



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:01 AM UTC

PDB ID : 8ACY / pdb_00008acy
Title : X-ray structure of Na⁺-NQR from *Vibrio cholerae* at 3.5 Å resolution
Authors : Fritz, G.
Deposited on : 2022-07-07
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

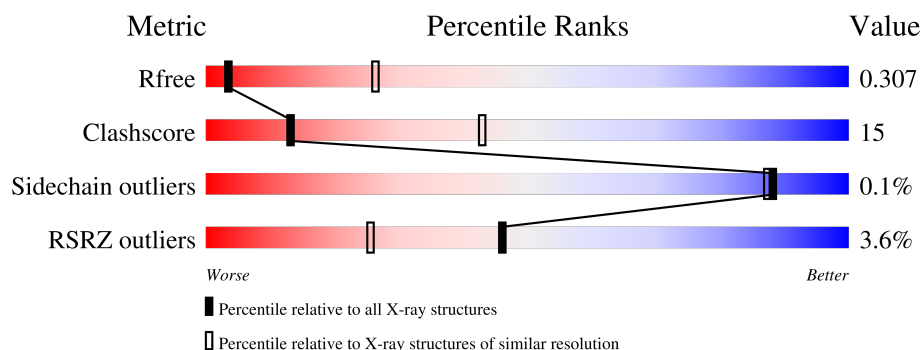
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	
2	B	415	
3	C	257	
4	D	210	
5	E	198	
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
11	FES	F	1502	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28808 atoms, of which 14464 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	6191	1946	3121	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	380	Total	C	H	N	O	S	0	0	0
			5818	1924	2907	475	490	22			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S	0	0	0
			3774	1192	1892	324	362	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	204	Total	C	H	N	O	S	0	0	0
			3208	1037	1646	247	268	10			

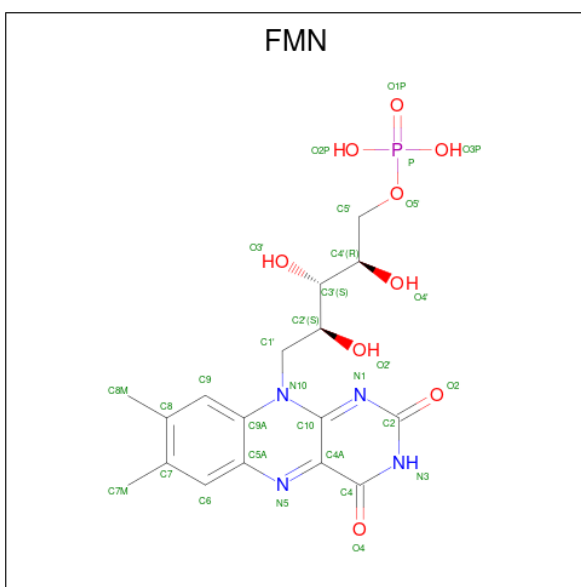
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

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.

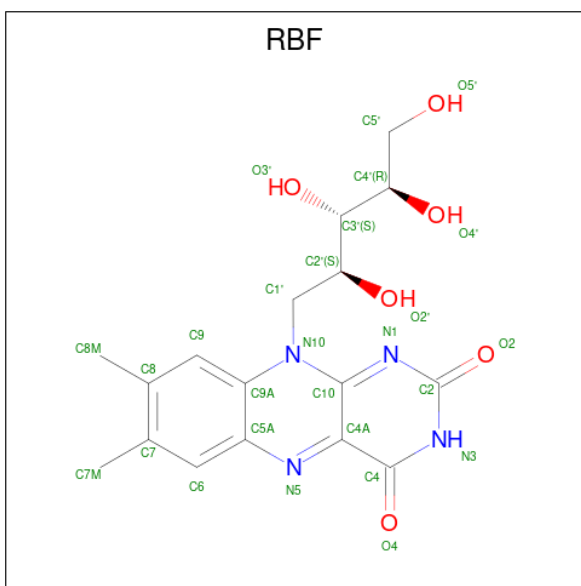
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	407	Total	C	H	N	O	S	0	0	0
			6259	2025	3098	518	594	24			

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



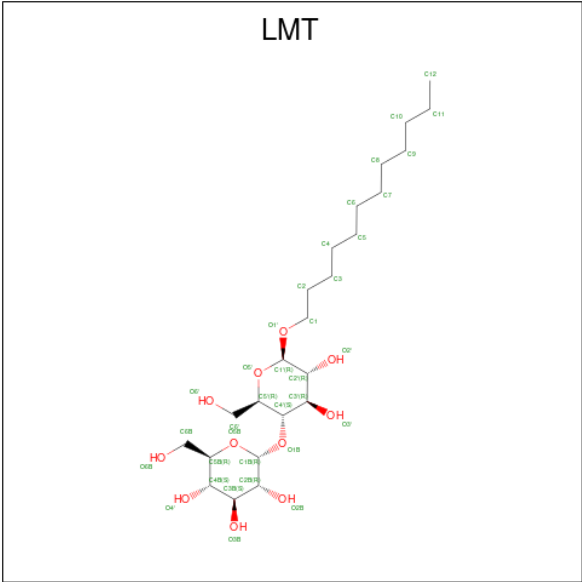
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	B	1	Total	C	H	N	O	P	0	0
			49	17	19	4	8	1		
7	C	1	Total	C	H	N	O	P	0	0
			49	17	19	4	8	1		

- 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: $C_{24}H_{46}O_{11}$).

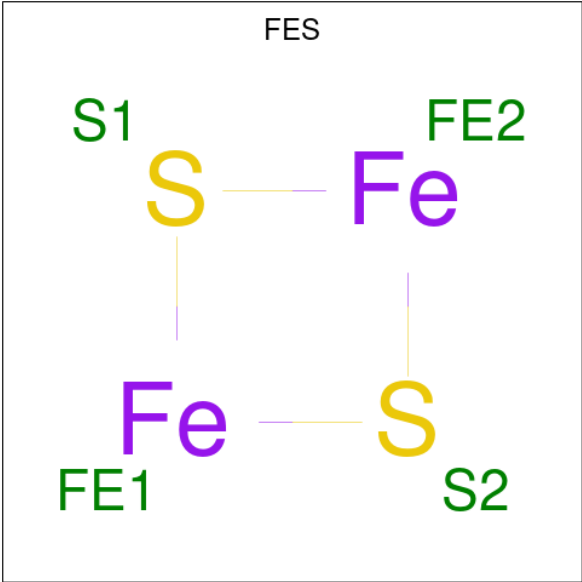


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			81	24	46	11		
9	B	1	Total	C	H	O	0	0
			81	24	46	11		
9	D	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

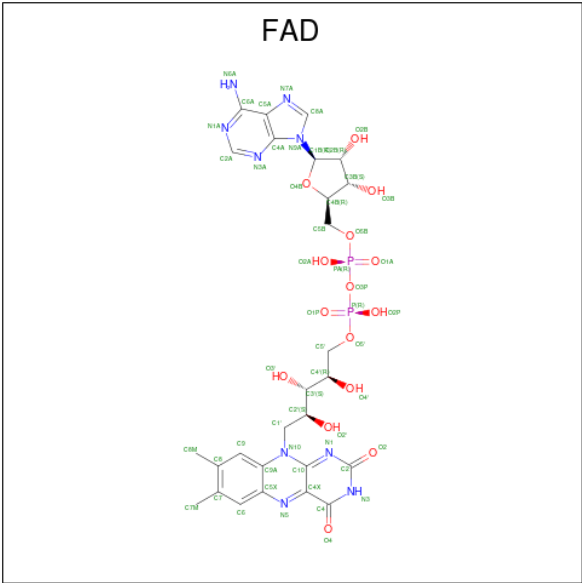
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Na	0	0
			1	1		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

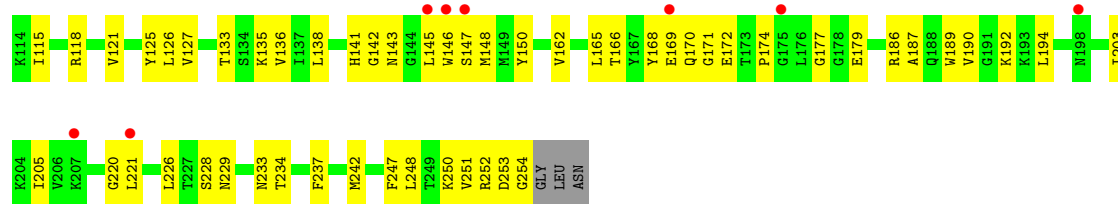


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	Fe	S	0	0
			4	2	2		
11	F	1	Total	Fe	S	0	0
			4	2	2		

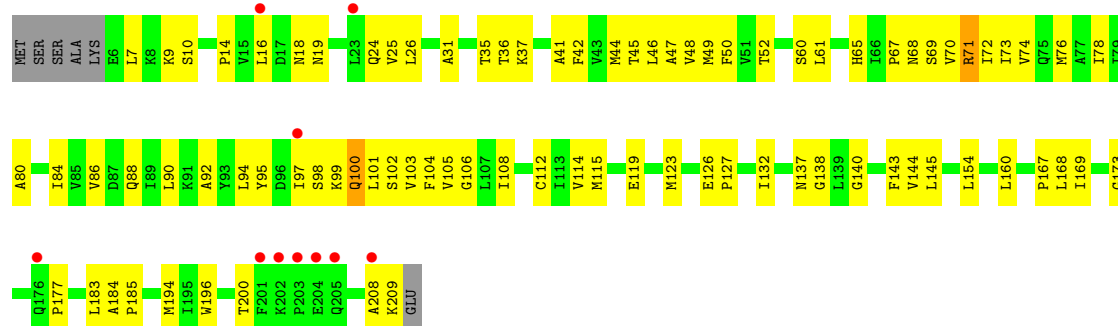
- Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



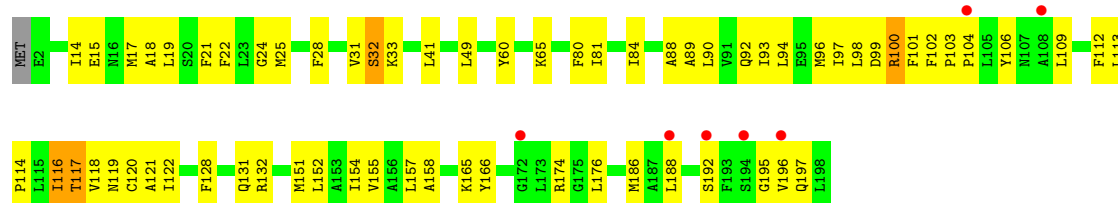
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		



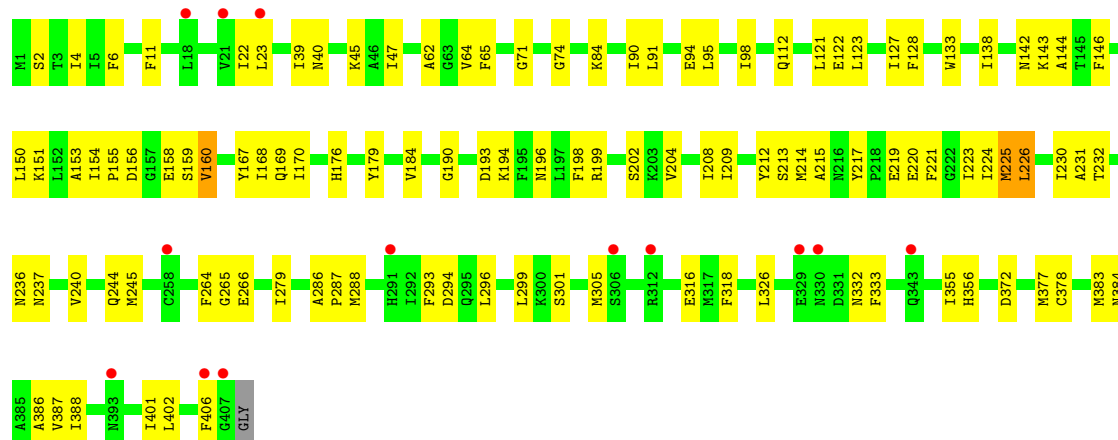
• Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D



