	1.03	4 (8%)
9	LMT	D	301	-	36,36,36	1.27	4 (11%)	47,47,47	1.03	1 (2%)
14	FES	D	302	4,5	0,4,4	-	-	-		
8	RBF	B	502	-	29,29,29	0.58	0	42,43,43	0.71	2 (4%)
9	LMT	B	503	-	36,36,36	1.28	5 (13%)	47,47,47	1.67	5 (10%)

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
15	FAD	F	1501	-	-	7/34/50/50	0/6/6/6
14	FES	F	1502	6	-	-	0/1/1/1
7	FMN	C	301	3	-	0/15/17/18	0/3/3/3
7	FMN	B	501	2	-	1/15/17/18	0/3/3/3
10	3PE	B	504	-	-	24/54/54/54	-
9	LMT	E	201	-	-	10/21/61/61	0/2/2/2
9	LMT	D	301	-	-	8/21/61/61	0/2/2/2
14	FES	D	302	4,5	-	-	0/1/1/1
8	RBF	B	502	-	-	0/14/14/14	0/3/3/3
9	LMT	B	503	-	-	7/21/61/61	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	201	LMT	O3'-C3'	-3.64	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	301	LMT	O2'-C2'	-3.53	1.34	1.43
7	B	501	FMN	C4A-N5	3.35	1.38	1.30
7	C	301	FMN	C4A-N5	3.30	1.37	1.30
9	B	503	LMT	O3'-C3'	-3.06	1.35	1.43
9	E	201	LMT	O2'-C2'	-2.93	1.35	1.43
9	D	301	LMT	O3'-C3'	-2.90	1.35	1.43
9	B	503	LMT	C3'-C2'	2.87	1.59	1.52
9	B	503	LMT	O2'-C2'	-2.74	1.36	1.43
7	C	301	FMN	C10-N1	2.61	1.38	1.33
7	B	501	FMN	C10-N1	2.53	1.38	1.33
9	B	503	LMT	O5'-C5'	-2.50	1.38	1.44
9	D	301	LMT	O2B-C2B	-2.42	1.37	1.43
9	E	201	LMT	O2B-C2B	-2.38	1.37	1.43
9	B	503	LMT	O2B-C2B	-2.35	1.37	1.43
9	E	201	LMT	C4B-C3B	2.25	1.58	1.52
9	E	201	LMT	O3B-C3B	-2.25	1.37	1.43
9	D	301	LMT	O3B-C3B	-2.16	1.37	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	LMT	O1'-C1'-C2'	7.74	120.03	108.27
7	B	501	FMN	C4-N3-C2	-3.54	119.35	125.64
7	B	501	FMN	C4'-C3'-C2'	-3.38	107.94	113.57
7	C	301	FMN	C4-N3-C2	-3.30	119.79	125.64
9	B	503	LMT	O5'-C1'-O1'	-3.28	102.30	110.04
7	C	301	FMN	C4A-C10-N10	3.17	121.02	116.48
9	B	503	LMT	C3'-C4'-C5'	-3.14	103.97	110.93
7	B	501	FMN	C4A-C10-N10	2.98	120.75	116.48
7	B	501	FMN	C10-C4A-N5	-2.70	119.29	124.81
7	B	501	FMN	C4A-C4-N3	2.69	120.11	113.25
9	E	201	LMT	C3'-C4'-C5'	-2.55	105.28	110.93
7	C	301	FMN	C4-C4A-C10	2.55	121.30	116.93
9	E	201	LMT	O1B-C1B-C2B	2.52	114.29	108.09
9	D	301	LMT	O1'-C1'-C2'	2.46	112.01	108.27
7	C	301	FMN	O4-C4-C4A	-2.44	120.10	126.53
7	C	301	FMN	C4A-C10-N1	-2.44	118.62	124.59
10	B	504	3PE	O12-P-O14	2.42	123.69	112.44
9	B	503	LMT	O5B-C5B-C4B	2.40	114.02	109.70
7	B	501	FMN	O4-C4-C4A	-2.36	120.30	126.53
7	C	301	FMN	C4A-C4-N3	2.32	119.16	113.25
7	B	501	FMN	C4A-C10-N1	-2.32	118.91	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	301	FMN	C5A-C9A-N10	2.30	120.05	117.97
7	B	501	FMN	C9A-C5A-N5	-2.21	120.11	122.45
8	B	502	RBF	C4-N3-C2	-2.18	121.76	125.64
9	B	503	LMT	O2'-C2'-C3'	-2.15	105.31	110.38
9	E	201	LMT	C1B-C2B-C3B	-2.10	105.59	110.01
7	C	301	FMN	C10-C4A-N5	-2.09	120.55	124.81
7	B	501	FMN	C4-C4A-C10	2.05	120.44	116.93
8	B	502	RBF	C4A-C4-N3	2.02	118.40	113.25
9	E	201	LMT	O5'-C5'-C6'	2.01	111.42	106.44

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	503	LMT	C2B-C1B-O1B-C4'
9	E	201	LMT	C2'-C1'-O1'-C1
10	B	504	3PE	C1-O11-P-O13
10	B	504	3PE	C1-O11-P-O14
10	B	504	3PE	C11-O13-P-O11
10	B	504	3PE	C11-O13-P-O14
10	B	504	3PE	O13-C11-C12-N
15	F	1501	FAD	C5'-O5'-P-O1P
15	F	1501	FAD	C5'-O5'-P-O2P
9	E	201	LMT	O5B-C1B-O1B-C4'
10	B	504	3PE	O32-C31-O31-C3
10	B	504	3PE	C32-C31-O31-C3
10	B	504	3PE	C22-C21-O21-C2
9	B	503	LMT	O5'-C1'-O1'-C1
9	D	301	LMT	O5'-C1'-O1'-C1
9	E	201	LMT	O5'-C1'-O1'-C1
9	B	503	LMT	C2'-C1'-O1'-C1
9	D	301	LMT	C2'-C1'-O1'-C1
10	B	504	3PE	O22-C21-O21-C2
9	E	201	LMT	C5'-C4'-O1B-C1B
9	D	301	LMT	C3-C4-C5-C6
9	B	503	LMT	C5-C6-C7-C8
9	E	201	LMT	C3'-C4'-O1B-C1B
10	B	504	3PE	C2A-C2B-C2C-C2D
10	B	504	3PE	C22-C23-C24-C25
9	B	503	LMT	C5'-C4'-O1B-C1B
9	E	201	LMT	C7-C8-C9-C10
10	B	504	3PE	C1-C2-C3-O31

