



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:01 am BST

PDB ID : 4P6V  
Title : Crystal structure of the Na<sup>+</sup>-translocating NADH: ubiquinone oxidoreductase from *Vibrio cholerae*  
Authors : Steuber, J.; Casutt, M.S.; Vohl, G.; Vorbürger, T.; Diederichs, K.; Fritz, G.  
Deposited on : 2014-03-25  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

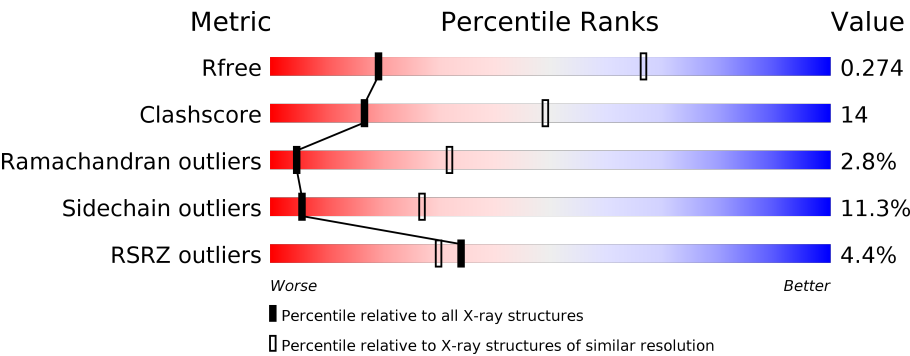
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	449	<div><div>0%</div><div><div>65%</div><div>21%</div><div>•</div><div>11%</div></div></div>
2	B	415	<div><div>3%</div><div><div>46%</div><div>31%</div><div>6%</div><div>16%</div></div></div>
3	C	257	<div><div>9%</div><div><div>70%</div><div>25%</div><div>••</div></div></div>
4	D	210	<div><div><div>39%</div><div>34%</div><div>10%</div><div>•</div><div>15%</div></div></div>
5	E	198	<div><div>4%</div><div><div>51%</div><div>33%</div><div>9%</div><div>•</div><div>5%</div></div></div>
6	F	408	<div><div>8%</div><div><div>75%</div><div>23%</div><div>•</div></div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	RBF	E	201	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13614 atoms, of which 0 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
1	A	400	Total	C	N	O	S	0	0	0
			3041	1927	516	584	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9KPS1
A	-1	PRO	-	expression tag	UNP Q9KPS1
A	0	HIS	-	expression tag	UNP Q9KPS1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	348	Total	C	N	O	S	0	0	0
			2619	1737	424	437	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	0
			1902	1204	327	367	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	179	Total	C	N	O	S	0	0	0
			1331	888	207	227	9			

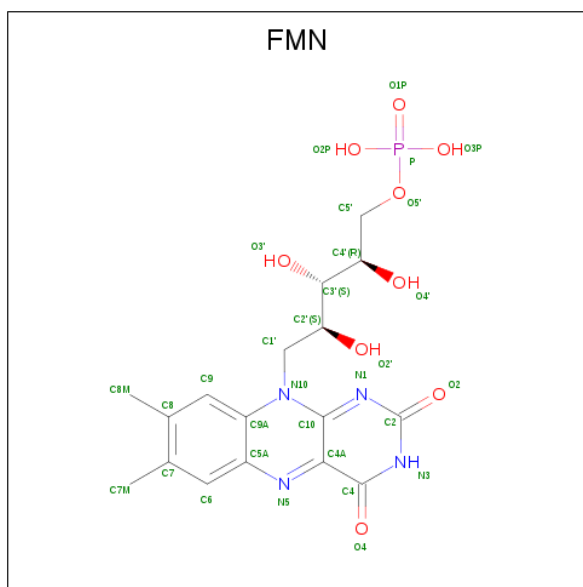
- Molecule 5 is a protein called Na(+)-translocating NADH-quinone reductase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	189	Total	C	N	O	S	0	0	0
			1429	960	218	241	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	N	O	S	0	0	0
			3146	2013	515	595	23			

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 30	C 17	N 4	O 8	P 1	0	0
7	C	1	Total 30	C 17	N 4	O 8	P 1	0	0

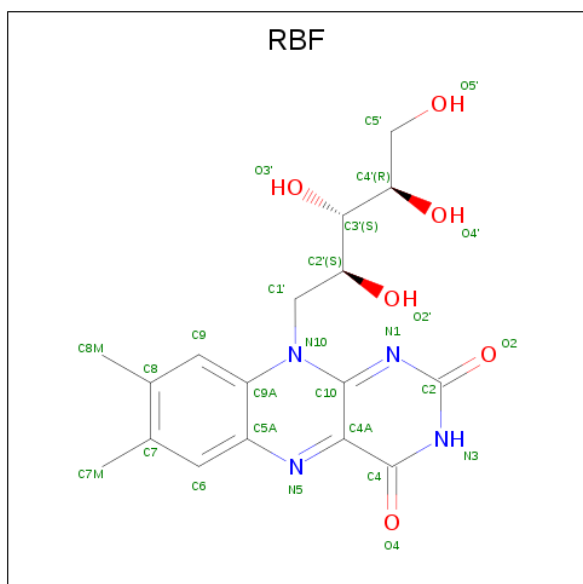
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

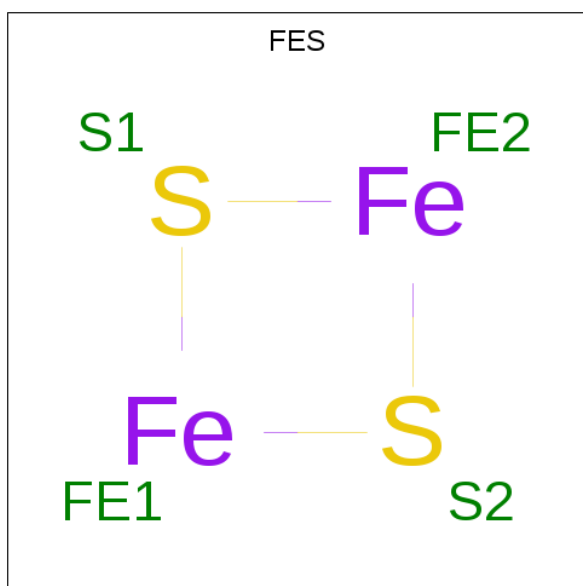
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total 1	Fe 1	0	0

- Molecule 10 is RIBOFLAVIN (three-letter code: RBF) (formula:  $C_{17}H_{20}N_4O_6$ ).