• 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	95.27Å 143.32Å 104.37Å 90.00° 110.98° 90.00°	Depositor
Resolution (Å)	48.73 – 3.50 48.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.73-3.50) 99.5 (48.73-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.266 , 0.290 (Not available) , 0.307	Depositor DCC
R_{free} test set	1647 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	165.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 103.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	28808	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: NA, FMN, FAD, LMT, RBF, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/3124	0.61	1/4236 (0.0%)
2	B	0.23	0/2998	0.61	2/4083 (0.0%)
3	C	0.29	0/1914	0.77	0/2583
4	D	0.31	0/1594	0.89	2/2164 (0.1%)
5	E	0.36	0/1537	0.94	7/2084 (0.3%)
6	F	0.28	0/3239	0.73	4/4384 (0.1%)
All	All	0.28	0/14406	0.73	16/19534 (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
4	D	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	117	THR	N-CA-C	-6.68	100.54	110.23
1	A	133	THR	N-CA-C	-6.51	99.03	109.96
5	E	132	ARG	N-CA-C	-5.97	101.09	109.69
6	F	226	LEU	N-CA-C	-5.83	99.84	108.99
2	B	244	GLY	N-CA-C	-5.45	100.26	113.18
5	E	116	ILE	N-CA-C	-5.41	105.26	110.72
6	F	225	MET	N-CA-CB	5.39	117.94	110.17
2	B	45	SER	N-CA-C	-5.37	102.09	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	100	GLN	CA-C-N	-5.31	111.84	120.72
4	D	100	GLN	C-N-CA	-5.31	111.84	120.72
5	E	33	LYS	N-CA-C	5.24	116.67	111.07
6	F	236	ASN	CB-CA-C	-5.10	99.93	109.72
5	E	100	ARG	N-CA-C	-5.04	107.27	113.41
6	F	160	VAL	N-CA-C	5.04	113.88	108.95
5	E	112	PHE	CA-C-N	-5.01	113.54	120.26
5	E	112	PHE	C-N-CA	-5.01	113.54	120.26

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	208	ALA	Peptide
5	E	32	SER	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	3121	3123	45	2
2	B	2911	2907	2907	69	0
3	C	1882	1892	1892	72	0
4	D	1562	1646	1648	91	0
5	E	1504	1574	1574	105	0
6	F	3161	3098	3098	95	2
7	B	30	19	19	5	0
7	C	30	19	19	1	0
8	B	27	19	20	2	0
9	B	70	92	84	8	0
9	D	35	46	43	1	0
10	B	1	0	0	0	0
11	E	4	0	0	0	0
11	F	4	0	0	2	0
12	F	53	31	31	3	0
All	All	14344	14464	14458	428	2

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 15.