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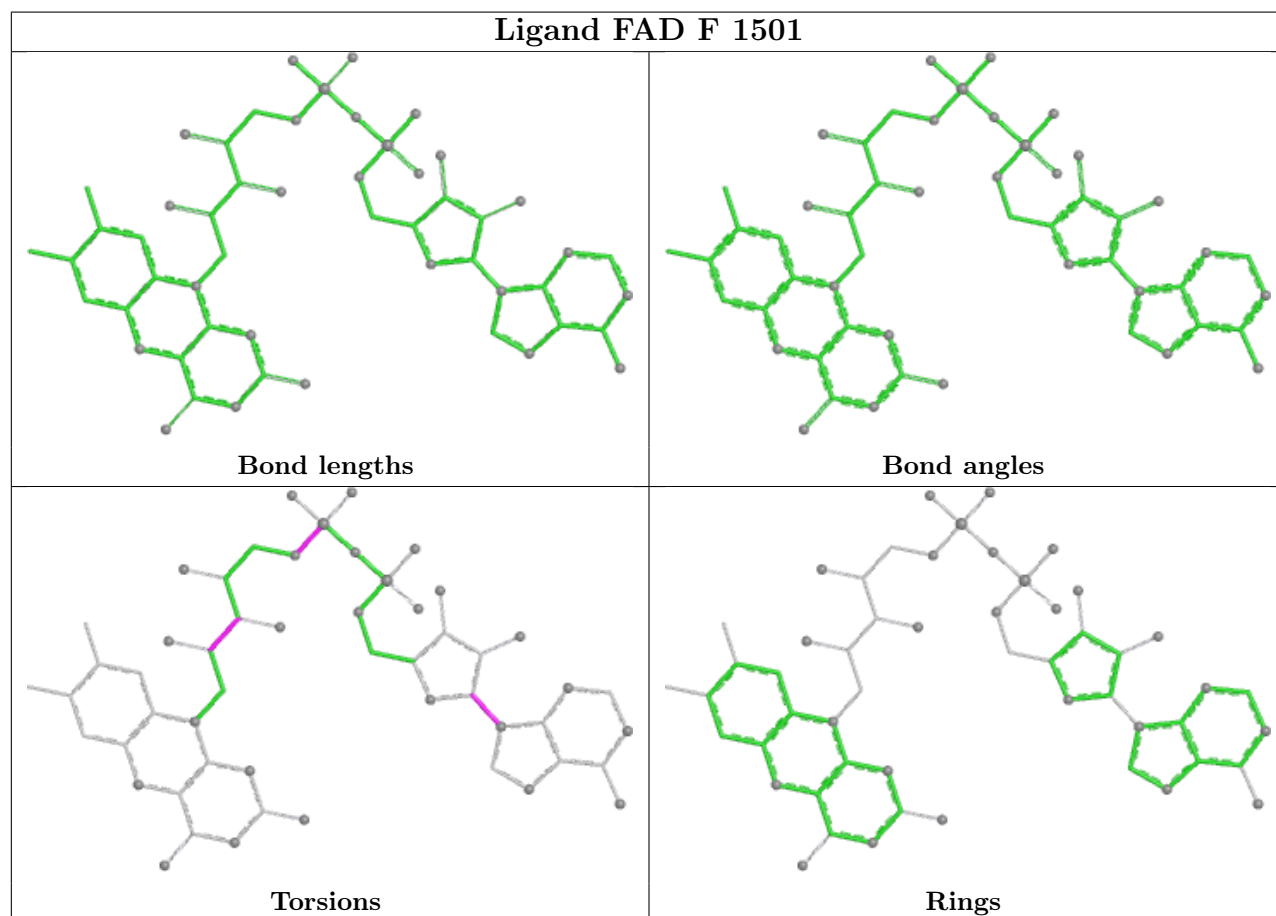
Mol	Chain	Res	Type	Atoms
9	D	301	LMT	O5'-C5'-C6'-O6'
9	D	301	LMT	C6-C7-C8-C9
10	B	504	3PE	O11-C1-C2-O21
10	B	504	3PE	C3D-C3E-C3F-C3G
9	E	201	LMT	O1'-C1-C2-C3
10	B	504	3PE	O11-C1-C2-C3
9	E	201	LMT	C9-C10-C11-C12
9	D	301	LMT	C4B-C5B-C6B-O6B
15	F	1501	FAD	C2B-C1B-N9A-C8A
9	B	503	LMT	C11-C10-C9-C8
9	B	503	LMT	C3'-C4'-O1B-C1B
10	B	504	3PE	C1-O11-P-O12
15	F	1501	FAD	C5'-O5'-P-O3P
10	B	504	3PE	C2-C1-O11-P
10	B	504	3PE	O21-C2-C3-O31
9	E	201	LMT	C3-C4-C5-C6
15	F	1501	FAD	O4B-C1B-N9A-C8A
7	B	501	FMN	C4'-C5'-O5'-P
10	B	504	3PE	C32-C33-C34-C35
9	D	301	LMT	C7-C8-C9-C10
9	D	301	LMT	C2-C1-O1'-C1'
10	B	504	3PE	C21-C22-C23-C24
10	B	504	3PE	C3C-C3D-C3E-C3F
10	B	504	3PE	C3E-C3F-C3G-C3H
10	B	504	3PE	C31-C32-C33-C34
15	F	1501	FAD	C2B-C1B-N9A-C4A
15	F	1501	FAD	O2'-C2'-C3'-C4'
9	E	201	LMT	C1-C2-C3-C4
10	B	504	3PE	C2B-C2C-C2D-C2E