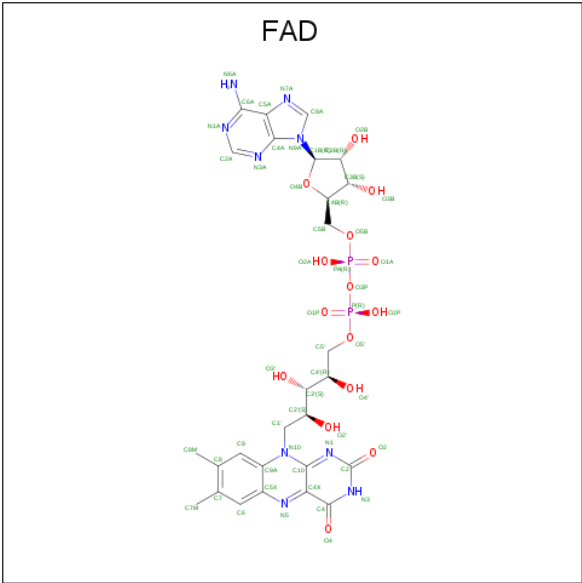
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	E	1	Total	C	N	O	0	0
			27	17	4	6		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

- Molecule 12 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).

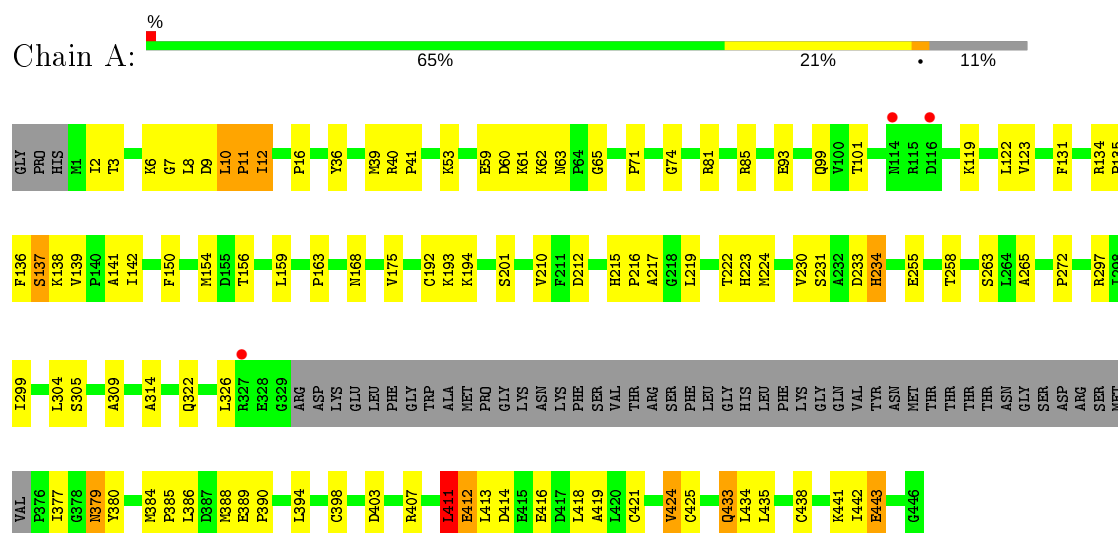


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0
			53	27	9	15	2	

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

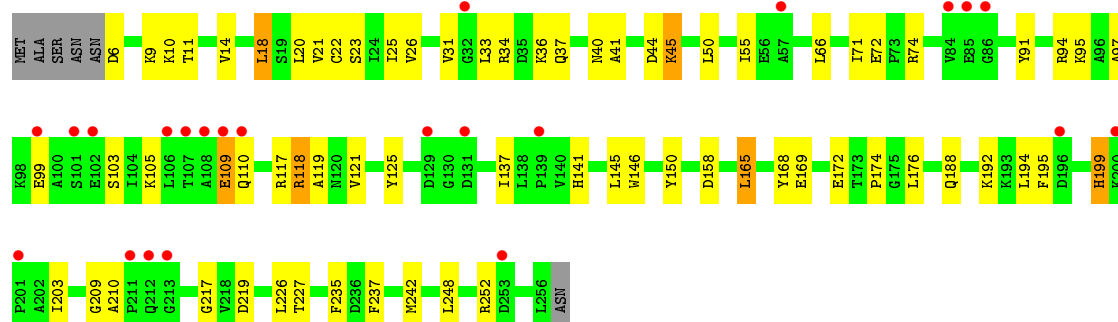
- Molecule 1: Na(+)-translocating NADH-quinone reductase subunit A



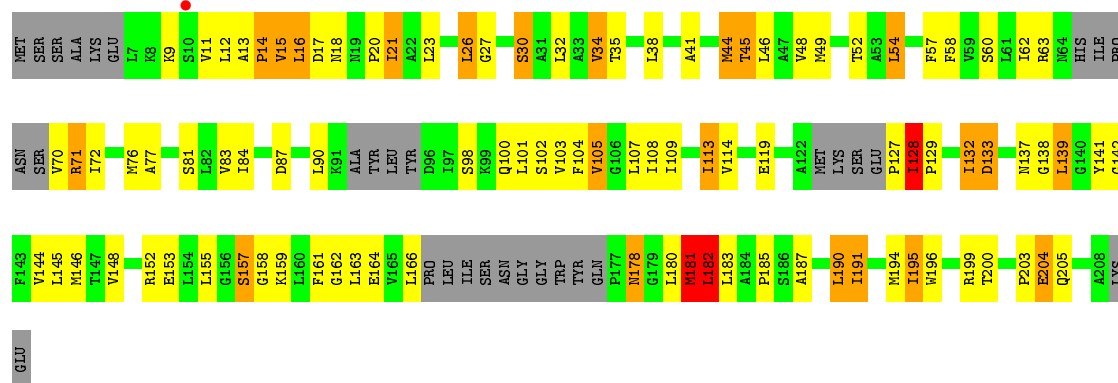




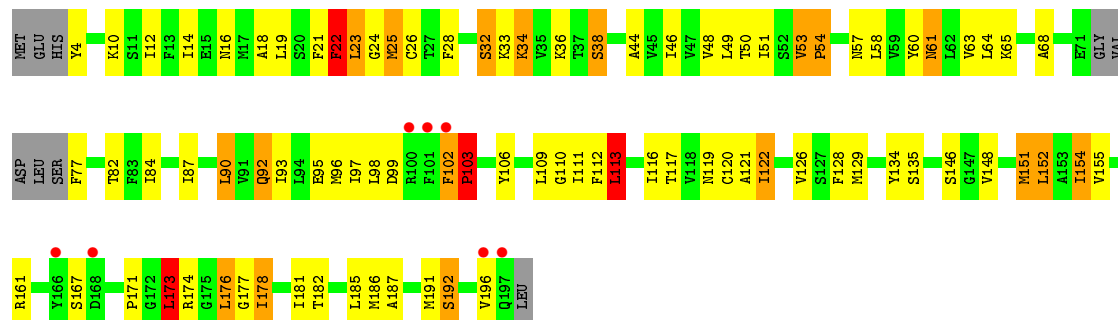
• Molecule 3: Na(+)-translocating NADH-quinone reductase subunit C