All (428) 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)
5:E:98:LEU:HD12	5:E:113:LEU:HD11	1.12	1.07
5:E:98:LEU:HD12	5:E:113:LEU:CD1	1.93	0.98
6:F:388:ILE:HD13	6:F:401:ILE:HD13	1.47	0.97
5:E:28:PHE:O	5:E:32:SER:OG	1.80	0.96
5:E:98:LEU:CD1	5:E:113:LEU:HD11	1.99	0.93
6:F:213:SER:O	6:F:226:LEU:HD12	1.71	0.89
5:E:98:LEU:O	5:E:102:PHE:N	2.09	0.85
5:E:117:THR:O	5:E:118:VAL:HG22	1.80	0.82
5:E:98:LEU:CD1	5:E:113:LEU:CD1	2.58	0.80
3:C:118:ARG:NH1	3:C:242:MET:O	2.14	0.80
3:C:252:ARG:O	3:C:252:ARG:NH1	2.13	0.80
1:A:433:GLN:OE1	2:B:40:VAL:HG13	1.81	0.79
6:F:244:GLN:NE2	12:F:1501:FAD:O1A	2.16	0.79
4:D:72:ILE:HG22	5:E:88:ALA:HB1	1.64	0.79
3:C:162:VAL:HG12	3:C:192:LYS:O	1.83	0.78
5:E:41:LEU:HD11	5:E:116:ILE:HD11	1.65	0.78
6:F:355:ILE:HD11	6:F:383:MET:SD	2.25	0.76
6:F:138:ILE:HD11	6:F:153:ALA:HB2	1.68	0.76
4:D:69:SER:O	5:E:92:GLN:NE2	2.19	0.75
5:E:103:PRO:HD2	5:E:104:PRO:HD2	1.67	0.75
5:E:99:ASP:O	5:E:100:ARG:NH2	2.20	0.74
4:D:61:LEU:HD23	4:D:127:PRO:HG2	1.69	0.74
3:C:145:LEU:HD22	3:C:146:TRP:NE1	2.03	0.74
5:E:113:LEU:HB3	5:E:114:PRO:HD3	1.68	0.74
1:A:34:GLU:HB2	2:B:39:LEU:HD13	1.70	0.74
4:D:26:LEU:HD22	4:D:112:CYS:HB3	1.68	0.74
9:B:503:LMT:O5B	9:B:503:LMT:O3'	2.06	0.73
4:D:90:LEU:HD12	4:D:101:LEU:HD11	1.67	0.73
1:A:134:ARG:HG3	1:A:230:VAL:HG21	1.70	0.73
3:C:145:LEU:HD23	5:E:128:PHE:HE1	1.54	0.72
5:E:98:LEU:O	5:E:100:ARG:N	2.23	0.72
1:A:392:LEU:HD13	2:B:401:VAL:HG21	1.73	0.71
5:E:114:PRO:O	5:E:117:THR:HG22	1.91	0.70
5:E:102:PHE:HB2	5:E:106:TYR:HB2	1.72	0.69
1:A:72:VAL:HG21	1:A:94:VAL:HG22	1.74	0.69
3:C:33:LEU:HB3	4:D:92:ALA:HB2	1.74	0.69
5:E:28:PHE:HA	5:E:154:ILE:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:LEU:HD21	4:D:143:PHE:CE2	2.28	0.69
2:B:336:PHE:HA	2:B:382:MET:HE3	1.75	0.68
4:D:90:LEU:O	4:D:98:SER:OG	2.11	0.68
1:A:374:MET:HG3	1:A:395:ARG:HD3	1.76	0.67
3:C:145:LEU:HD12	3:C:226:LEU:HB2	1.75	0.67
4:D:72:ILE:HB	5:E:92:GLN:OE1	1.94	0.67
6:F:90:ILE:HG21	6:F:95:LEU:HD21	1.77	0.66
5:E:119:ASN:HB3	5:E:122:ILE:HG12	1.77	0.66
6:F:168:ILE:HD13	6:F:224:ILE:HG21	1.78	0.66
4:D:80:ALA:HB3	5:E:81:ILE:HD12	1.77	0.66
6:F:232:THR:O	12:F:1501:FAD:O3B	2.14	0.65
6:F:194:LYS:HA	6:F:194:LYS:HE3	1.77	0.65
4:D:72:ILE:HG21	5:E:117:THR:HG21	1.78	0.65
4:D:61:LEU:HD23	4:D:127:PRO:CG	2.25	0.65
5:E:98:LEU:C	5:E:102:PHE:HB3	2.21	0.65
1:A:433:GLN:CD	2:B:40:VAL:HG13	2.23	0.64
5:E:98:LEU:O	5:E:101:PHE:N	2.30	0.64
3:C:127:VAL:HB	3:C:135:LYS:HG3	1.79	0.64
6:F:159:SER:HB3	6:F:221:PHE:HB2	1.79	0.64
5:E:24:GLY:HA2	5:E:119:ASN:OD1	1.96	0.64
6:F:90:ILE:HD11	6:F:94:GLU:HB3	1.79	0.64
1:A:43:MET:HE2	1:A:79:ILE:HD13	1.78	0.64
3:C:250:LYS:O	3:C:253:ASP:OD1	2.15	0.64
2:B:213:PHE:HA	2:B:220:ILE:HG21	1.80	0.63
4:D:72:ILE:HG12	4:D:115:MET:HE1	1.80	0.63
3:C:253:ASP:OD1	3:C:254:GLY:N	2.31	0.63
6:F:219:GLU:O	6:F:221:PHE:HD1	1.81	0.63
1:A:133:THR:O	1:A:137:SER:N	2.31	0.63
3:C:145:LEU:HD22	3:C:146:TRP:CE2	2.33	0.63
6:F:40:ASN:N	6:F:121:LEU:O	2.29	0.62
1:A:133:THR:O	1:A:137:SER:HA	1.99	0.62
2:B:274:GLU:OE1	7:B:501:FMN:O3'	2.17	0.62
5:E:118:VAL:HG23	5:E:118:VAL:O	1.97	0.62
4:D:44:MET:HE2	4:D:104:PHE:CE2	2.35	0.62
3:C:143:ASN:HB2	3:C:148:MET:HE2	1.81	0.61
6:F:160:VAL:HG21	6:F:224:ILE:HD11	1.82	0.61
3:C:141:HIS:HB3	3:C:150:TYR:CD2	2.35	0.61
6:F:212:TYR:HB3	6:F:226:LEU:HD11	1.82	0.61
1:A:392:LEU:CD1	2:B:401:VAL:HG21	2.30	0.61
4:D:72:ILE:CG2	5:E:117:THR:HG21	2.30	0.61
5:E:99:ASP:HA	5:E:102:PHE:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:SER:OG	4:D:132:ILE:HG21	2.01	0.60
1:A:283:LEU:HD12	1:A:309:ALA:CB	2.32	0.60
6:F:40:ASN:HA	6:F:122:GLU:HA	1.83	0.60
2:B:375:ASN:ND2	5:E:192:SER:O	2.34	0.60
6:F:212:TYR:CB	6:F:226:LEU:HD21	2.32	0.60
5:E:103:PRO:CD	5:E:104:PRO:HD2	2.32	0.60
1:A:374:MET:CG	1:A:395:ARG:HD3	2.32	0.60
3:C:115:ILE:HG22	3:C:148:MET:HE1	1.83	0.59
2:B:236:THR:HG21	7:B:501:FMN:C5'	2.33	0.59
6:F:160:VAL:CG2	6:F:224:ILE:HD11	2.33	0.59
3:C:179:GLU:HB2	3:C:221:LEU:HD12	1.85	0.58
2:B:308:LEU:HD23	2:B:369:VAL:HB	1.85	0.58
6:F:384:ASN:O	6:F:388:ILE:HG22	2.03	0.58
4:D:169:ILE:HG13	4:D:173:GLY:O	2.04	0.58
2:B:272:ILE:O	2:B:272:ILE:HG23	2.03	0.58
3:C:145:LEU:HD12	3:C:226:LEU:HD12	1.86	0.57
3:C:170:GLN:OE1	3:C:172:GLU:N	2.37	0.57
2:B:395:LEU:HD21	9:B:503:LMT:H41	1.87	0.57
3:C:145:LEU:HD23	5:E:128:PHE:CE1	2.38	0.57
6:F:293:PHE:CE1	6:F:326:LEU:HD11	2.40	0.57
1:A:43:MET:CE	1:A:79:ILE:HD13	2.35	0.56
1:A:134:ARG:CG	1:A:230:VAL:HG21	2.35	0.56
2:B:237:ALA:HB1	2:B:249:LEU:HD21	1.88	0.56
2:B:129:PHE:HB2	2:B:272:ILE:HD13	1.88	0.56
3:C:145:LEU:CD1	3:C:226:LEU:HD12	2.36	0.56
4:D:41:ALA:O	4:D:45:THR:HG23	2.05	0.56
2:B:238:LEU:HB2	7:B:501:FMN:O1P	2.07	0.55
6:F:156:ASP:OD1	6:F:158:GLU:N	2.36	0.55
6:F:214:MET:HE1	6:F:224:ILE:HD12	1.89	0.55
5:E:14:ILE:CG1	5:E:196:VAL:HG11	2.36	0.55
5:E:14:ILE:HG12	5:E:196:VAL:HG11	1.88	0.55
6:F:196:ASN:HB2	6:F:199:ARG:CZ	2.36	0.55
6:F:215:ALA:O	6:F:225:MET:HE3	2.06	0.55
6:F:223:ILE:O	6:F:223:ILE:HG13	2.07	0.55
3:C:126:LEU:HD23	3:C:136:VAL:HG13	1.89	0.55
4:D:126:GLU:OE1	4:D:126:GLU:HA	2.07	0.55
5:E:93:ILE:O	5:E:97:ILE:HG13	2.07	0.55
3:C:99:GLU:O	3:C:103:SER:OG	2.22	0.54
3:C:113:ALA:HA	3:C:233:ASN:HB3	1.89	0.54
5:E:31:VAL:HG21	5:E:41:LEU:HD22	1.89	0.54
2:B:327:TRP:CD1	9:B:504:LMT:H12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:ILE:HG21	3:C:228:SER:HB2	1.88	0.54
4:D:76:MET:HE3	5:E:118:VAL:CG1	2.37	0.54
6:F:159:SER:HB3	6:F:221:PHE:CB	2.38	0.54
4:D:168:LEU:HD22	4:D:177:PRO:HG3	1.90	0.54
3:C:44:ASP:OD2	4:D:99:LYS:NZ	2.40	0.54
4:D:97:ILE:O	4:D:100:GLN:HB2	2.07	0.54
5:E:117:THR:O	5:E:118:VAL:CG2	2.55	0.54
1:A:133:THR:O	1:A:137:SER:CA	2.56	0.54
3:C:165:LEU:HD22	3:C:189:TRP:CD2	2.42	0.54
1:A:37:VAL:HG12	1:A:138:LYS:HE3	1.90	0.54
6:F:64:VAL:HG21	6:F:123:LEU:HD12	1.89	0.54
6:F:179:TYR:OH	6:F:231:ALA:O	2.26	0.54
9:B:504:LMT:O2B	9:B:504:LMT:H5B	2.08	0.54
4:D:72:ILE:HG23	4:D:115:MET:HE1	1.89	0.53
5:E:90:LEU:O	5:E:93:ILE:HG12	2.08	0.53
6:F:90:ILE:CG2	6:F:95:LEU:HD21	2.39	0.53
4:D:76:MET:HE3	5:E:118:VAL:HG11	1.90	0.53
1:A:97:ASP:OD1	1:A:97:ASP:O	2.26	0.53
6:F:71:GLY:O	11:F:1502:FES:S2	2.67	0.53
2:B:246:ALA:O	2:B:249:LEU:HB2	2.07	0.53
5:E:32:SER:O	5:E:158:ALA:HA	2.09	0.53
6:F:156:ASP:OD1	6:F:156:ASP:C	2.50	0.53
1:A:10:LEU:CD2	2:B:47:VAL:HG21	2.39	0.53
1:A:291:ILE:HG21	1:A:296:VAL:HG21	1.90	0.53
3:C:113:ALA:HB2	3:C:237:PHE:HB3	1.91	0.53
6:F:133:TRP:HB3	6:F:154:ILE:CD1	2.39	0.53
4:D:47:ALA:HB1	4:D:108:ILE:HD13	1.89	0.53
4:D:168:LEU:CD2	4:D:177:PRO:HG3	2.39	0.53
2:B:241:TRP:CH2	2:B:246:ALA:HB2	2.44	0.53
4:D:74:VAL:O	4:D:78:ILE:HG12	2.09	0.53
4:D:168:LEU:O	4:D:173:GLY:N	2.42	0.52
2:B:329:TRP:O	2:B:333:LEU:HG	2.08	0.52
6:F:170:ILE:O	6:F:209:ILE:HD12	2.09	0.52
5:E:151:MET:HA	5:E:154:ILE:HG22	1.92	0.52
6:F:217:TYR:CE2	6:F:219:GLU:HB2	2.44	0.52
3:C:71:ILE:HG23	3:C:125:TYR:HB3	1.90	0.52
5:E:60:TYR:O	5:E:65:LYS:N	2.43	0.52
5:E:89:ALA:HA	6:F:22:ILE:HD11	1.90	0.52
6:F:220:GLU:HB3	6:F:223:ILE:HD11	1.92	0.52
1:A:216:PRO:HG3	1:A:420:LEU:HD12	1.91	0.52
6:F:47:ILE:HD12	6:F:62:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:O	2:B:272:ILE:O	2.28	0.52
3:C:18:LEU:HD11	4:D:78:ILE:HD11	1.92	0.52
6:F:169:GLN:HB3	6:F:209:ILE:HD11	1.91	0.52
4:D:72:ILE:HG12	4:D:115:MET:CE	2.40	0.52
2:B:260:TRP:HA	2:B:329:TRP:CH2	2.45	0.52
1:A:1:MET:HA	1:A:1:MET:HE2	1.91	0.51
1:A:135:PRO:O	1:A:136:PHE:CD1	2.64	0.51
3:C:143:ASN:OD1	5:E:131:GLN:NE2	2.41	0.51
1:A:149:ILE:HD12	1:A:185:THR:HB	1.90	0.51
2:B:370:LEU:O	2:B:374:VAL:HG22	2.11	0.51
5:E:98:LEU:C	5:E:100:ARG:N	2.69	0.51
2:B:371:ILE:HD11	5:E:192:SER:HB2	1.93	0.51
3:C:145:LEU:HD22	3:C:146:TRP:CD1	2.45	0.51
1:A:135:PRO:HA	1:A:411:LEU:O	2.11	0.51
6:F:196:ASN:CG	6:F:199:ARG:NH2	2.69	0.51
2:B:368:CYS:SG	2:B:382:MET:HE2	2.51	0.51
6:F:212:TYR:CB	6:F:226:LEU:HD11	2.41	0.51
3:C:33:LEU:O	3:C:37:GLN:HG3	2.11	0.51
2:B:54:LYS:HD3	2:B:157:GLU:HG2	1.93	0.51
4:D:72:ILE:HG22	5:E:88:ALA:CB	2.38	0.51
5:E:99:ASP:CA	5:E:102:PHE:HB3	2.40	0.51
6:F:286:ALA:HB3	6:F:287:PRO:CD	2.41	0.51
5:E:117:THR:C	5:E:118:VAL:HG13	2.36	0.50
1:A:32:LEU:HD23	1:A:89:SER:HB3	1.93	0.50
3:C:150:TYR:HB3	3:C:168:TYR:CZ	2.46	0.50
6:F:74:GLY:HA2	11:F:1502:FES:S1	2.52	0.50
1:A:428:LYS:NZ	2:B:51:VAL:O	2.38	0.50
4:D:42:PHE:CE1	4:D:46:LEU:HD11	2.45	0.50
4:D:60:SER:HB2	4:D:127:PRO:HG3	1.94	0.50
5:E:102:PHE:HD2	5:E:106:TYR:HB3	1.75	0.50
4:D:80:ALA:HB3	5:E:81:ILE:CD1	2.42	0.50
4:D:73:ILE:HD13	5:E:88:ALA:HB3	1.94	0.50
4:D:184:ALA:HB3	5:E:22:PHE:CZ	2.46	0.50
6:F:168:ILE:CD1	6:F:224:ILE:HG21	2.42	0.50
1:A:428:LYS:HD2	2:B:48:ARG:HD2	1.93	0.49
3:C:30:ALA:O	3:C:34:ARG:HB2	2.12	0.49
4:D:44:MET:HE2	4:D:104:PHE:CD2	2.47	0.49
1:A:283:LEU:HD12	1:A:309:ALA:HB2	1.94	0.49
3:C:77:ASP:O	3:C:81:GLY:N	2.41	0.49
6:F:196:ASN:CB	6:F:199:ARG:CZ	2.90	0.49
6:F:221:PHE:N	6:F:221:PHE:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:LEU:C	5:E:100:ARG:H	2.20	0.49
5:E:102:PHE:CD1	5:E:103:PRO:HD3	2.47	0.49
2:B:64:VAL:HG12	2:B:342:PHE:CD2	2.47	0.49
5:E:96:MET:O	5:E:99:ASP:HB2	2.12	0.49
3:C:31:VAL:HB	6:F:4:ILE:HD11	1.94	0.49
5:E:19:LEU:HD11	5:E:186:MET:HE2	1.94	0.49
6:F:215:ALA:HB2	6:F:286:ALA:HB1	1.94	0.49
6:F:39:ILE:HB	6:F:45:LYS:HB3	1.95	0.49
6:F:402:LEU:N	6:F:402:LEU:HD12	2.28	0.49
4:D:18:ASN:OD1	4:D:24:GLN:HG3	2.12	0.49
5:E:100:ARG:HA	5:E:100:ARG:NE	2.28	0.49