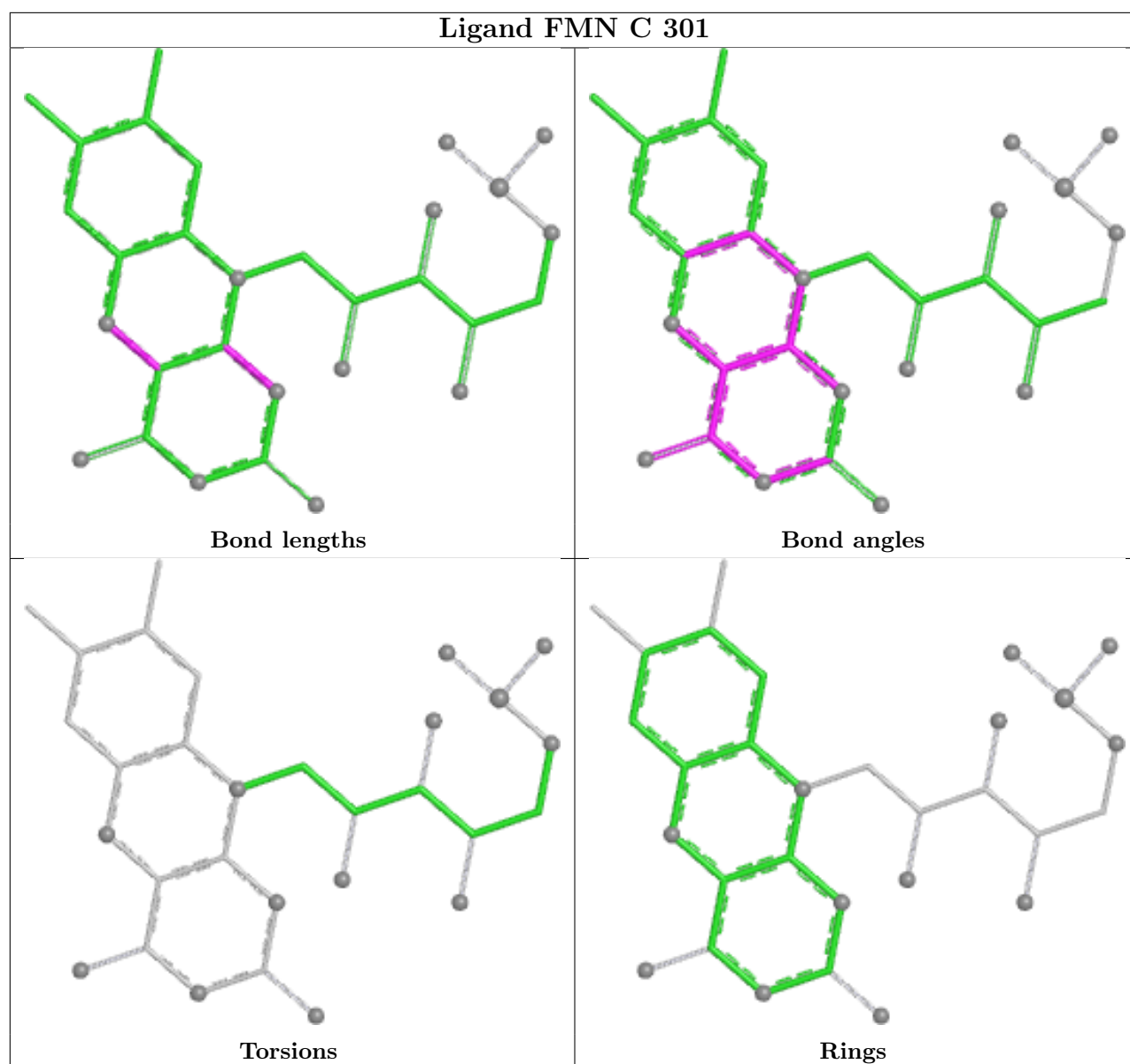
There are no ring outliers.

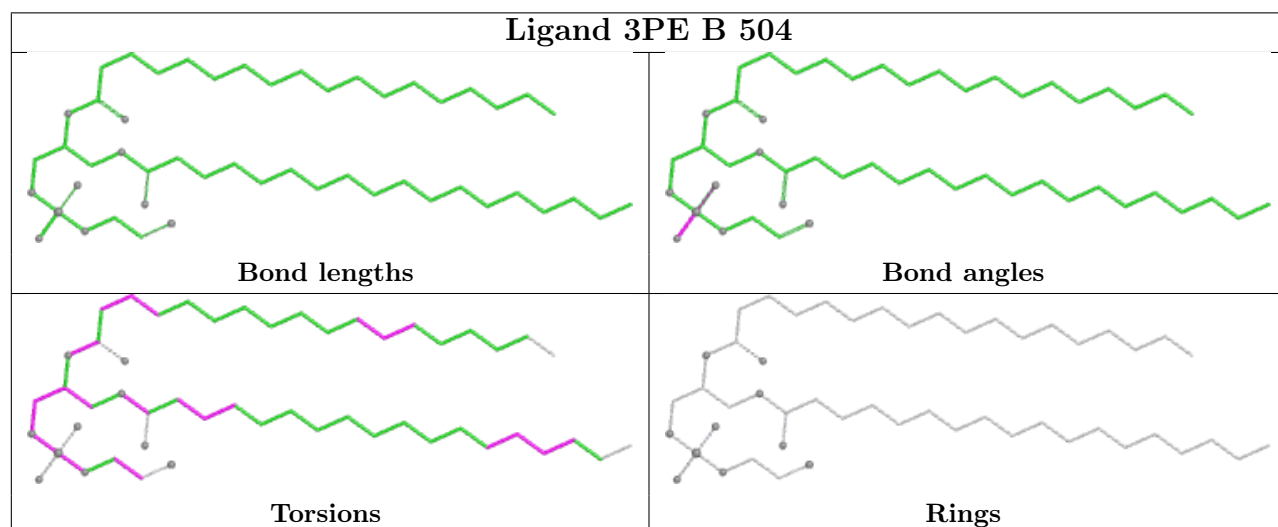
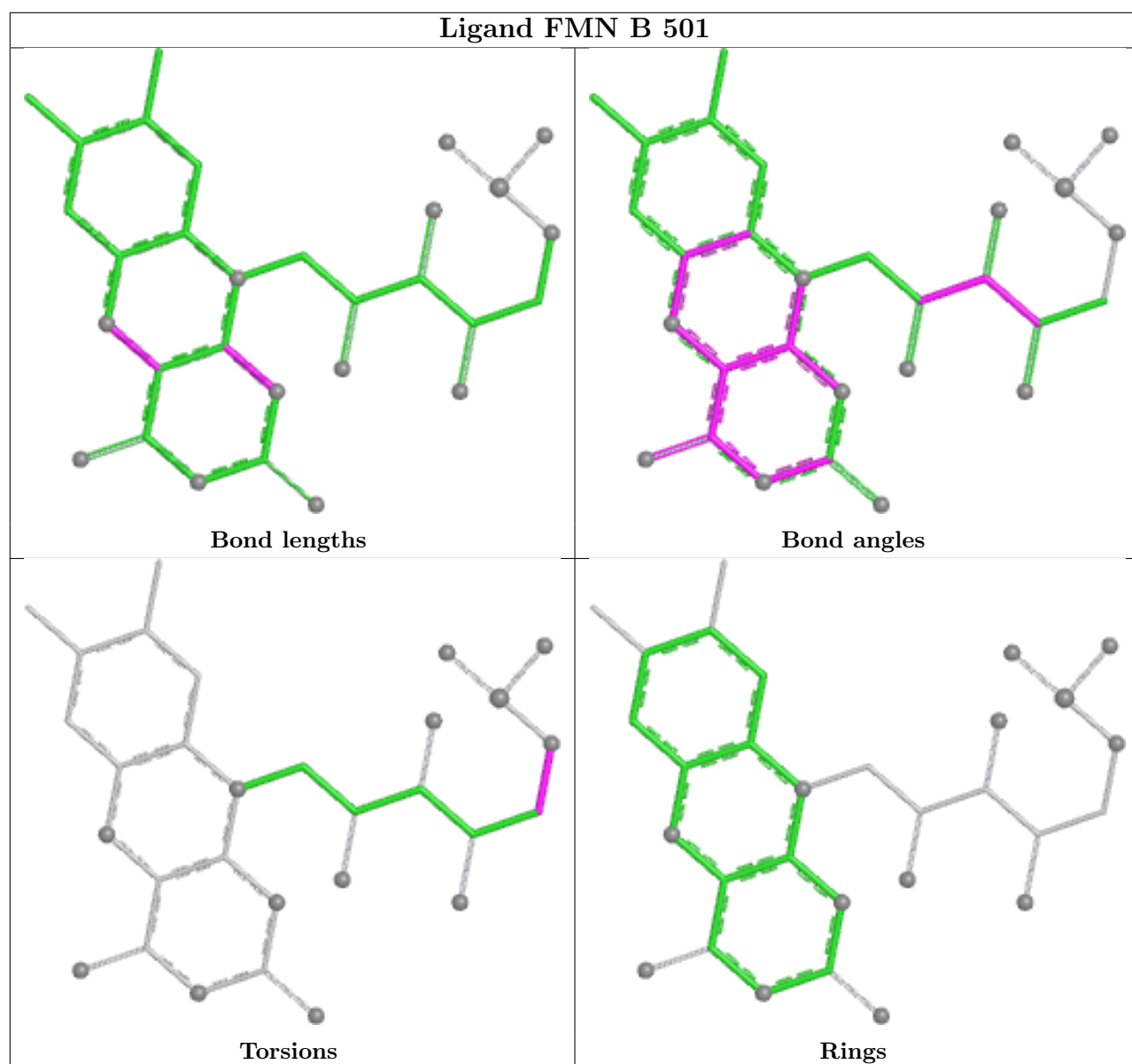
7 monomers are involved in 18 short contacts:

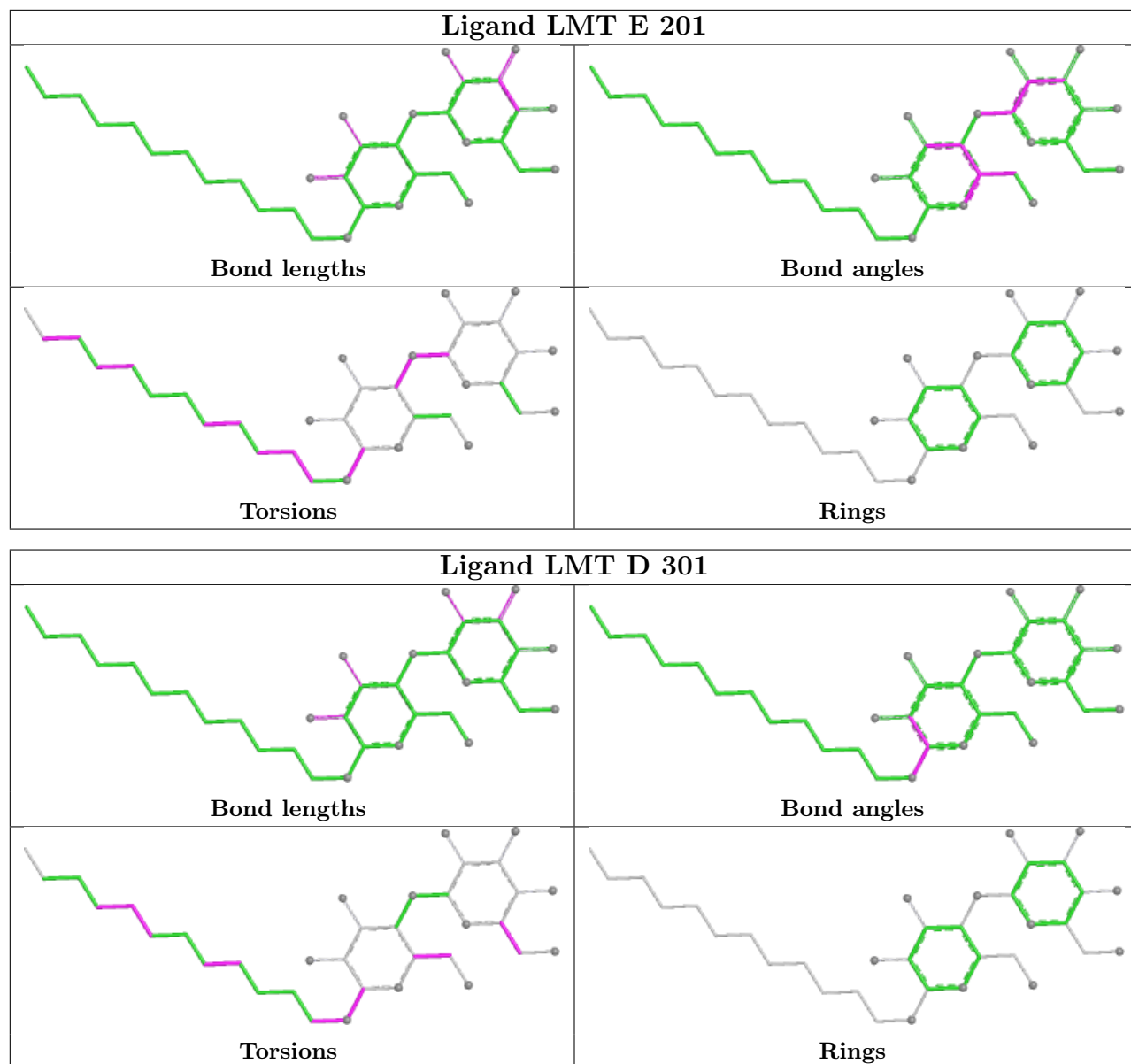
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	1501	FAD	1	0
7	C	301	FMN	6	0
10	B	504	3PE	2	0
9	E	201	LMT	3	0
9	D	301	LMT	2	0
8	B	502	RBF	1	0
9	B	503	LMT	3	0

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.