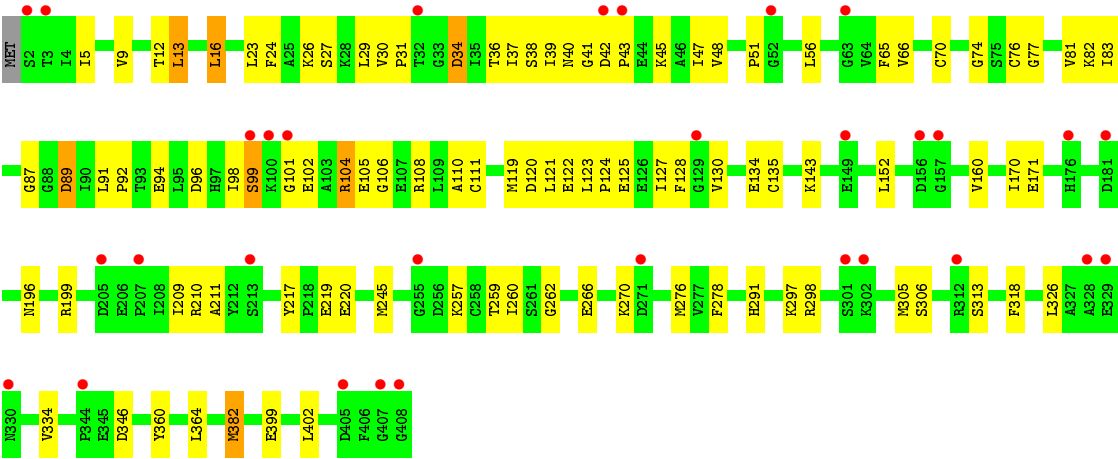
• Molecule 4: Na(+)-translocating NADH-quinone reductase subunit D