6:F:65:PHE:O	6:F:127:ILE:HG23	2.12	0.48
9:B:503:LMT:H22	5:E:155:VAL:HG11	1.94	0.48
3:C:172:GLU:HB2	3:C:177:GLY:C	2.39	0.48
4:D:25:VAL:CG2	5:E:176:LEU:HD13	2.44	0.48
4:D:90:LEU:C	4:D:98:SER:OG	2.56	0.48
2:B:392:PHE:CE1	5:E:152:LEU:HD21	2.49	0.48
3:C:45:LYS:HD3	3:C:45:LYS:N	2.29	0.48
2:B:56:ILE:HG23	2:B:292:ILE:HG12	1.96	0.48
3:C:126:LEU:HB3	3:C:133:THR:HG22	1.94	0.48
3:C:50:LEU:HD12	3:C:63:ILE:HG23	1.95	0.47
4:D:19:ASN:OD1	4:D:144:VAL:HG21	2.14	0.47
5:E:99:ASP:N	5:E:102:PHE:HB3	2.29	0.47
2:B:383:MET:O	2:B:387:LEU:HG	2.14	0.47
4:D:31:ALA:O	4:D:35:THR:OG1	2.20	0.47
1:A:278:VAL:HG22	1:A:279:MET:N	2.29	0.47
2:B:343:MET:HA	8:B:502:RBF:O4	2.15	0.47
2:B:54:LYS:CD	2:B:157:GLU:HG2	2.43	0.47
2:B:86:LEU:HD11	2:B:232:TYR:HD1	1.79	0.47
2:B:340:MET:HE3	2:B:341:PHE:CZ	2.50	0.47
4:D:154:LEU:HB2	4:D:160:LEU:HD21	1.97	0.47
4:D:169:ILE:HA	4:D:173:GLY:O	2.15	0.47
6:F:94:GLU:O	6:F:98:ILE:HD12	2.14	0.47
4:D:14:PRO:HB2	4:D:137:ASN:HA	1.97	0.47
4:D:90:LEU:HD23	4:D:94:LEU:HB2	1.96	0.47
4:D:119:GLU:O	4:D:123:MET:HB2	2.15	0.47
6:F:133:TRP:CG	6:F:154:ILE:HD11	2.50	0.47
6:F:144:ALA:HB1	6:F:316:GLU:HA	1.96	0.47
5:E:25:MET:HE2	5:E:25:MET:HA	1.97	0.46
5:E:90:LEU:HA	5:E:93:ILE:HG12	1.97	0.46
4:D:196:TRP:O	4:D:200:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:ILE:N	5:E:92:GLN:OE1	2.45	0.46
5:E:102:PHE:O	5:E:106:TYR:N	2.43	0.46
6:F:91:LEU:HD13	6:F:112:GLN:HG3	1.97	0.46
1:A:384:MET:HE3	1:A:384:MET:HB3	1.87	0.46
4:D:168:LEU:HD22	4:D:177:PRO:CG	2.45	0.46
6:F:143:LYS:HB3	6:F:318:PHE:CG	2.50	0.46
1:A:403:ASP:O	1:A:407:ARG:HG3	2.16	0.46
2:B:241:TRP:CZ2	2:B:246:ALA:HB2	2.50	0.46
5:E:32:SER:OG	5:E:157:LEU:HD23	2.16	0.46
6:F:64:VAL:HG21	6:F:123:LEU:CD1	2.45	0.46
4:D:25:VAL:O	4:D:26:LEU:HD23	2.15	0.46
3:C:21:VAL:HG23	3:C:22:CYS:N	2.31	0.45
4:D:115:MET:SD	5:E:118:VAL:HG11	2.56	0.45
3:C:171:GLY:O	4:D:103:VAL:CG1	2.64	0.45
5:E:41:LEU:HD13	5:E:109:LEU:HD21	1.99	0.45
3:C:91:TYR:OH	3:C:121:VAL:O	2.28	0.45
3:C:253:ASP:OD1	3:C:253:ASP:C	2.60	0.45
4:D:50:PHE:CE1	4:D:86:VAL:HG21	2.51	0.45
5:E:118:VAL:O	5:E:118:VAL:CG2	2.64	0.45
1:A:77:VAL:HG23	1:A:78:GLU:HG2	1.99	0.45
4:D:95:TYR:HE1	4:D:99:LYS:HZ3	1.63	0.45
1:A:61:LYS:NZ	6:F:372:ASP:OD1	2.49	0.45
2:B:274:GLU:OE2	2:B:334:GLY:C	2.60	0.45
2:B:375:ASN:OD1	5:E:195:GLY:HA3	2.16	0.45
4:D:14:PRO:O	4:D:140:GLY:HA3	2.16	0.45
5:E:31:VAL:HG11	5:E:109:LEU:CD2	2.46	0.45
6:F:84:LYS:HE3	6:F:122:GLU:HB2	1.98	0.45
2:B:63:ALA:HB2	2:B:287:ILE:HG23	1.98	0.45
5:E:24:GLY:CA	5:E:119:ASN:OD1	2.65	0.45
1:A:389:GLU:OE1	2:B:353:THR:HG22	2.17	0.45
3:C:40:ASN:HD22	4:D:95:TYR:HB2	1.82	0.45
3:C:138:LEU:HD11	3:C:248:LEU:HD21	1.99	0.45
2:B:370:LEU:C	2:B:370:LEU:HD23	2.41	0.44
5:E:116:ILE:O	5:E:119:ASN:HB2	2.17	0.44
2:B:334:GLY:HA3	2:B:380:GLU:OE1	2.17	0.44
6:F:190:GLY:HA2	6:F:193:ASP:OD2	2.18	0.44
6:F:237:ASN:OD1	6:F:240:VAL:HG23	2.18	0.44
6:F:377:MET:SD	6:F:387:VAL:HG11	2.57	0.44
3:C:44:ASP:OD2	4:D:99:LYS:HE3	2.17	0.44
6:F:2:SER:O	6:F:6:PHE:CD2	2.70	0.44
6:F:265:GLY:C	6:F:266:GLU:HG3	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:HG21	8:B:502:RBF:HC82	1.99	0.44
2:B:238:LEU:HD12	7:B:501:FMN:O1P	2.17	0.44
4:D:25:VAL:HG22	5:E:176:LEU:HD13	2.00	0.44
2:B:82:ALA:HB3	2:B:229:ALA:HB2	1.98	0.44
4:D:184:ALA:N	4:D:185:PRO:CD	2.80	0.44
5:E:99:ASP:HA	5:E:102:PHE:CD1	2.53	0.44
5:E:102:PHE:N	5:E:103:PRO:CD	2.81	0.44
2:B:130:LEU:HB2	2:B:131:PRO:HD3	2.00	0.44
5:E:98:LEU:O	5:E:99:ASP:C	2.61	0.44
2:B:250:ILE:CD1	2:B:257:THR:HG22	2.48	0.44
2:B:274:GLU:CD	7:B:501:FMN:HO3'	2.23	0.44
9:B:504:LMT:O3'	9:B:504:LMT:O5B	2.35	0.44
4:D:52:THR:HG22	4:D:114:VAL:HG22	2.00	0.44
3:C:150:TYR:HB2	3:C:169:GLU:HB3	1.99	0.44
3:C:44:ASP:OD2	4:D:99:LYS:CE	2.66	0.43
4:D:31:ALA:O	4:D:35:THR:CG2	2.65	0.43
6:F:167:TYR:N	6:F:264:PHE:O	2.47	0.43
6:F:279:ILE:CG2	6:F:355:ILE:HD12	2.48	0.43
6:F:286:ALA:HB3	6:F:287:PRO:HD3	2.00	0.43
7:C:1000:FMN:H9	7:C:1000:FMN:H1'1	1.76	0.43
4:D:167:PRO:HB2	4:D:173:GLY:HA3	2.00	0.43
6:F:142:ASN:ND2	6:F:184:VAL:HG13	2.33	0.43
1:A:53:LYS:O	1:A:70:SER:O	2.36	0.43
1:A:374:MET:O	1:A:376:PRO:HD3	2.18	0.43
3:C:174:PRO:HG2	4:D:104:PHE:CE1	2.53	0.43
6:F:179:TYR:HB3	6:F:198:PHE:HA	2.00	0.43
6:F:305:MET:HB3	6:F:333:PHE:HD1	1.84	0.43
4:D:31:ALA:O	4:D:35:THR:HG23	2.18	0.43
4:D:68:ASN:HA	4:D:71:ARG:HG2	1.99	0.43
9:D:301:LMT:O1B	9:D:301:LMT:O6'	2.36	0.43
1:A:99:GLN:OE1	1:A:255:GLU:HB3	2.19	0.43
2:B:86:LEU:CD1	2:B:232:TYR:HB2	2.48	0.43
3:C:60:SER:O	3:C:64:VAL:HG23	2.18	0.43
4:D:49:MET:HG3	4:D:138:GLY:HA3	2.01	0.43
5:E:49:LEU:HG	5:E:122:ILE:HD12	2.01	0.43
3:C:150:TYR:HB3	3:C:168:TYR:CE2	2.54	0.43
2:B:70:TRP:CD1	2:B:276:SER:HB2	2.54	0.43
4:D:52:THR:CG2	4:D:114:VAL:HG22	2.48	0.43
9:B:504:LMT:O2B	9:B:504:LMT:H4'	2.17	0.43
5:E:17:MET:HE3	5:E:121:ALA:HA	2.01	0.43
6:F:301:SER:O	6:F:332:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:GLU:CG	2:B:381:GLY:N	2.82	0.43
5:E:84:ILE:HD12	5:E:84:ILE:HA	1.87	0.43
3:C:174:PRO:CG	4:D:102:SER:HB3	2.49	0.43
4:D:184:ALA:CB	5:E:22:PHE:CE2	3.01	0.43
4:D:209:LYS:HG2	5:E:174:ARG:CZ	2.49	0.43
6:F:204:VAL:HG22	6:F:244:GLN:HB2	2.01	0.43
6:F:240:VAL:CG1	12:F:1501:FAD:N3A	2.82	0.43
9:B:503:LMT:O3'	9:B:503:LMT:C1B	2.65	0.42
3:C:12:LEU:HD11	6:F:23:LEU:CD1	2.48	0.42
2:B:259:THR:HG23	2:B:262:ASP:H	1.83	0.42
6:F:215:ALA:HB2	6:F:286:ALA:CB	2.49	0.42
1:A:394:LEU:HD22	1:A:431:TYR:CD1	2.53	0.42
6:F:45:LYS:HB3	6:F:45:LYS:HE3	1.83	0.42
6:F:128:PHE:CD2	6:F:128:PHE:C	2.96	0.42
3:C:44:ASP:O	3:C:48:LYS:HG2	2.18	0.42
4:D:72:ILE:CB	5:E:92:GLN:OE1	2.65	0.42
3:C:147:SER:HA	5:E:131:GLN:OE1	2.19	0.42
3:C:229:ASN:ND2	5:E:197:GLN:NE2	2.68	0.42
4:D:65:HIS:O	4:D:67:PRO:HD3	2.20	0.42
5:E:93:ILE:HA	5:E:96:MET:CE	2.49	0.42
3:C:11:THR:O	3:C:15:VAL:HG22	2.20	0.42
3:C:165:LEU:HD22	3:C:189:TRP:CE2	2.54	0.42
6:F:208:ILE:HD12	6:F:245:MET:HB2	2.02	0.42
3:C:247:PHE:CE2	3:C:251:VAL:HG21	2.55	0.42
2:B:136:VAL:HG21	2:B:166:PHE:HD2	1.85	0.41
3:C:62:GLN:O	3:C:66:LEU:HD23	2.20	0.41
3:C:71:ILE:CG2	3:C:125:TYR:HB3	2.50	0.41
4:D:67:PRO:HB2	4:D:70:VAL:HG22	2.02	0.41
6:F:4:ILE:HD12	6:F:4:ILE:H	1.85	0.41
6:F:294:ASP:OD1	6:F:299:LEU:HD23	2.20	0.41
1:A:29:VAL:CG1	1:A:71:PRO:HG2	2.50	0.41
2:B:111:THR:HG23	2:B:116:ALA:HB2	2.02	0.41
3:C:94:ARG:NE	3:C:150:TYR:CE2	2.89	0.41
4:D:7:LEU:HD23	4:D:9:LYS:HE2	2.02	0.41
6:F:217:TYR:CE1	6:F:220:GLU:CG	3.03	0.41
1:A:134:ARG:HD2	1:A:412:GLU:O	2.20	0.41
4:D:97:ILE:HA	4:D:100:GLN:HG3	2.02	0.41
4:D:105:VAL:HG23	4:D:106:GLY:H	1.86	0.41
2:B:404:ASN:O	2:B:404:ASN:ND2	2.53	0.41
4:D:84:ILE:O	4:D:88:GLN:HG2	2.20	0.41
6:F:288:MET:HG2	6:F:378:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:356:HIS:CD2	6:F:386:ALA:HB1	2.55	0.41
2:B:65:PHE:HA	2:B:68:MET:HE2	2.02	0.41
2:B:86:LEU:HD11	2:B:232:TYR:HB2	2.02	0.41
2:B:392:PHE:CE1	5:E:152:LEU:CD2	3.04	0.41
3:C:205:ILE:HG23	3:C:220:GLY:HA2	2.03	0.41
4:D:31:ALA:HA	4:D:145:LEU:CD1	2.51	0.41
5:E:14:ILE:HG12	5:E:196:VAL:CG1	2.50	0.41
5:E:93:ILE:HA	5:E:96:MET:HE2	2.02	0.41
6:F:151:LYS:HE3	6:F:225:MET:CG	2.50	0.41
1:A:43:MET:HE3	1:A:43:MET:HB3	1.98	0.41
1:A:229:PRO:O	2:B:411:ARG:NH2	2.53	0.41
1:A:384:MET:HE1	1:A:386:LEU:HB2	2.03	0.41
2:B:217:PRO:O	2:B:221:SER:OG	2.36	0.41
3:C:171:GLY:O	4:D:103:VAL:HG11	2.21	0.41
4:D:48:VAL:O	4:D:52:THR:HG23	2.20	0.41
6:F:159:SER:HB3	6:F:221:PHE:CA	2.50	0.41
6:F:176:HIS:ND1	6:F:202:SER:O	2.52	0.41
2:B:86:LEU:HD11	2:B:232:TYR:CD1	2.55	0.41
2:B:271:SER:CB	2:B:274:GLU:OE1	2.68	0.41
4:D:72:ILE:HG23	4:D:115:MET:CE	2.51	0.41
4:D:105:VAL:HG23	5:E:80:PHE:HE2	1.85	0.41
5:E:81:ILE:HG12	6:F:11:PHE:CE2	2.56	0.41
6:F:217:TYR:CE1	6:F:293:PHE:CD2	3.08	0.41
2:B:39:LEU:O	2:B:40:VAL:C	2.63	0.41
3:C:166:THR:HA	3:C:186:ARG:HD2	2.03	0.41
5:E:98:LEU:CD1	5:E:113:LEU:HD12	2.49	0.41
5:E:165:LYS:HG3	5:E:166:TYR:N	2.35	0.41
6:F:213:SER:HB2	6:F:406:PHE:CZ	2.55	0.41
1:A:74:GLY:HA3	1:A:93:GLU:O	2.20	0.41
2:B:44:SER:O	2:B:45:SER:C	2.63	0.41
2:B:333:LEU:O	2:B:372:ARG:NH2	2.51	0.41
6:F:154:ILE:HD12	6:F:155:PRO:HD2	2.02	0.41
6:F:217:TYR:CE1	6:F:293:PHE:HD2	2.38	0.41
6:F:217:TYR:CE1	6:F:220:GLU:HG2	2.55	0.41
6:F:296:LEU:HD12	6:F:326:LEU:HD13	2.02	0.41
3:C:142:GLY:HA3	3:C:234:THR:OG1	2.21	0.41
5:E:102:PHE:HB2	5:E:106:TYR:CD2	2.56	0.41
2:B:55:ARG:O	2:B:59:MET:HG2	2.21	0.40
4:D:144:VAL:HA	4:D:194:MET:HE1	2.03	0.40
5:E:15:GLU:HB3	5:E:21:PHE:CE1	2.56	0.40
5:E:18:ALA:O	5:E:22:PHE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:ILE:HG13	5:E:94:LEU:N	2.36	0.40
5:E:154:ILE:HG23	5:E:155:VAL:N	2.37	0.40
6:F:212:TYR:HB3	6:F:226:LEU:HD21	2.00	0.40
3:C:115:ILE:O	3:C:115:ILE:HG13	2.21	0.40
6:F:146:PHE:HB3	6:F:230:ILE:HG22	2.02	0.40
6:F:150:LEU:O	6:F:225:MET:HA	2.21	0.40
2:B:271:SER:HB2	2:B:274:GLU:OE1	2.21	0.40
3:C:141:HIS:CB	3:C:150:TYR:CD2	3.04	0.40
3:C:187:ALA:O	3:C:190:VAL:HG22	2.22	0.40
3:C:194:LEU:HA	3:C:203:ILE:HG12	2.03	0.40
5:E:24:GLY:H	5:E:120:CYS:HB2	1.87	0.40
5:E:117:THR:O	5:E:118:VAL:CB	2.69	0.40
3:C:205:ILE:N	3:C:205:ILE:HD12	2.37	0.40
4:D:36:THR:HG23	4:D:37:LYS:HG3	2.03	0.40
4:D:60:SER:HB2	4:D:127:PRO:CG	2.52	0.40
5:E:96:MET:HE3	5:E:96:MET:HB2	1.77	0.40
5:E:102:PHE:HB2	5:E:106:TYR:HD2	1.86	0.40
3:C:174:PRO:HG3	4:D:102:SER:CB	2.52	0.40
4:D:42:PHE:CZ	4:D:46:LEU:HD11	2.57	0.40
4:D:183:LEU:HB2	4:D:185:PRO:HD2	2.03	0.40
5:E:99:ASP:C	5:E:100:ARG:CZ	2.95	0.40
5:E:188:LEU:HD12	5:E:188:LEU:HA	1.95	0.40