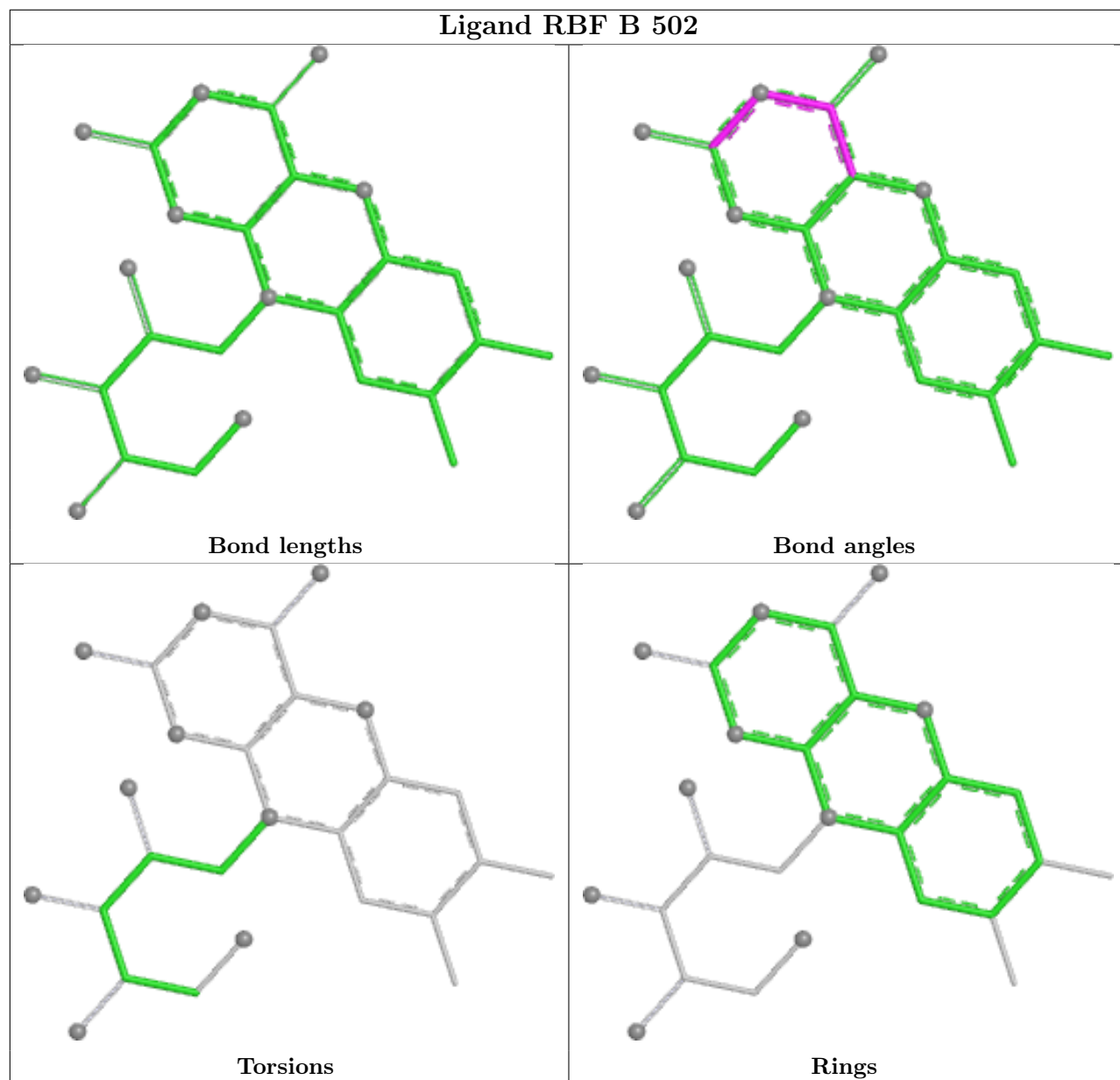


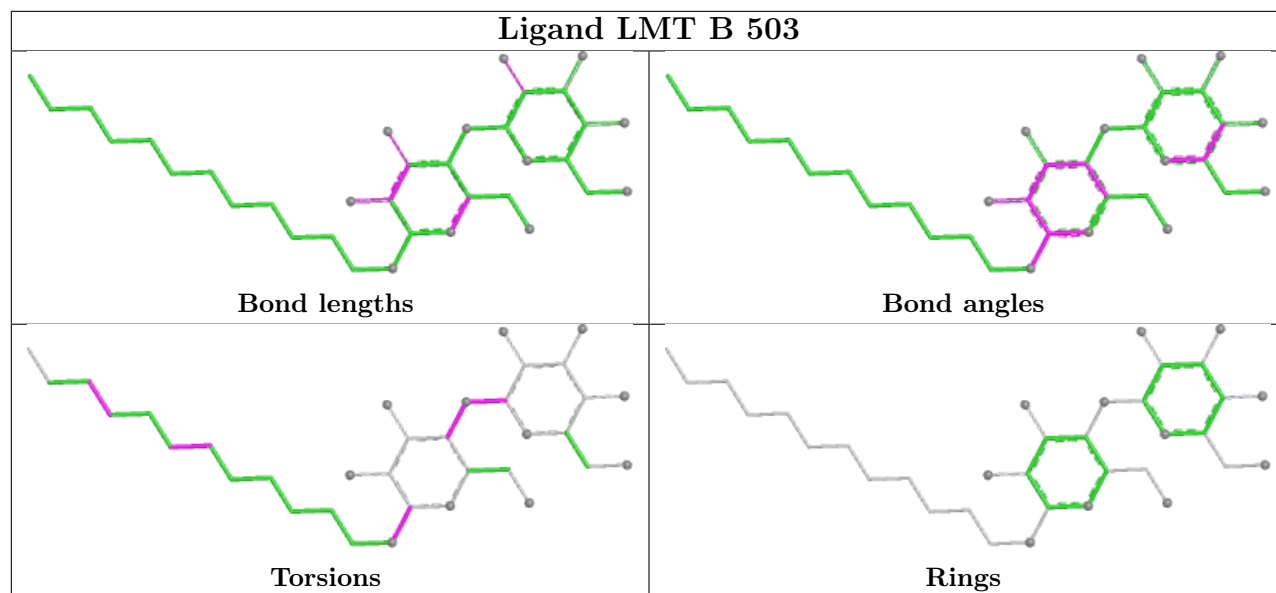






Ligand RBF B 502





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%)	0.11	17 (4%) 40 22	101, 124, 157, 295	0
2	B	384/415 (92%)	0.09	7 (1%) 67 46	103, 145, 199, 244	0
3	C	247/257 (96%)	0.54	25 (10%) 12 6	149, 187, 232, 250	0
4	D	202/210 (96%)	-0.05	3 (1%) 72 52	111, 152, 209, 255	0
5	E	197/198 (99%)	0.20	6 (3%) 52 32	103, 138, 174, 243	0
6	F	406/408 (99%)	0.19	23 (5%) 29 16	101, 150, 191, 224	0
All	All	1839/1956 (94%)	0.17	81 (4%) 39 21	101, 145, 206, 295	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	SER	6.6
1	A	198	LEU	6.2
5	E	194	SER	5.2
6	F	212	TYR	4.7
1	A	207	GLU	4.5
6	F	406	PHE	4.3
6	F	405	ASP	4.3
1	A	106	GLU	4.1
2	B	377	ALA	4.1
3	C	127	VAL	4.0
6	F	379	GLY	4.0
3	C	53	ALA	4.0
3	C	155	VAL	3.8
6	F	150	LEU	3.7
1	A	187	GLY	3.7
3	C	194	LEU	3.7
2	B	378	TYR	3.6
3	C	71	ILE	3.6
6	F	147	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	199	PRO	3.6
6	F	254	ALA	3.5
1	A	377	ILE	3.5
1	A	376	PRO	3.5
3	C	160	ASN	3.4
1	A	107	ALA	3.4
4	D	11	VAL	3.4
6	F	258	CYS	3.3
3	C	137	ILE	3.2
3	C	195	PHE	3.2
3	C	154	ALA	3.1