• 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, $\alpha$ , $\beta$ , $\gamma$	95.35Å 143.38Å 104.49Å 90.00° 110.96° 90.00°	Depositor
Resolution (Å)	24.98 – 3.50 24.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.98-3.50) 100.0 (24.98-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 3.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.246 , 0.276 0.246 , 0.274	Depositor DCC
$R_{free}$ test set	1943 reflections (5.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	155.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 112.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, FMN, FE, RBF, FAD, 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	0.28	0/3095	0.55	0/4199
2	B	0.28	0/2691	0.47	0/3662
3	C	0.32	0/1934	0.65	1/2610 (0.0%)
4	D	0.28	0/1351	0.55	1/1831 (0.1%)
5	E	0.29	0/1459	0.56	2/1980 (0.1%)
6	F	0.29	1/3224 (0.0%)	0.55	0/4367
All	All	0.29	1/13754 (0.0%)	0.55	4/18649 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
5	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	160	VAL	C-N	5.01	1.43	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	182	LEU	CA-CB-CG	6.27	129.72	115.30
5	E	113	LEU	CA-CB-CG	6.05	129.22	115.30
5	E	173	LEU	CA-CB-CG	5.67	128.34	115.30
3	C	199	HIS	C-N-CA	-5.06	109.05	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	346	ASP	Peptide
5	E	103	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3041	0	3079	61	0
2	B	2619	0	2594	99	0
3	C	1902	0	1910	52	0
4	D	1331	0	1399	74	0
5	E	1429	0	1495	66	0
6	F	3146	0	3056	67	0
7	B	30	0	19	5	0
7	C	30	0	19	2	0
8	C	1	0	0	0	0
9	D	1	0	0	0	0
10	E	27	0	20	2	0
11	F	4	0	0	1	0
12	F	53	0	29	3	0
All	All	13614	0	13620	385	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (385) 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)
4:D:72:ILE:HG21	5:E:117:THR:HG21	1.56	0.85
5:E:64:LEU:HG	5:E:65:LYS:H	1.46	0.81
4:D:128:ILE:H	4:D:129:PRO:HD2	1.47	0.78
1:A:193:LYS:HG3	1:A:210:VAL:HG22	1.67	0.77
2:B:213:PHE:HA	2:B:220:ILE:HG21	1.64	0.77
3:C:118:ARG:NH1	3:C:119:ALA:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TYR:HE2	1:A:394:LEU:HD12	1.52	0.74
4:D:83:VAL:HG21	4:D:109:ILE:HG12	1.68	0.74
2:B:169:ILE:O	2:B:209:ARG:NH1	2.21	0.73
1:A:299:ILE:HD11	2:B:47:VAL:HG11	1.70	0.72
1:A:81:ARG:NH1	1:A:85:ARG:O	2.23	0.72
1:A:156:THR:HG21	1:A:217:ALA:HB3	1.72	0.71
2:B:326:PRO:HG2	2:B:330:HIS:HB2	1.73	0.71
7:C:301:FMN:HM81	5:E:23:LEU:HD13	1.72	0.71
6:F:39:ILE:HD11	6:F:45:LYS:HB3	1.73	0.71
5:E:99:ASP:HA	5:E:103:PRO:HG3	1.73	0.71
6:F:36:THR:HG22	6:F:48:VAL:HG12	1.73	0.71
1:A:7:GLY:HA3	1:A:385:PRO:HG3	1.71	0.70
6:F:270:LYS:HE3	6:F:402:LEU:HD11	1.74	0.69
3:C:118:ARG:HH11	3:C:118:ARG:HG2	1.59	0.68
4:D:32:LEU:HD12	5:E:23:LEU:HD21	1.76	0.68
4:D:9:LYS:HG2	4:D:12:LEU:HD12	1.76	0.68
4:D:34:VAL:HG21	4:D:44:MET:HG3	1.75	0.67
2:B:399:VAL:HG22	10:E:201:RBF:HC82	1.75	0.67
4:D:157:SER:OG	4:D:158:GLY:N	2.27	0.67
1:A:398:CYS:HA	1:A:434:LEU:HD21	1.77	0.67
2:B:391:LEU:HD22	5:E:186:MET:HG2	1.75	0.67
4:D:70:VAL:N	5:E:92:GLN:OE1	2.27	0.67
4:D:14:PRO:O	4:D:18:ASN:N	2.27	0.67
2:B:137:PHE:HA	2:B:159:PHE:HE2	1.60	0.66
1:A:438:CYS:HA	1:A:441:LYS:HD2	1.78	0.66
5:E:109:LEU:HD11	5:E:113:LEU:HG	1.77	0.66
5:E:28:PHE:HA	5:E:154:ILE:HD11	1.76	0.66
6:F:134:GLU:OE2	6:F:257:LYS:NZ	2.29	0.65
1:A:216:PRO:HB2	1:A:222:THR:HG21	1.77	0.65
2:B:215:ALA:HA	4:D:181:MET:H	1.62	0.65
6:F:81:VAL:HG11	6:F:110:ALA:HB2	1.78	0.65
2:B:314:VAL:HG22	2:B:315:ILE:HG23	1.80	0.64
3:C:25:ILE:HG21	4:D:81:SER:HB2	1.79	0.64
4:D:71:ARG:NH2	4:D:119:GLU:OE1	2.31	0.64
6:F:143:LYS:HB3	6:F:318:PHE:CG	2.33	0.64
2:B:136:VAL:HG13	2:B:183:ILE:HG21	1.80	0.64
2:B:169:ILE:HG22	2:B:338:PHE:HE2	1.63	0.64
2:B:375:ASN:ND2	5:E:192:SER:O	2.30	0.63
4:D:76:MET:HB3	5:E:84:ILE:HD13	1.79	0.63
1:A:8:LEU:HB3	1:A:9:ASP:HB3	1.81	0.63
3:C:110:GLN:NE2	3:C:242:MET:SD	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ASN:ND2	6:F:43:PRO:O	2.31	0.63
2:B:293:ALA:HB1	2:B:294:SER:HB2	1.81	0.62
1:A:138:LYS:NZ	1:A:443:GLU:OE2	2.32	0.62
4:D:38:LEU:N	4:D:153:GLU:OE1	2.21	0.62
1:A:65:GLY:HA3	1:A:142:ILE:HD13	1.81	0.62
5:E:102:PHE:HB3	5:E:103:PRO:HA	1.81	0.62
2:B:106:GLU:HA	2:B:110:GLY:H	1.65	0.62
3:C:94:ARG:NH1	3:C:169:GLU:OE1	2.26	0.62
5:E:28:PHE:O	5:E:32:SER:OG	2.17	0.62
2:B:101:HIS:HB3	2:B:127:THR:HB	1.80	0.61
3:C:23:SER:HA	6:F:9:VAL:HG22	1.82	0.61
6:F:104:ARG:HD3	6:F:105:GLU:HG2	1.82	0.61
4:D:13:ALA:HA	4:D:16:LEU:HD23	1.82	0.61
6:F:24:PHE:HA	6:F:27:SER:HB3	1.83	0.61
2:B:313:ASN:HD21	2:B:326:PRO:HA	1.65	0.61
2:B:318:ASP:O	2:B:320:ASN:N	2.33	0.61
6:F:70:CYS:HB3	6:F:76:CYS:HB3	1.82	0.60
2:B:139:VAL:HG13	2:B:183:ILE:HD11	1.82	0.60
2:B:380:GLU:HG2	2:B:382:MET:H	1.65	0.60