All (2) 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:168:ASN:O	6:F:199:ARG:NH1[2_444]	1.90	0.30
1:A:168:ASN:O	6:F:199:ARG:HH11[2_444]	1.49	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/395 (86%)	339 (100%)	0	100	100
2	B	292/320 (91%)	292 (100%)	0	100	100
3	C	198/205 (97%)	198 (100%)	0	100	100
4	D	171/176 (97%)	170 (99%)	1 (1%)	78	79
5	E	164/165 (99%)	164 (100%)	0	100	100
6	F	337/337 (100%)	337 (100%)	0	100	100
All	All	1501/1598 (94%)	1500 (100%)	1 (0%)	88	87

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

Mol	Chain	Res	Type
4	D	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	209	HIS
1	A	234	HIS
2	B	84	ASN
3	C	40	ASN
3	C	110	GLN
3	C	216	HIS
3	C	229	ASN
4	D	68	ASN
4	D	88	GLN
5	E	197	GLN
6	F	356	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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
7	FMN	B	501	2	29,32,33	1.12	2 (6%)	41,47,50	1.67	8 (19%)
8	RBF	B	502	-	29,29,29	0.63	0	42,43,43	0.73	1 (2%)
11	FES	F	1502	6	0,4,4	-	-	-	-	-
9	LMT	D	301	-	36,36,36	1.20	5 (13%)	47,47,47	1.03	1 (2%)
9	LMT	B	503	-	36,36,36	1.16	4 (11%)	47,47,47	1.13	4 (8%)
9	LMT	B	504	-	36,36,36	1.22	5 (13%)	47,47,47	1.21	2 (4%)
7	FMN	C	1000	3	29,32,33	1.13	2 (6%)	41,47,50	1.48	10 (24%)
11	FES	E	1001	4,5	0,4,4	-	-	-	-	-
12	FAD	F	1501	-	58,58,58	0.31	0	85,89,89	0.35	0

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
7	FMN	B	501	2	-	1/15/17/18	0/3/3/3
8	RBF	B	502	-	-	2/14/14/14	0/3/3/3
11	FES	F	1502	6	-	-	0/1/1/1
9	LMT	D	301	-	-	9/21/61/61	0/2/2/2
9	LMT	B	503	-	-	7/21/61/61	0/2/2/2
9	LMT	B	504	-	-	10/21/61/61	0/2/2/2
7	FMN	C	1000	3	-	0/15/17/18	0/3/3/3
11	FES	E	1001	4,5	-	-	0/1/1/1
12	FAD	F	1501	-	-	7/34/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	FMN	C4A-N5	3.60	1.38	1.30
7	C	1000	FMN	C4A-N5	3.39	1.38	1.30
9	D	301	LMT	O3'-C3'	-3.10	1.35	1.43
9	D	301	LMT	O2'-C2'	-3.05	1.35	1.43
9	B	504	LMT	O2'-C2'	-2.98	1.35	1.43
9	B	503	LMT	O3'-C3'	-2.92	1.35	1.43
9	B	504	LMT	O3'-C3'	-2.87	1.35	1.43
7	C	1000	FMN	C10-N1	2.78	1.38	1.33
9	B	503	LMT	O3B-C3B	-2.75	1.36	1.43
9	B	504	LMT	O2B-C2B	-2.68	1.36	1.43
7	B	501	FMN	C10-N1	2.66	1.38	1.33
9	B	504	LMT	O3B-C3B	-2.41	1.37	1.43
9	B	504	LMT	O5'-C5'	-2.32	1.38	1.44
9	B	503	LMT	O2'-C2'	-2.27	1.37	1.43
9	D	301	LMT	O3B-C3B	-2.22	1.37	1.43
9	D	301	LMT	O2B-C2B	-2.20	1.37	1.43
9	B	503	LMT	O2B-C2B	-2.16	1.37	1.43
9	D	301	LMT	O4'-C4B	-2.15	1.37	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	FMN	C4'-C3'-C2'	-4.96	105.32	113.57
9	B	504	LMT	O5'-C1'-O1'	-4.48	99.45	110.04
7	C	1000	FMN	C4-N3-C2	-3.68	119.11	125.64
7	B	501	FMN	C4-N3-C2	-3.58	119.29	125.64
9	B	503	LMT	C3'-C4'-C5'	-3.50	103.17	110.93
9	D	301	LMT	C1'-O5'-C5'	-3.09	107.68	113.72
7	B	501	FMN	C4A-C4-N3	2.84	120.47	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	LMT	O5B-C5B-C4B	2.83	114.81	109.70
7	B	501	FMN	O4-C4-C4A	-2.82	119.09	126.53
7	C	1000	FMN	C4A-C10-N1	-2.79	117.75	124.59
7	B	501	FMN	C4A-C10-N10	2.79	120.47	116.48
7	C	1000	FMN	C4A-C4-N3	2.77	120.31	113.25
7	B	501	FMN	C10-C4A-N5	-2.70	119.30	124.81
7	C	1000	FMN	C5A-C9A-N10	2.66	120.38	117.97
7	C	1000	FMN	O4-C4-C4A	-2.64	119.56	126.53
7	C	1000	FMN	C4A-C10-N10	2.54	120.12	116.48
7	C	1000	FMN	C4-C4A-C10	2.39	121.04	116.93
7	C	1000	FMN	C9A-C5A-N5	-2.34	119.97	122.45
9	B	503	LMT	O5'-C1'-O1'	-2.34	104.52	110.04
7	C	1000	FMN	C10-C4A-N5	-2.33	120.05	124.81
7	B	501	FMN	C4A-C10-N1	-2.28	119.00	124.59
9	B	503	LMT	O5B-C5B-C4B	2.25	113.75	109.70
7	C	1000	FMN	C10-N1-C2	2.09	121.38	116.85
8	B	502	RBF	C4-N3-C2	-2.09	121.93	125.64
9	B	503	LMT	O1B-C4'-C3'	2.08	112.53	107.23
7	B	501	FMN	C10-N1-C2	2.05	121.29	116.85

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	504	LMT	C2B-C1B-O1B-C4'
12	F	1501	FAD	N10-C1'-C2'-O2'
9	B	503	LMT	C3'-C4'-O1B-C1B
8	B	502	RBF	C3'-C4'-C5'-O5'
9	D	301	LMT	C4'-C5'-C6'-O6'
9	D	301	LMT	O5'-C5'-C6'-O6'
9	B	504	LMT	O5B-C5B-C6B-O6B
9	B	503	LMT	O5'-C1'-O1'-C1
9	B	504	LMT	C7-C8-C9-C10
9	B	503	LMT	C2'-C1'-O1'-C1
9	B	504	LMT	C4B-C5B-C6B-O6B
12	F	1501	FAD	O4B-C4B-C5B-O5B
9	B	503	LMT	O5B-C1B-O1B-C4'
8	B	502	RBF	O4'-C4'-C5'-O5'
9	B	503	LMT	O5B-C5B-C6B-O6B
9	D	301	LMT	C6-C7-C8-C9
9	D	301	LMT	O5B-C5B-C6B-O6B
9	B	504	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
9	B	504	LMT	C5'-C4'-O1B-C1B
12	F	1501	FAD	C3B-C4B-C5B-O5B
9	B	504	LMT	C3'-C4'-O1B-C1B
9	B	504	LMT	C11-C10-C9-C8
12	F	1501	FAD	C2B-C1B-N9A-C8A
12	F	1501	FAD	N10-C1'-C2'-C3'
9	B	504	LMT	O1'-C1-C2-C3
9	D	301	LMT	C5'-C4'-O1B-C1B
12	F	1501	FAD	O4B-C1B-N9A-C8A
12	F	1501	FAD	O4B-C1B-N9A-C4A
7	B	501	FMN	C4'-C5'-O5'-P
9	D	301	LMT	C7-C8-C9-C10
9	D	301	LMT	C3-C4-C5-C6
9	B	503	LMT	C6-C7-C8-C9
9	D	301	LMT	C11-C10-C9-C8
9	D	301	LMT	C9-C10-C11-C12
9	B	504	LMT	C5-C6-C7-C8
9	B	503	LMT	C2B-C1B-O1B-C4'