6	F	152	LEU	3.1
1	A	196	THR	3.1
6	F	381	PRO	3.1
1	A	186	THR	3.0
3	C	125	TYR	3.0
3	C	152	PHE	2.9
2	B	107	MET	2.9
6	F	228	VAL	2.8
6	F	255	GLY	2.8
6	F	137	VAL	2.7
2	B	293	ALA	2.7
1	A	329	GLY	2.7
3	C	49	ILE	2.7
4	D	104	PHE	2.6
5	E	196	VAL	2.6
3	C	248	LEU	2.6
3	C	199	HIS	2.5
3	C	138	LEU	2.5
3	C	136	VAL	2.5
1	A	208	GLU	2.4
6	F	271	ASP	2.3
3	C	239	LEU	2.3
1	A	188	LYS	2.3
3	C	45	LYS	2.3
1	A	195	GLY	2.3
3	C	151	ALA	2.3
3	C	197	GLU	2.3
6	F	209	ILE	2.3
5	E	191	MET	2.3
3	C	196	ASP	2.3
6	F	388	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	198	ASN	2.2
3	C	211	PRO	2.2
4	D	107	LEU	2.2
6	F	384	ASN	2.2
5	E	192	SER	2.1
6	F	353	GLY	2.1
5	E	98	LEU	2.1
6	F	194	LYS	2.1
1	A	144	SER	2.1
1	A	193	LYS	2.1
6	F	385	ALA	2.1
6	F	380	PRO	2.1
2	B	35	TYR	2.1
2	B	336	PHE	2.1
5	E	27	THR	2.1
3	C	67	PHE	2.1
3	C	244	PHE	2.1
2	B	282	ILE	2.0
6	F	139	SER	2.0
6	F	242	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

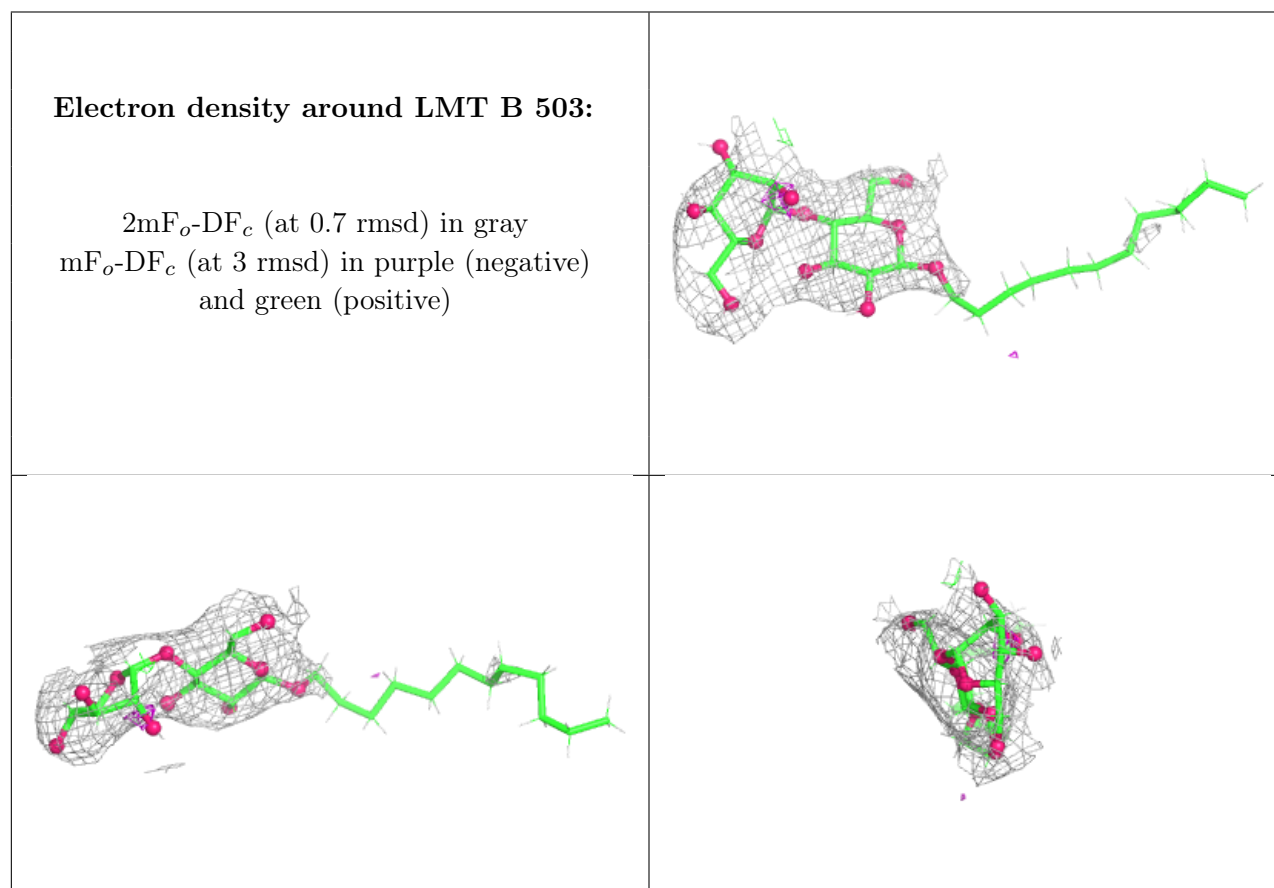
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NA	B	505	1/1	0.50	0.36	127,127,127,127	0
12	K	B	506	1/1	0.63	0.41	133,133,133,133	0
9	LMT	B	503	35/35	0.65	0.14	112,143,171,190	0