3:C:146:TRP:HD1	3:C:172:GLU:HA	1.66	0.60
3:C:50:LEU:HD22	3:C:55:ILE:HG21	1.83	0.60
4:D:152:ARG:NH2	4:D:183:LEU:O	2.34	0.60
2:B:292:ILE:HG22	2:B:293:ALA:H	1.67	0.59
4:D:21:ILE:HD11	4:D:137:ASN:O	2.01	0.59
4:D:77:ALA:O	4:D:81:SER:OG	2.17	0.59
4:D:195:ILE:HD12	5:E:176:LEU:HD23	1.84	0.59
1:A:16:PRO:HA	1:A:272:PRO:HB2	1.84	0.59
6:F:196:ASN:O	6:F:199:ARG:HG2	2.03	0.59
4:D:196:TRP:CD1	5:E:173:LEU:HD11	2.38	0.59
1:A:411:LEU:O	1:A:413:LEU:N	2.36	0.59
4:D:48:VAL:HG21	4:D:141:TYR:HD2	1.68	0.59
2:B:308:LEU:HD22	2:B:366:VAL:HG13	1.85	0.58
1:A:39:MET:O	1:A:40:ARG:NH1	2.30	0.58
4:D:128:ILE:H	4:D:129:PRO:CD	2.17	0.58
4:D:16:LEU:HD22	4:D:139:LEU:HD22	1.85	0.58
5:E:173:LEU:H	5:E:173:LEU:HD13	1.69	0.58
2:B:175:PRO:HB2	2:B:177:TRP:CD1	2.39	0.58
1:A:175:VAL:HG13	1:A:201:SER:HA	1.85	0.58
4:D:199:ARG:HG2	4:D:204:GLU:HG3	1.86	0.58
3:C:31:VAL:HB	6:F:5:ILE:HD11	1.85	0.58
1:A:101:THR:HG22	1:A:255:GLU:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:21:PHE:HA	5:E:22:PHE:O	2.04	0.58
2:B:367:MET:O	2:B:371:ILE:HG12	2.04	0.57
6:F:135:CYS:HB3	6:F:152:LEU:HB3	1.87	0.57
4:D:21:ILE:H	4:D:21:ILE:HD12	1.67	0.57
2:B:232:TYR:HE1	2:B:250:ILE:HB	1.69	0.57
3:C:210:ALA:H	3:C:219:ASP:HA	1.70	0.57
6:F:382:MET:N	6:F:382:MET:SD	2.71	0.57
2:B:372:ARG:HE	2:B:380:GLU:HG3	1.69	0.57
4:D:105:VAL:O	4:D:109:ILE:HG13	2.04	0.57
2:B:209:ARG:HH22	7:B:600:FMN:H1'2	1.70	0.57
4:D:127:PRO:HB2	4:D:129:PRO:HD2	1.86	0.57
3:C:18:LEU:HD23	6:F:16:LEU:HD21	1.86	0.57
2:B:105:THR:HG21	2:B:124:LEU:HD13	1.86	0.56
6:F:270:LYS:NZ	6:F:399:GLU:O	2.22	0.56
4:D:104:PHE:O	4:D:108:ILE:HG13	2.05	0.56
3:C:150:TYR:HB3	3:C:168:TYR:CZ	2.41	0.56
5:E:112:PHE:O	5:E:116:ILE:HG13	2.05	0.56
5:E:50:THR:O	5:E:54:PRO:HD2	2.06	0.56
1:A:389:GLU:OE2	2:B:353:THR:OG1	2.23	0.56
2:B:372:ARG:NH2	2:B:380:GLU:OE2	2.38	0.56
4:D:185:PRO:HG3	5:E:187:ALA:HB3	1.87	0.56
2:B:202:LEU:HD21	5:E:185:LEU:HB3	1.87	0.56
3:C:6:ASP:OD1	3:C:9:LYS:N	2.34	0.55
5:E:24:GLY:HA3	5:E:121:ALA:HB2	1.87	0.55
4:D:98:SER:HA	4:D:101:LEU:HB2	1.87	0.55
2:B:318:ASP:HB2	2:B:323:PHE:HB2	1.89	0.55
2:B:85:HIS:CE1	2:B:250:ILE:HG21	2.41	0.55
4:D:144:VAL:O	4:D:148:VAL:HG12	2.06	0.55
5:E:53:VAL:HB	5:E:126:VAL:HG12	1.87	0.55
4:D:195:ILE:HD11	5:E:177:GLY:HA2	1.89	0.55
2:B:232:TYR:CE1	2:B:250:ILE:HB	2.43	0.54
5:E:103:PRO:HB2	5:E:106:TYR:H	1.72	0.54
6:F:297:LYS:HE2	6:F:326:LEU:HD21	1.89	0.54
4:D:52:THR:HG22	4:D:114:VAL:HA	1.88	0.54
4:D:11:VAL:O	4:D:15:VAL:HG22	2.07	0.54
6:F:36:THR:HA	6:F:48:VAL:HA	1.90	0.54
2:B:172:PRO:HD3	2:B:226:TRP:CZ3	2.43	0.54
5:E:34:LYS:O	5:E:38:SER:OG	2.25	0.54
1:A:384:MET:HG3	1:A:390:PRO:HG3	1.89	0.54
5:E:109:LEU:O	5:E:111:ILE:N	2.41	0.54
3:C:41:ALA:HA	3:C:44:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HB3	1:A:265:ALA:HB3	1.89	0.54
6:F:92:PRO:O	6:F:96:ASP:HB2	2.08	0.54
6:F:82:LYS:O	6:F:121:LEU:HA	2.09	0.53
3:C:194:LEU:HA	3:C:203:ILE:HG12	1.90	0.53
5:E:23:LEU:HD23	5:E:25:MET:HG2	1.90	0.53
4:D:71:ARG:HG3	4:D:72:ILE:HG13	1.89	0.53
1:A:63:ASN:ND2	1:A:139:VAL:O	2.42	0.53
1:A:137:SER:OG	1:A:414:ASP:OD2	2.27	0.53
3:C:95:LYS:O	3:C:99:GLU:HG2	2.08	0.53
6:F:123:LEU:O	6:F:125:GLU:N	2.41	0.53
3:C:6:ASP:HB3	3:C:9:LYS:HB3	1.91	0.53
1:A:304:LEU:O	1:A:419:ALA:HB1	2.08	0.53
2:B:217:PRO:HA	2:B:220:ILE:HG22	1.91	0.52
1:A:193:LYS:O	1:A:210:VAL:HA	2.08	0.52
2:B:315:ILE:HB	2:B:316:GLY:HA2	1.92	0.52
3:C:36:LYS:O	3:C:40:ASN:ND2	2.41	0.52
5:E:60:TYR:HA	5:E:63:VAL:HG12	1.90	0.52
6:F:217:TYR:CE1	6:F:220:GLU:HG3	2.44	0.52
5:E:49:LEU:HD13	5:E:122:ILE:HG13	1.92	0.52
2:B:372:ARG:NE	2:B:380:GLU:HG3	2.24	0.52
5:E:92:GLN:HB3	6:F:23:LEU:HD21	1.91	0.52
6:F:276:MET:HB2	6:F:305:MET:HG2	1.92	0.51
5:E:93:ILE:O	5:E:97:ILE:HG13	2.09	0.51
4:D:204:GLU:HB2	4:D:205:GLN:HB2	1.91	0.51
5:E:53:VAL:O	5:E:57:ASN:N	2.43	0.51
2:B:156:ASN:OD1	2:B:157:GLU:N	2.44	0.51
2:B:380:GLU:HG2	2:B:382:MET:N	2.25	0.51
4:D:152:ARG:NH2	4:D:182:LEU:O	2.42	0.51
4:D:187:ALA:O	4:D:191:ILE:HG23	2.10	0.51
1:A:154:MET:HA	1:A:163:PRO:HG2	1.93	0.51
5:E:36:LYS:HG3	10:E:201:RBF:O4	2.11	0.51
6:F:89:ASP:N	6:F:89:ASP:OD1	2.44	0.51
2:B:370:LEU:HD23	2:B:371:ILE:HD13	1.93	0.51
5:E:61:ASN:HD22	5:E:61:ASN:N	2.09	0.51
2:B:395:LEU:O	2:B:399:VAL:HG23	2.11	0.51
4:D:101:LEU:HD23	4:D:104:PHE:HD2	1.74	0.51
3:C:118:ARG:HD3	3:C:237:PHE:CZ	2.46	0.50
5:E:93:ILE:HG22	5:E:97:ILE:HD11	1.93	0.50
6:F:5:ILE:O	6:F:9:VAL:HG23	2.11	0.50
3:C:118:ARG:HH11	3:C:118:ARG:CG	2.24	0.50
3:C:125:TYR:HB2	3:C:137:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:VAL:N	6:F:31:PRO:HD2	2.27	0.50
1:A:263:SER:HB3	1:A:322:GLN:HB2	1.93	0.50
3:C:158:ASP:O	3:C:252:ARG:HG2	2.11	0.50
3:C:97:ALA:O	3:C:117:ARG:HB2	2.12	0.50
6:F:210:ARG:HB3	12:F:502:FAD:O2'	2.12	0.50
1:A:411:LEU:C	1:A:413:LEU:H	2.15	0.50