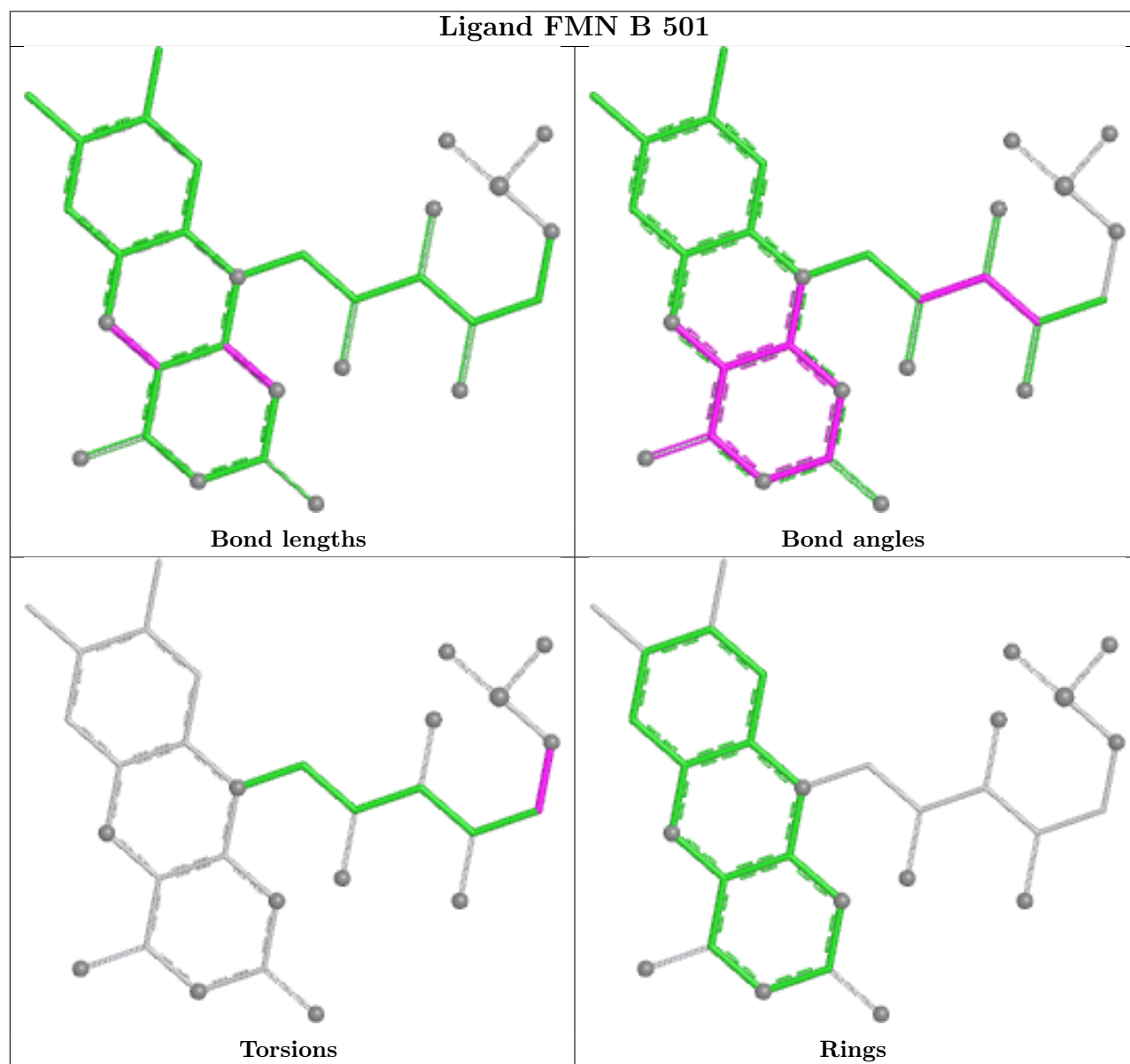
There are no ring outliers.

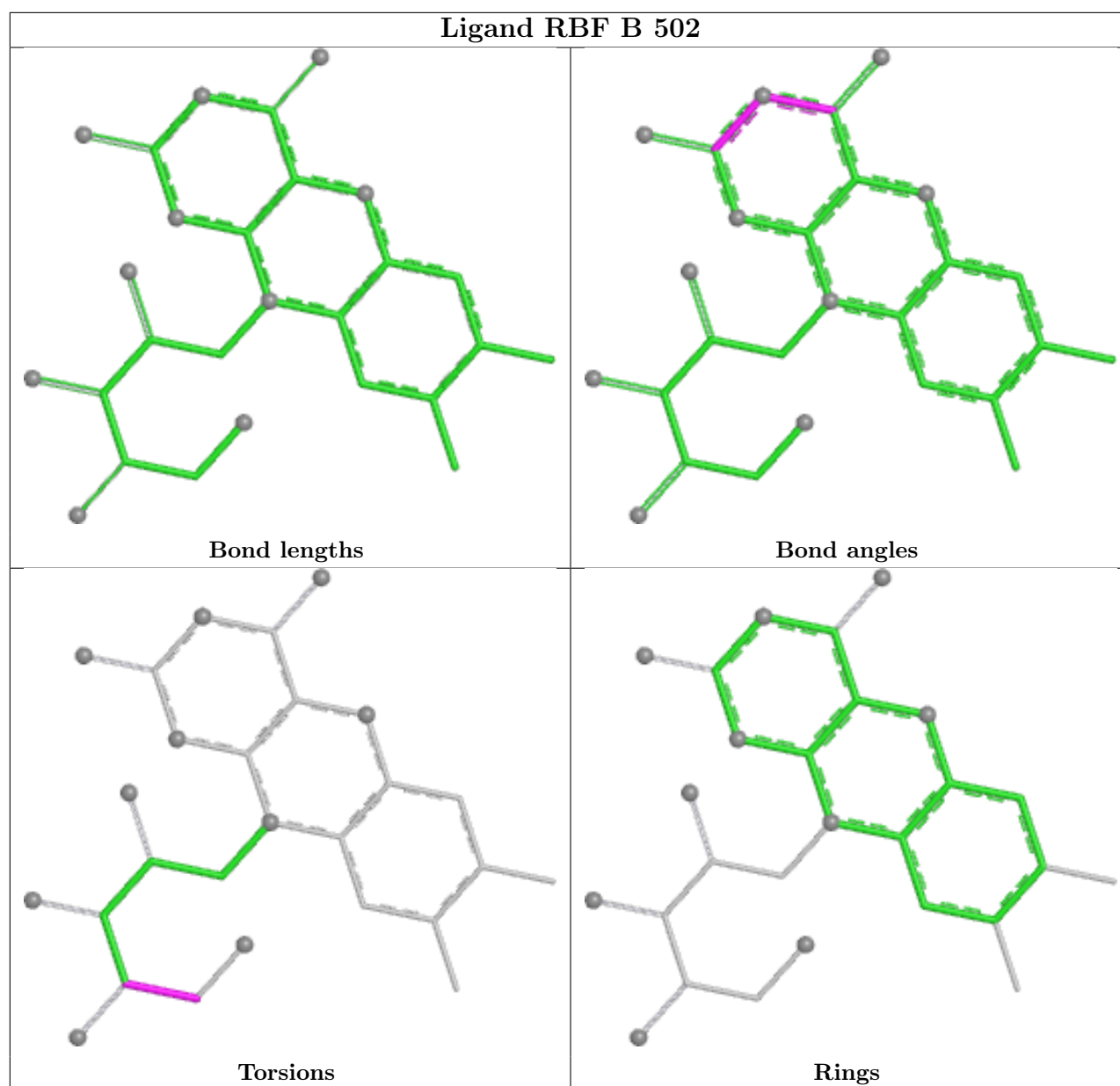
8 monomers are involved in 22 short contacts:

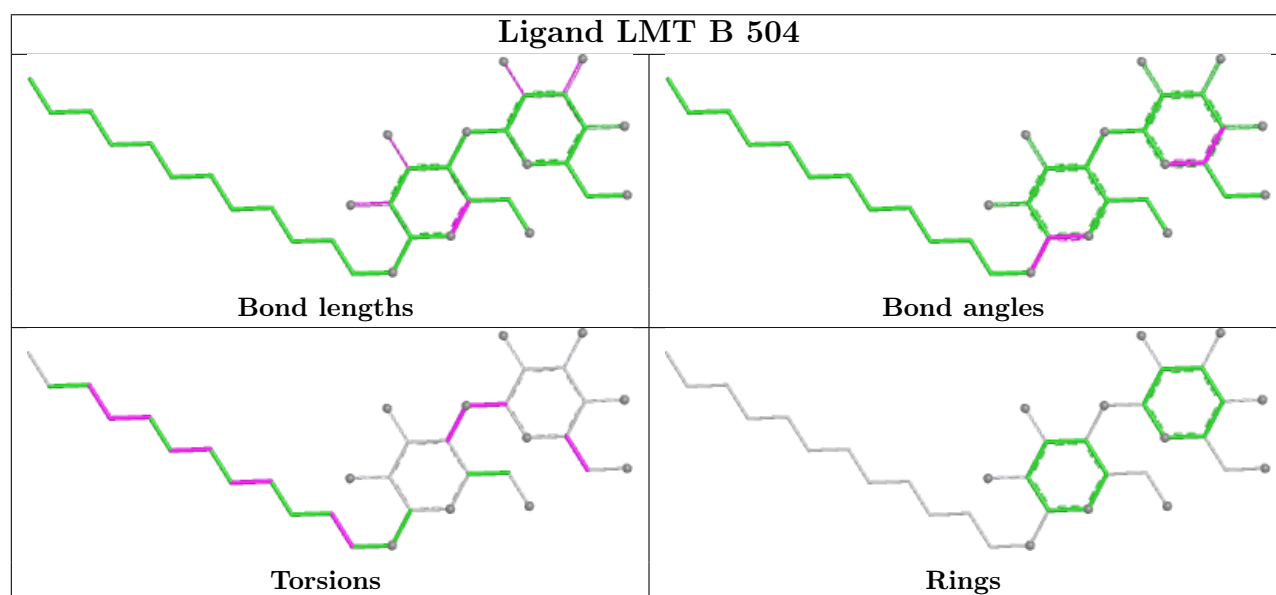
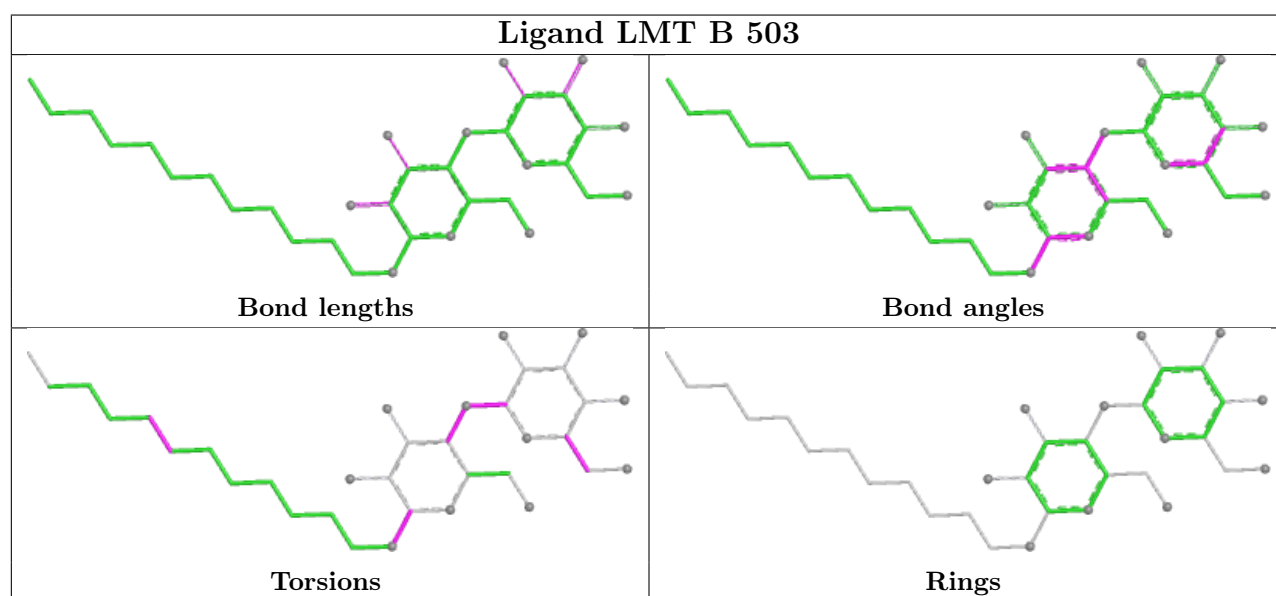
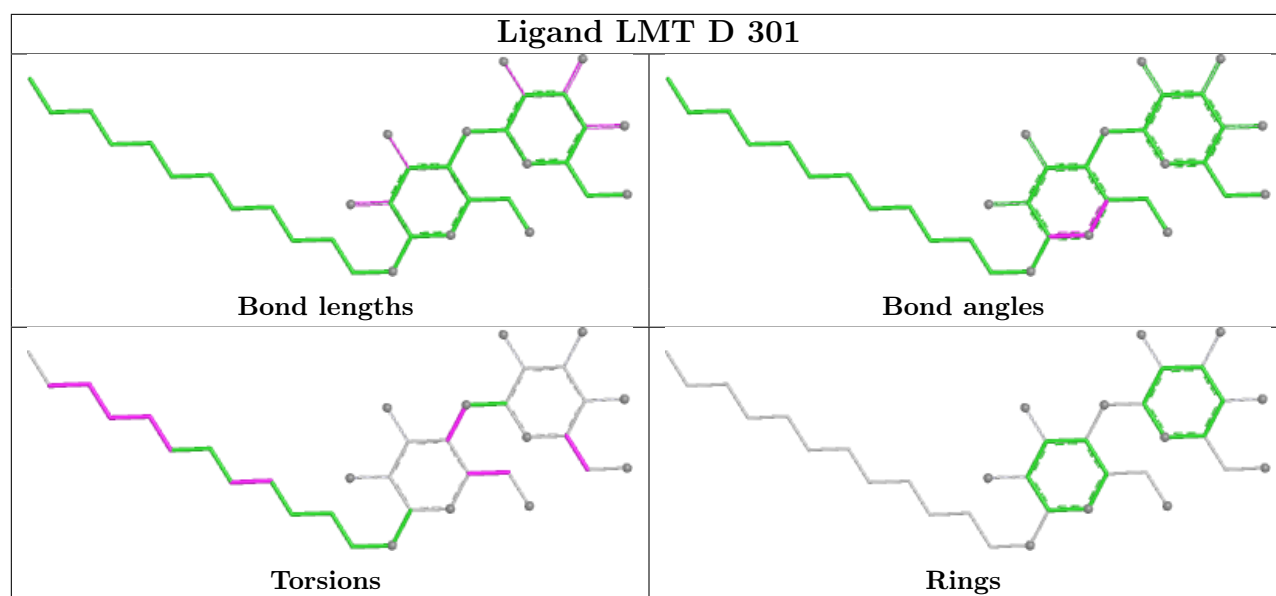
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	FMN	5	0
8	B	502	RBF	2	0
11	F	1502	FES	2	0
9	D	301	LMT	1	0
9	B	503	LMT	4	0
9	B	504	LMT	4	0
7	C	1000	FMN	1	0
12	F	1501	FAD	3	0