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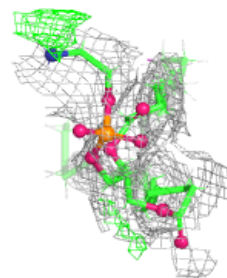
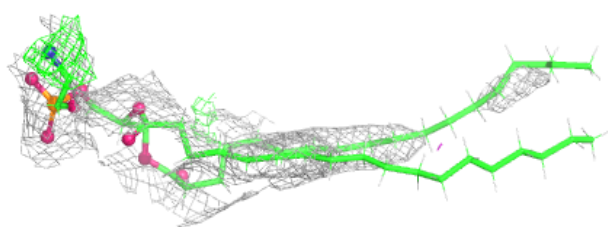
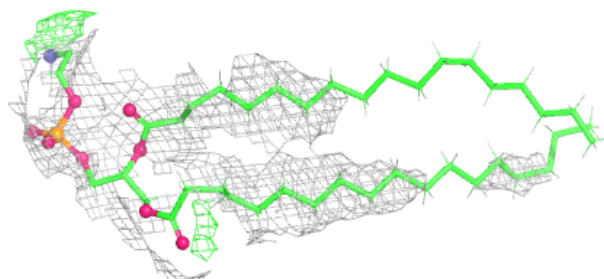
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	3PE	B	504	51/51	0.71	0.20	109,144,197,224	0
9	LMT	D	301	35/35	0.72	0.14	102,140,169,170	0
9	LMT	E	201	35/35	0.82	0.12	96,134,168,179	0
8	RBF	B	502	27/27	0.87	0.12	118,135,166,172	0
15	FAD	F	1501	53/53	0.87	0.12	107,133,163,179	0
7	FMN	C	301	30/31	0.89	0.14	133,164,196,205	0
7	FMN	B	501	30/31	0.93	0.09	109,121,147,151	0
13	BR	C	302	1/1	0.96	0.05	165,165,165,165	0
14	FES	D	302	4/4	0.97	0.05	115,115,117,118	0
14	FES	F	1502	4/4	0.98	0.05	161,162,162,193	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.

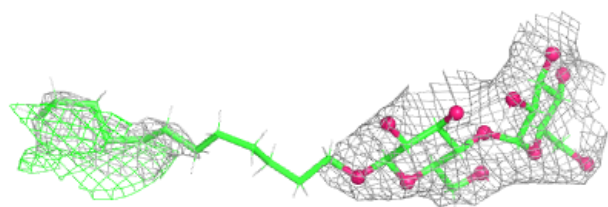
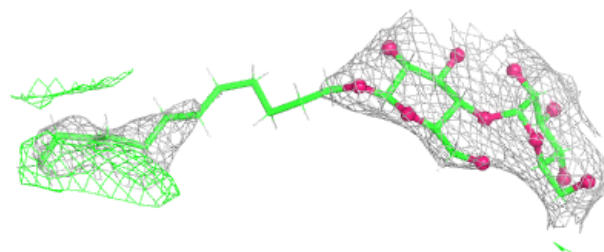


Electron density around 3PE B 504:

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

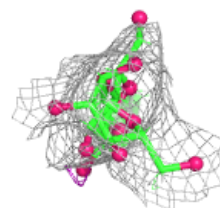
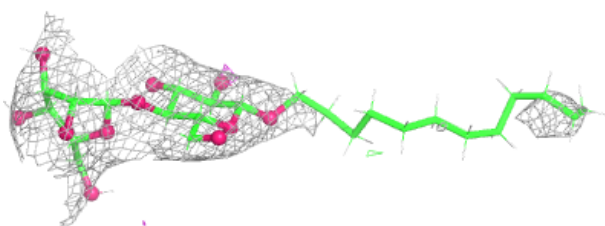
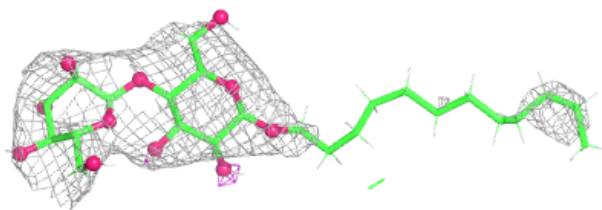
**Electron density around LMT D 301:**