4:D:21:ILE:HD13	4:D:141:TYR:HB2	1.92	0.50
5:E:36:LYS:H	5:E:36:LYS:HD2	1.76	0.50
2:B:175:PRO:HD2	2:B:178:GLN:HG3	1.92	0.50
6:F:26:LYS:HZ2	6:F:30:VAL:HG21	1.77	0.50
6:F:37:ILE:N	6:F:47:ILE:O	2.44	0.50
2:B:222:GLY:HA2	2:B:226:TRP:HE1	1.76	0.50
4:D:152:ARG:HG3	4:D:190:LEU:HD23	1.94	0.49
6:F:170:ILE:HG12	6:F:260:ILE:HG22	1.94	0.49
6:F:42:ASP:HB2	6:F:43:PRO:HD3	1.95	0.49
2:B:145:VAL:HG22	2:B:155:VAL:HG21	1.93	0.49
4:D:17:ASP:O	4:D:20:PRO:HD3	2.11	0.49
5:E:87:ILE:HA	5:E:90:LEU:HD11	1.93	0.49
3:C:103:SER:HA	3:C:119:ALA:HA	1.95	0.49
2:B:76:GLY:HA3	2:B:121:LYS:O	2.13	0.49
3:C:192:LYS:NZ	3:C:217:GLY:O	2.23	0.49
5:E:16:ASN:OD1	5:E:196:VAL:HB	2.12	0.49
1:A:71:PRO:HA	1:A:258:THR:HG21	1.94	0.49
4:D:72:ILE:H	5:E:92:GLN:HE22	1.61	0.49
2:B:238:LEU:HD22	2:B:380:GLU:HB2	1.95	0.49
4:D:104:PHE:CD1	4:D:107:LEU:HD11	2.48	0.49
5:E:19:LEU:HD23	5:E:146:SER:HB2	1.94	0.49
6:F:77:GLY:N	11:F:501:FES:S2	2.85	0.49
1:A:135:PRO:HB2	1:A:411:LEU:O	2.13	0.48
2:B:280:LEU:HD11	2:B:341:PHE:HB2	1.95	0.48
5:E:51:ILE:HG22	5:E:90:LEU:HD22	1.95	0.48
1:A:122:LEU:HD13	1:A:131:PHE:HE2	1.78	0.48
2:B:318:ASP:HB2	2:B:323:PHE:CB	2.43	0.48
5:E:32:SER:O	5:E:161:ARG:HG3	2.13	0.48
6:F:217:TYR:CE2	6:F:219:GLU:HB2	2.49	0.48
6:F:26:LYS:NZ	6:F:30:VAL:HG21	2.28	0.48
3:C:248:LEU:O	3:C:252:ARG:HG3	2.13	0.48
1:A:234:HIS:ND1	1:A:234:HIS:N	2.62	0.48
1:A:309:ALA:HB1	1:A:314:ALA:HA	1.94	0.48
6:F:130:VAL:HG12	6:F:130:VAL:O	2.13	0.48
2:B:382:MET:HG2	7:B:600:FMN:HM72	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD22	1:A:215:HIS:H	1.78	0.48
2:B:169:ILE:HD12	2:B:170:VAL:HG13	1.95	0.48
3:C:118:ARG:HD3	3:C:237:PHE:HZ	1.79	0.48
4:D:49:MET:HG3	4:D:138:GLY:HA3	1.96	0.48
5:E:25:MET:HA	5:E:28:PHE:HB3	1.96	0.48
2:B:80:ILE:HD13	2:B:111:THR:HG23	1.96	0.47
1:A:418:LEU:HD12	1:A:435:LEU:HB2	1.95	0.47
4:D:20:PRO:HG2	4:D:23:LEU:HB3	1.95	0.47
2:B:203:ASN:HB3	2:B:206:LEU:HB2	1.96	0.47
3:C:145:LEU:HD13	3:C:226:LEU:HD13	1.95	0.47
5:E:18:ALA:O	5:E:21:PHE:N	2.46	0.47
2:B:159:PHE:HE1	2:B:187:VAL:HG21	1.79	0.47
2:B:206:LEU:HD13	2:B:386:ILE:HG21	1.96	0.47
4:D:113:ILE:HD11	4:D:137:ASN:HB3	1.97	0.47
5:E:46:ILE:HD11	5:E:151:MET:HG2	1.96	0.47
2:B:172:PRO:HG2	2:B:220:ILE:HD12	1.96	0.47
2:B:46:HIS:NE2	2:B:48:ARG:O	2.45	0.47
2:B:236:THR:HG21	7:B:600:FMN:O3P	2.15	0.47
6:F:399:GLU:H	6:F:399:GLU:CD	2.17	0.47
2:B:367:MET:HB3	2:B:385:ALA:HB1	1.96	0.47
4:D:54:LEU:H	4:D:54:LEU:HD13	1.79	0.47
2:B:175:PRO:O	2:B:177:TRP:N	2.46	0.47
1:A:134:ARG:HA	1:A:135:PRO:HA	1.66	0.47
1:A:53:LYS:HE2	1:A:99:GLN:HB3	1.96	0.47
4:D:148:VAL:HG23	4:D:190:LEU:HB3	1.96	0.47
6:F:56:LEU:HD22	6:F:111:CYS:HB3	1.97	0.47
2:B:60:VAL:HG12	2:B:287:ILE:HG21	1.96	0.47
3:C:34:ARG:HA	3:C:37:GLN:HE21	1.79	0.47
4:D:142:GLY:O	4:D:146:MET:N	2.46	0.47
5:E:119:ASN:HB3	5:E:122:ILE:HB	1.96	0.46
1:A:231:SER:OG	1:A:412:GLU:OE2	2.30	0.46
2:B:294:SER:HB3	2:B:297:ILE:HB	1.98	0.46
6:F:171:GLU:HG2	6:F:259:THR:O	2.16	0.46
6:F:83:ILE:HD12	6:F:108:ARG:HB2	1.97	0.46
2:B:353:THR:HG23	2:B:356:GLY:H	1.81	0.46
6:F:65:PHE:CD2	6:F:128:PHE:HB2	2.50	0.46
1:A:36:TYR:HB2	1:A:39:MET:HB2	1.97	0.46
4:D:48:VAL:HG21	4:D:141:TYR:CD2	2.47	0.46
5:E:33:LYS:HE3	5:E:33:LYS:HB2	1.72	0.46
3:C:66:LEU:HD23	3:C:66:LEU:HA	1.63	0.46
4:D:142:GLY:O	4:D:146:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:GLU:OE1	3:C:227:THR:OG1	2.26	0.46
1:A:134:ARG:HD2	1:A:135:PRO:HA	1.98	0.46
2:B:185:PHE:CD2	2:B:211:PHE:HB2	2.51	0.46
6:F:219:GLU:CD	6:F:298:ARG:HG3	2.36	0.46
6:F:98:ILE:HG22	6:F:98:ILE:O	2.16	0.45
2:B:49:ASP:OD1	2:B:50:SER:N	2.49	0.45
3:C:45:LYS:HE2	3:C:168:TYR:CE2	2.50	0.45
4:D:142:GLY:HA2	4:D:145:LEU:HG	1.99	0.45
2:B:99:ASN:HB3	2:B:101:HIS:ND1	2.32	0.45
5:E:48:VAL:HG13	5:E:90:LEU:HD13	1.98	0.45
2:B:52:ASP:O	2:B:53:LEU:HB2	2.15	0.45
1:A:222:THR:HG22	1:A:386:LEU:HD11	1.98	0.45
6:F:245:MET:H	12:F:502:FAD:P	2.39	0.45
6:F:91:LEU:HB2	6:F:94:GLU:H	1.82	0.45
2:B:224:LEU:HA	2:B:225:VAL:HA	1.53	0.45
2:B:401:VAL:O	2:B:404:ASN:HB3	2.16	0.45
3:C:72:GLU:OE2	3:C:74:ARG:HD3	2.17	0.45
2:B:297:ILE:O	2:B:301:VAL:HG12	2.17	0.45
5:E:178:ILE:O	5:E:182:THR:HG23	2.17	0.45
2:B:174:LEU:O	2:B:176:LEU:N	2.45	0.45
3:C:105:LYS:HB2	3:C:117:ARG:NH1	2.32	0.45
6:F:38:SER:HB3	6:F:120:ASP:HA	1.98	0.45
3:C:172:GLU:O	4:D:103:VAL:HG11	2.17	0.45
6:F:211:ALA:HB3	12:F:502:FAD:C8	2.47	0.44
3:C:25:ILE:HG13	3:C:26:VAL:N	2.31	0.44
6:F:13:LEU:HD12	6:F:16:LEU:HD22	1.98	0.44
7:B:600:FMN:H1'1	7:B:600:FMN:H9	1.62	0.44
3:C:146:TRP:CZ3	5:E:128:PHE:HE1	2.35	0.44
6:F:96:ASP:O	6:F:99:SER:HB3	2.17	0.44
1:A:150:PHE:CZ	1:A:224:MET:HG2	2.52	0.44
1:A:62:LYS:HE2	6:F:399:GLU:OE2	2.17	0.44
5:E:60:TYR:CZ	5:E:64:LEU:HD22	2.53	0.44
1:A:297:ARG:HD3	1:A:297:ARG:HA	1.89	0.44