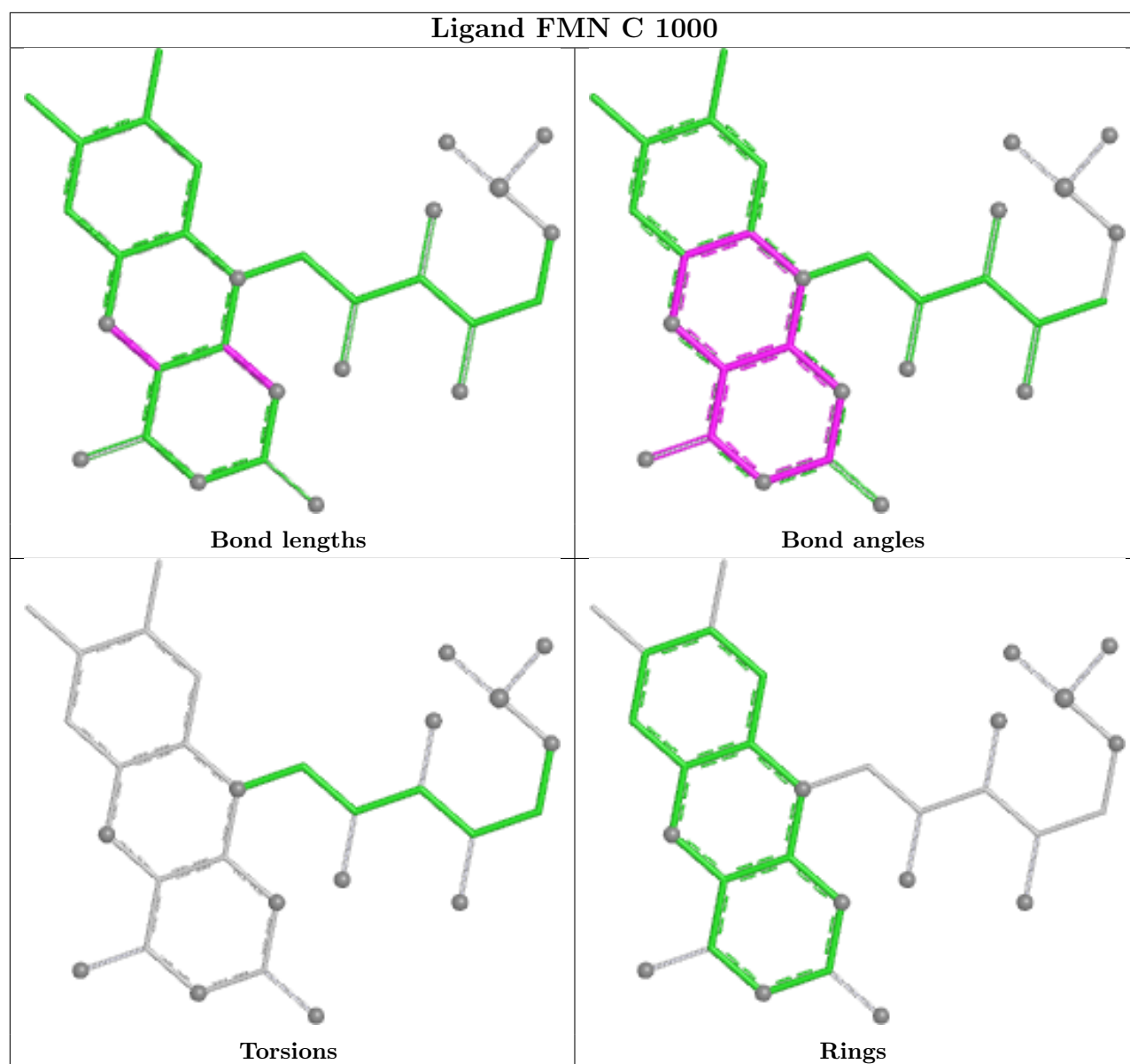
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

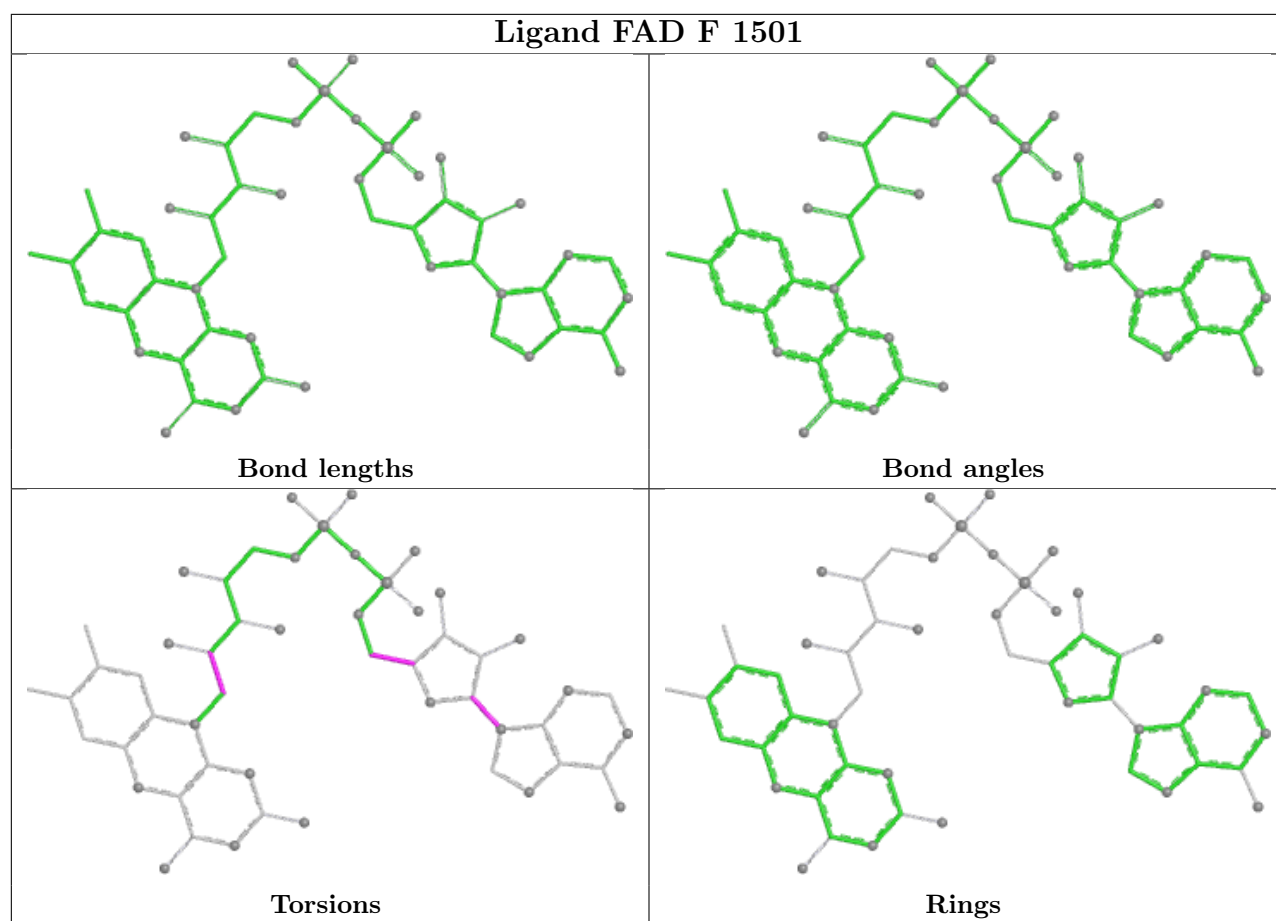
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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%)	-0.14	10 (2%) 58 35	141, 172, 206, 276	0
2	B	380/415 (91%)	-0.03	16 (4%) 40 22	132, 178, 227, 259	0
3	C	248/257 (96%)	-0.02	10 (4%) 42 23	178, 221, 253, 279	0
4	D	204/210 (97%)	0.01	10 (4%) 35 19	138, 178, 221, 245	0
5	E	197/198 (99%)	-0.05	7 (3%) 46 25	125, 166, 218, 241	0
6	F	407/408 (99%)	0.02	13 (3%) 50 29	158, 221, 284, 317	0
All	All	1839/1956 (94%)	-0.04	66 (3%) 46 25	125, 187, 253, 317	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	108	ALA	6.1
5	E	196	VAL	5.1
1	A	383	VAL	4.8
4	D	204	GLU	4.6
6	F	407	GLY	4.5
2	B	173	THR	4.0
1	A	83	ALA	3.9
2	B	272	ILE	3.8
4	D	97	ILE	3.8
2	B	216	TYR	3.7
3	C	146	TRP	3.5
1	A	220	ALA	3.4
2	B	292	ILE	3.2
6	F	18	LEU	3.2
5	E	194	SER	3.1
6	F	258	CYS	3.0
2	B	212	LEU	2.9
2	B	273	GLY	2.9
1	A	117	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	77	VAL	2.8
3	C	198	ASN	2.8
2	B	98	GLY	2.8
6	F	343	GLN	2.8
6	F	21	VAL	2.8
2	B	94	ALA	2.7
2	B	228	ALA	2.7
2	B	171	PRO	2.6
6	F	330	ASN	2.6
1	A	91	VAL	2.6
2	B	97	ALA	2.6
1	A	8	LEU	2.6
4	D	23	LEU	2.6
1	A	385	PRO	2.5
4	D	205	GLN	2.5
4	D	201	PHE	2.5
3	C	147	SER	2.5
5	E	192	SER	2.5
4	D	176	GLN	2.4
6	F	329	GLU	2.4
3	C	221	LEU	2.4
3	C	169	GLU	2.4
2	B	170	VAL	2.3
3	C	8	ILE	2.3
2	B	172	PRO	2.3
4	D	16	LEU	2.3
5	E	104	PRO	2.3
2	B	220	ILE	2.2
5	E	172	GLY	2.2
4	D	208	ALA	2.2
3	C	207	LYS	2.2
3	C	145	LEU	2.2
5	E	188	LEU	2.2
6	F	23	LEU	2.2
4	D	203	PRO	2.2
6	F	406	PHE	2.1
1	A	134	ARG	2.1
2	B	227	THR	2.1
3	C	9	LYS	2.1
2	B	219	GLN	2.1
6	F	393	ASN	2.1
6	F	312	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	175	GLY	2.0
1	A	238	SER	2.0
6	F	306	SER	2.0
4	D	202	LYS	2.0
6	F	291	HIS	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](#)