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



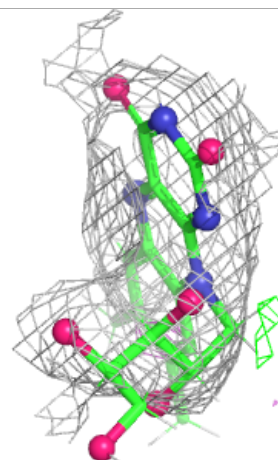
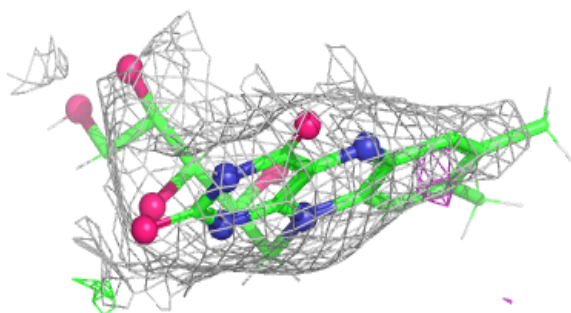
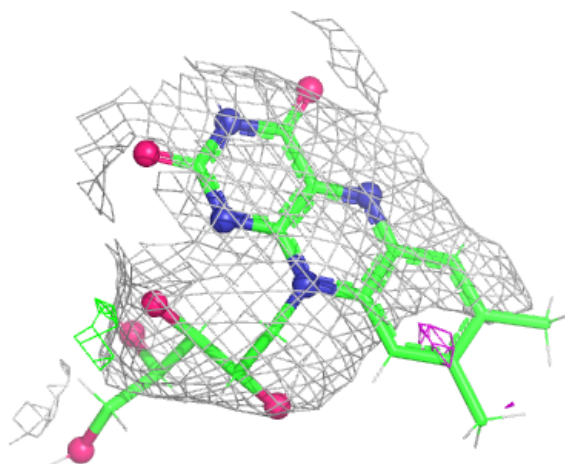
Electron density around LMT E 201:

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



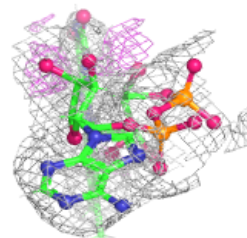
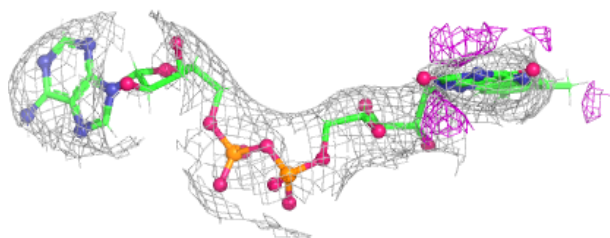
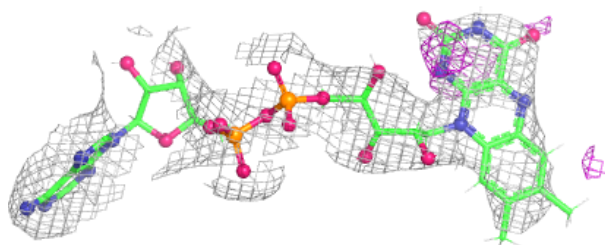
Electron density around RBF B 502:

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

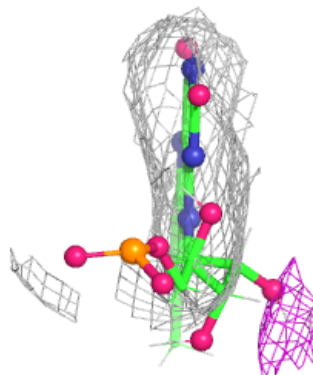
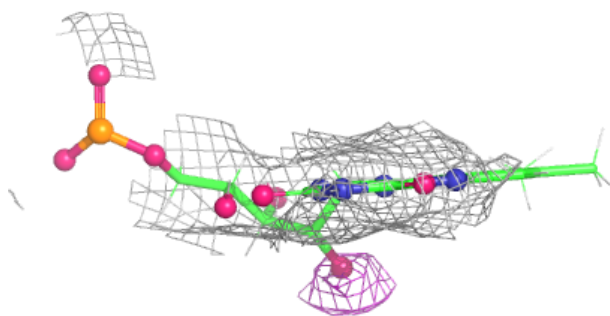
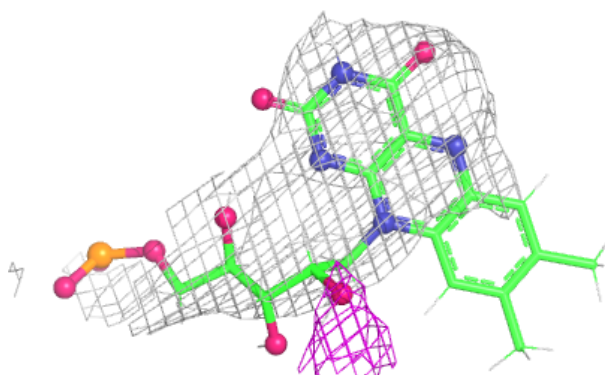


Electron density around FAD F 1501:

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

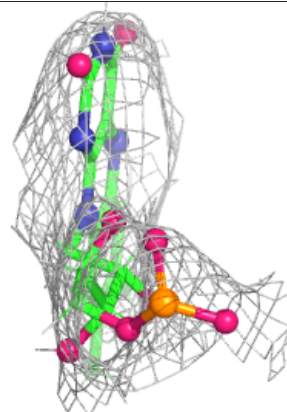
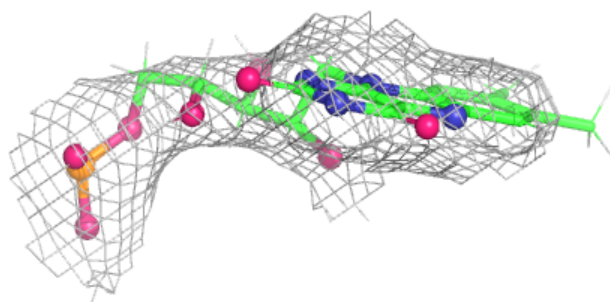
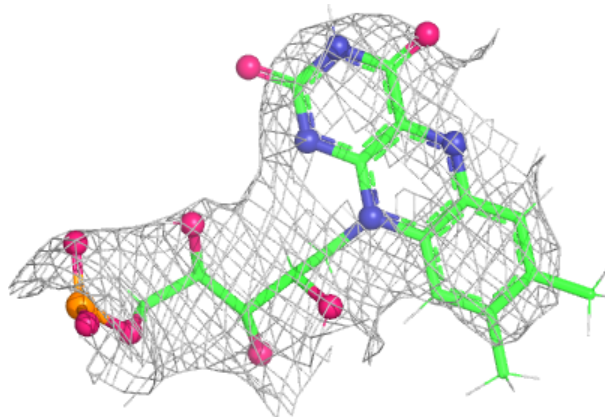
**Electron density around FMN C 301:**

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



Electron density around 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.