2:B:314:VAL:HG13	2:B:315:ILE:HG12	1.99	0.44
2:B:395:LEU:HD11	5:E:155:VAL:O	2.17	0.44
6:F:134:GLU:HA	6:F:259:THR:HA	1.99	0.44
2:B:214:PHE:HZ	2:B:384:LEU:HD21	1.82	0.44
4:D:60:SER:HB2	4:D:127:PRO:N	2.33	0.44
1:A:304:LEU:HA	2:B:46:HIS:CE1	2.52	0.44
4:D:71:ARG:HH12	4:D:119:GLU:HG2	1.83	0.44
5:E:10:LYS:O	5:E:14:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:ILE:HG12	5:E:148:VAL:HG23	1.99	0.44
6:F:39:ILE:HG12	6:F:45:LYS:O	2.18	0.44
1:A:39:MET:HG2	1:A:60:ASP:CG	2.39	0.44
3:C:71:ILE:HG23	3:C:125:TYR:HB3	2.00	0.44
1:A:41:PRO:HA	1:A:59:GLU:O	2.18	0.43
1:A:192:CYS:HB3	1:A:223:HIS:CE1	2.53	0.43
3:C:109:GLU:OE2	3:C:110:GLN:HG3	2.18	0.43
3:C:188:GLN:HE22	3:C:219:ASP:CG	2.21	0.43
4:D:196:TRP:HA	5:E:173:LEU:HG	2.00	0.43
4:D:30:SER:O	4:D:34:VAL:HG23	2.18	0.43
5:E:87:ILE:HD13	5:E:122:ILE:HG23	2.01	0.43
1:A:305:SER:HB3	1:A:416:GLU:OE1	2.19	0.43
2:B:59:MET:HG2	2:B:292:ILE:HD11	2.00	0.43
6:F:74:GLY:HA2	6:F:111:CYS:SG	2.59	0.43
1:A:119:LYS:O	1:A:123:VAL:HG23	2.18	0.43
2:B:380:GLU:O	7:B:600:FMN:N3	2.51	0.43
3:C:22:CYS:SG	6:F:9:VAL:HA	2.59	0.43
6:F:65:PHE:HZ	6:F:123:LEU:HD13	1.83	0.43
2:B:131:PRO:O	2:B:135:THR:HG22	2.19	0.43
2:B:284:ALA:O	2:B:288:VAL:HG12	2.18	0.43
6:F:278:PHE:HE2	6:F:291:HIS:HB3	1.84	0.43
6:F:34:ASP:N	6:F:34:ASP:OD1	2.52	0.43
6:F:170:ILE:O	6:F:209:ILE:HA	2.19	0.43
2:B:54:LYS:HE3	2:B:157:GLU:HG3	2.00	0.43
2:B:407:ARG:HA	2:B:408:ARG:C	2.39	0.43
3:C:11:THR:HG21	6:F:24:PHE:CE1	2.54	0.43
1:A:74:GLY:HA3	1:A:93:GLU:O	2.19	0.42
2:B:248:ALA:HB1	2:B:267:ASN:O	2.19	0.42
6:F:12:THR:O	6:F:16:LEU:HB3	2.19	0.42
2:B:103:TRP:C	2:B:103:TRP:CD1	2.92	0.42
4:D:191:ILE:HD12	4:D:195:ILE:HD13	2.01	0.42
4:D:41:ALA:O	4:D:45:THR:HG22	2.18	0.42
5:E:53:VAL:HG22	5:E:54:PRO:HD3	2.02	0.42
7:C:301:FMN:H9	7:C:301:FMN:H1'1	1.82	0.42
6:F:306:SER:HA	6:F:334:VAL:O	2.19	0.42
1:A:41:PRO:O	1:A:61:LYS:NZ	2.53	0.42
3:C:165:LEU:HD13	3:C:235:PHE:HZ	1.84	0.42
5:E:44:ALA:O	5:E:48:VAL:HG23	2.20	0.42
2:B:48:ARG:HA	2:B:48:ARG:NE	2.34	0.42
2:B:53:LEU:HB3	2:B:54:LYS:H	1.64	0.42
1:A:36:TYR:O	1:A:39:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:53:VAL:HG13	5:E:54:PRO:CD	2.50	0.42
5:E:53:VAL:HG13	5:E:54:PRO:HD2	2.01	0.42
3:C:174:PRO:HG3	4:D:100:GLN:HB3	2.01	0.41
3:C:209:GLY:HA2	3:C:219:ASP:HA	2.01	0.41
4:D:26:LEU:HA	4:D:27:GLY:HA2	1.57	0.41
4:D:71:ARG:HH22	4:D:119:GLU:HG2	1.84	0.41
6:F:65:PHE:CG	6:F:128:PHE:HB2	2.55	0.41
2:B:73:TYR:HA	2:B:122:MET:HA	2.02	0.41
2:B:392:PHE:HE1	5:E:152:LEU:HD12	1.85	0.41
4:D:152:ARG:HH21	4:D:182:LEU:C	2.24	0.41
2:B:338:PHE:CE1	2:B:342:PHE:HD2	2.38	0.41
5:E:109:LEU:CD1	5:E:113:LEU:HG	2.46	0.41
1:A:154:MET:HE1	1:A:217:ALA:HB1	2.02	0.41
3:C:195:PHE:HB3	3:C:199:HIS:HA	2.02	0.41
4:D:132:ILE:HG13	4:D:133:ASP:N	2.34	0.41
4:D:98:SER:O	4:D:102:SER:N	2.52	0.41
5:E:28:PHE:CD1	5:E:154:ILE:HG12	2.55	0.41
3:C:18:LEU:HG	6:F:16:LEU:HD11	2.01	0.41
3:C:141:HIS:HB3	3:C:150:TYR:CD2	2.56	0.41
4:D:161:PHE:CG	4:D:162:GLY:N	2.88	0.41
4:D:35:THR:HG21	4:D:148:VAL:HG13	2.03	0.41
6:F:360:TYR:HA	6:F:364:LEU:HB2	2.02	0.41
2:B:165:LEU:HA	2:B:165:LEU:HD23	1.82	0.41
2:B:211:PHE:CE1	4:D:180:LEU:HD11	2.56	0.41
2:B:311:LEU:HA	2:B:311:LEU:HD22	1.89	0.41
1:A:63:ASN:OD1	1:A:141:ALA:HA	2.21	0.41
1:A:154:MET:CA	1:A:163:PRO:HG2	2.51	0.41
2:B:354:ASN:HD22	2:B:354:ASN:HA	1.53	0.41
1:A:433:GLN:OE1	2:B:43:ARG:HG2	2.20	0.41
4:D:45:THR:O	4:D:49:MET:HB2	2.21	0.41
2:B:380:GLU:HA	2:B:381:GLY:HA3	1.87	0.41
3:C:11:THR:HA	3:C:14:VAL:HG12	2.02	0.41
6:F:94:GLU:OE2	6:F:108:ARG:NH1	2.53	0.41
1:A:134:ARG:HG3	1:A:224:MET:SD	2.61	0.41
4:D:90:LEU:HD13	4:D:90:LEU:HA	1.94	0.41
6:F:313:SER:HB2	6:F:346:ASP:OD2	2.21	0.41
2:B:57:MET:HG2	2:B:157:GLU:O	2.20	0.40
2:B:187:VAL:O	2:B:191:LYS:HB3	2.20	0.40
4:D:190:LEU:HD12	4:D:190:LEU:HA	1.75	0.40
4:D:72:ILE:H	5:E:92:GLN:NE2	2.19	0.40
1:A:134:ARG:CD	1:A:135:PRO:HA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:THR:N	2:B:198:GLY:HA3	2.36	0.40
2:B:183:ILE:HD12	2:B:184:THR:N	2.36	0.40
2:B:211:PHE:HE1	4:D:180:LEU:HD11	1.87	0.40
1:A:377:ILE:HG23	2:B:347:PRO:HG2	2.04	0.40
3:C:91:TYR:OH	3:C:121:VAL:O	2.24	0.40
1:A:10:LEU:HA	1:A:11:PRO:HD3	1.88	0.40
1:A:136:PHE:HE1	1:A:442:ILE:HD11	1.87	0.40
3:C:21:VAL:O	3:C:25:ILE:HG23	2.22	0.40
3:C:33:LEU:O	3:C:37:GLN:HG3	2.22	0.40
5:E:161:ARG:HE	5:E:161:ARG:HB3	1.65	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/449 (88%)	380 (96%)	9 (2%)	7 (2%)	8	41
2	B	340/415 (82%)	287 (84%)	39 (12%)	14 (4%)	3	23
3	C	249/257 (97%)	236 (95%)	13 (5%)	0	100	100
4	D	169/210 (80%)	145 (86%)	16 (10%)	8 (5%)	2	20
5	E	185/198 (93%)	155 (84%)	18 (10%)	12 (6%)	1	14
6	F	405/408 (99%)	371 (92%)	26 (6%)	8 (2%)	7	39
All	All	1744/1937 (90%)	1574 (90%)	121 (7%)	49 (3%)	5	32