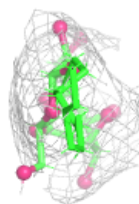
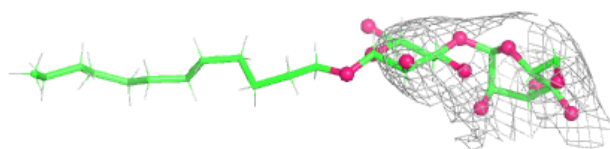
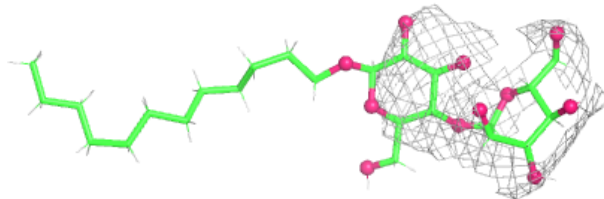
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	LMT	B	504	35/35	0.62	0.11	149,185,216,236	0
9	LMT	D	301	35/35	0.74	0.14	165,205,238,246	0
10	NA	B	505	1/1	0.76	0.14	138,138,138,138	0
12	FAD	F	1501	53/53	0.79	0.12	196,220,264,284	0
8	RBF	B	502	27/27	0.84	0.12	159,191,246,264	0
9	LMT	B	503	35/35	0.85	0.08	130,169,236,250	0
7	FMN	B	501	30/31	0.92	0.09	145,170,204,209	0
11	FES	E	1001	4/4	0.94	0.05	143,144,146,147	0
11	FES	F	1502	4/4	0.94	0.05	260,274,274,275	0
7	FMN	C	1000	30/31	0.94	0.10	160,182,213,220	0

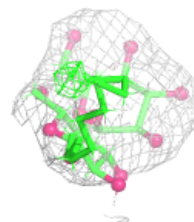
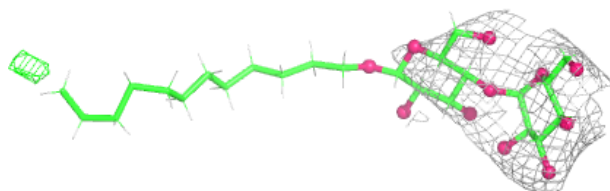
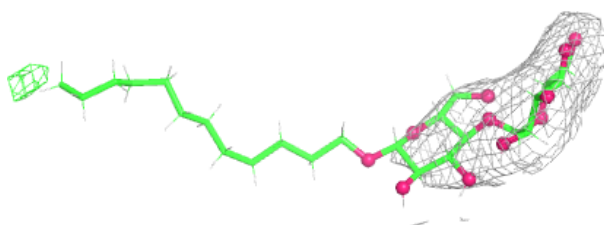
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

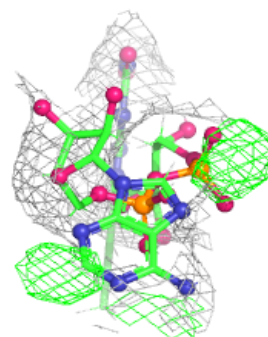
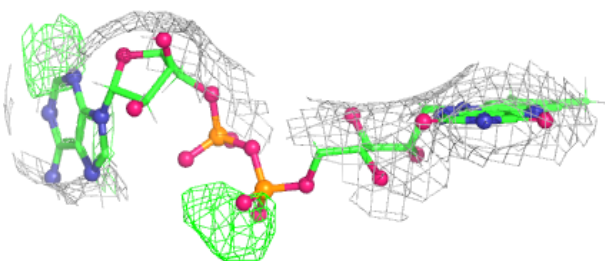
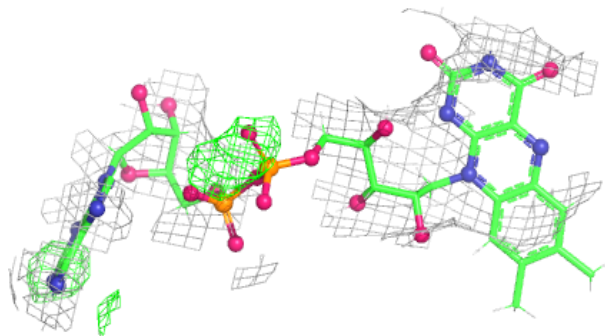
**Electron density around LMT D 301:**

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



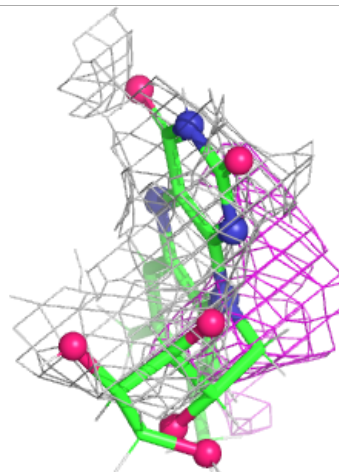
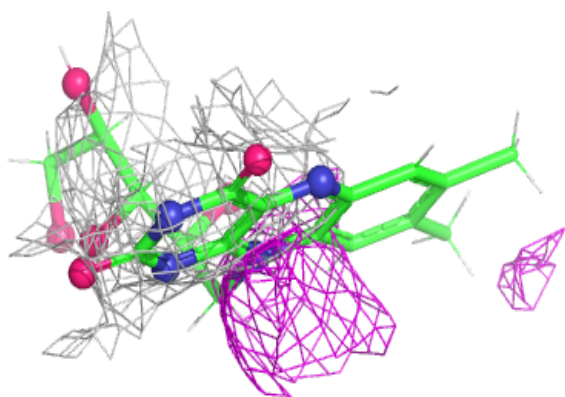
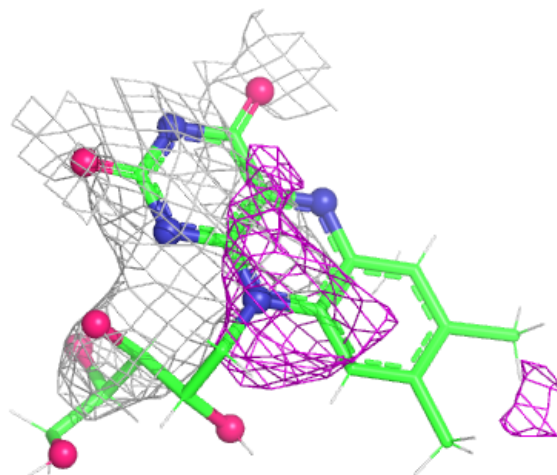
Electron density around FAD F 1501:

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



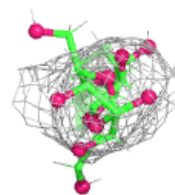
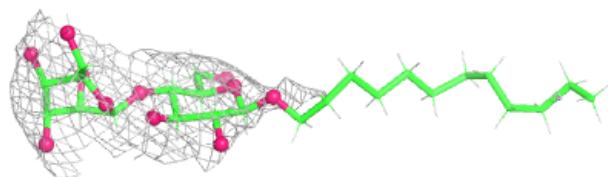
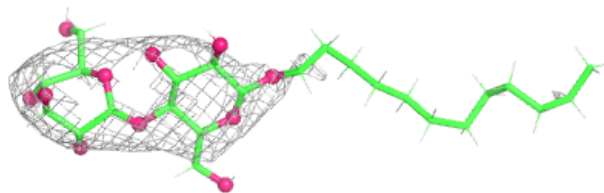
Electron density around RBF B 502:

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



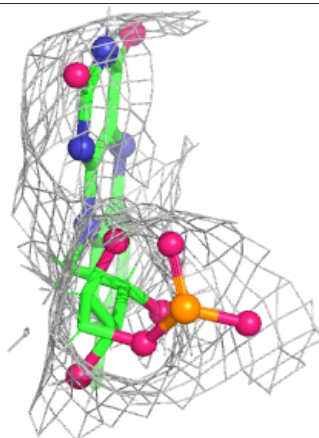
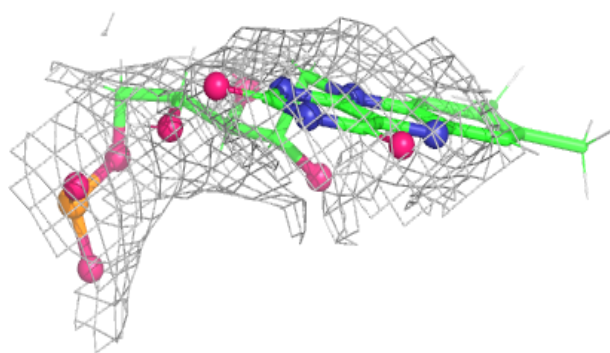
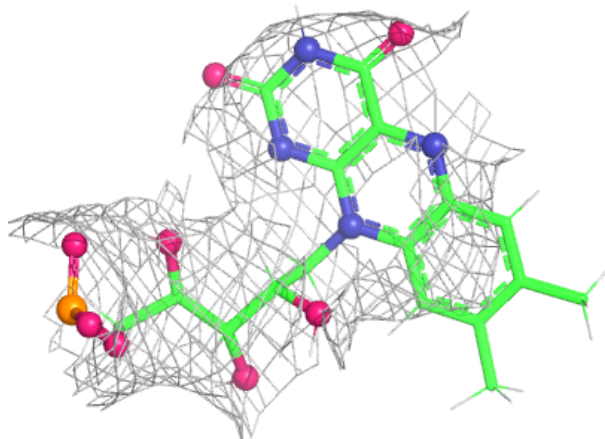
Electron density around LMT B 503:

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

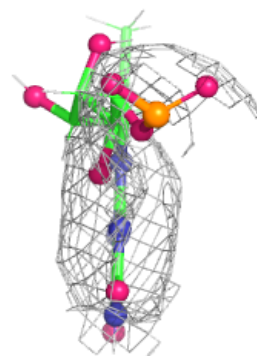
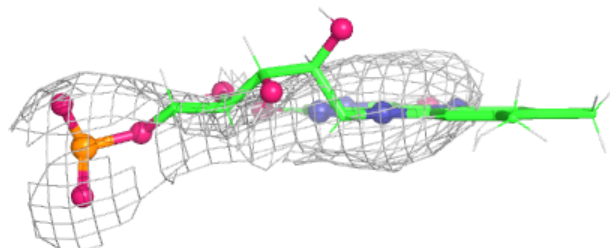
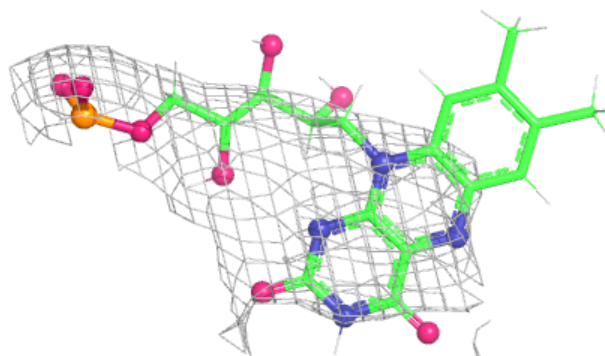


Electron density around FMN B 501:

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

**Electron density around FMN C 1000:**

$2mF_o-DF_c$ (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.