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	12	ILE

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Mol	Chain	Res	Type
2	B	236	THR
2	B	319	THR
4	D	159	LYS
4	D	181	MET
5	E	22	PHE
5	E	102	PHE
5	E	110	GLY
6	F	101	GLY
1	A	412	GLU
1	A	424	VAL
2	B	53	LEU
2	B	200	ASN
2	B	292	ILE
4	D	157	SER
4	D	178	ASN
5	E	25	MET
5	E	68	ALA
6	F	87	GLY
6	F	127	ILE
6	F	262	GLY
1	A	411	LEU
2	B	45	SER
2	B	46	HIS
2	B	353	THR
2	B	377	ALA
4	D	128	ILE
4	D	164	GLU
5	E	26	CYS
5	E	34	LYS
1	A	379	ASN
1	A	425	CYS
2	B	109	GLY
2	B	376	PRO
5	E	103	PRO
5	E	167	SER
5	E	174	ARG
6	F	106	GLY
2	B	270	GLY
2	B	331	LEU
4	D	105	VAL
5	E	135	SER
5	E	171	PRO

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Mol	Chain	Res	Type
6	F	51	PRO
4	D	203	PRO
2	B	172	PRO
6	F	41	GLY
6	F	124	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	334/378 (88%)	311 (93%)	23 (7%)	15	47
2	B	256/320 (80%)	206 (80%)	50 (20%)	1	7
3	C	200/205 (98%)	192 (96%)	8 (4%)	31	64
4	D	143/176 (81%)	108 (76%)	35 (24%)	0	4
5	E	154/165 (93%)	123 (80%)	31 (20%)	1	6
6	F	333/337 (99%)	320 (96%)	13 (4%)	32	64
All	All	1420/1581 (90%)	1260 (89%)	160 (11%)	6	27

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	THR
1	A	6	LYS
1	A	10	LEU
1	A	12	ILE
1	A	137	SER
1	A	168	ASN
1	A	194	LYS
1	A	212	ASP
1	A	219	LEU
1	A	230	VAL
1	A	233	ASP
1	A	234	HIS

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Mol	Chain	Res	Type
1	A	326	LEU
1	A	379	ASN
1	A	388	MET
1	A	403	ASP
1	A	407	ARG
1	A	411	LEU
1	A	421	CYS
1	A	424	VAL
1	A	433	GLN
1	A	443	GLU
2	B	40	VAL
2	B	49	ASP
2	B	51	VAL
2	B	55	ARG
2	B	57	MET
2	B	62	LEU
2	B	74	ASN
2	B	78	GLN
2	B	101	HIS
2	B	103	TRP
2	B	111	THR
2	B	112	MET
2	B	122	MET
2	B	123	LEU
2	B	127	THR
2	B	137	PHE
2	B	139	VAL
2	B	146	LEU
2	B	149	MET
2	B	154	GLU
2	B	157	GLU
2	B	170	VAL
2	B	173	THR
2	B	200	ASN
2	B	203	ASN
2	B	224	LEU
2	B	225	VAL
2	B	227	THR
2	B	249	LEU
2	B	278	LEU
2	B	280	LEU
2	B	286	PHE

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Mol	Chain	Res	Type
2	B	290	MET
2	B	303	ILE
2	B	307	LEU
2	B	311	LEU
2	B	325	MET
2	B	343	MET
2	B	353	THR
2	B	354	ASN
2	B	355	SER
2	B	370	LEU
2	B	373	VAL
2	B	374	VAL
2	B	378	TYR
2	B	383	MET
2	B	406	LYS
2	B	407	ARG
2	B	408	ARG
2	B	409	LEU
3	C	10	LYS
3	C	18	LEU
3	C	20	LEU
3	C	45	LYS
3	C	109	GLU
3	C	118	ARG
3	C	165	LEU
3	C	176	LEU
4	D	14	PRO
4	D	15	VAL
4	D	16	LEU
4	D	21	ILE
4	D	26	LEU
4	D	30	SER
4	D	34	VAL
4	D	44	MET
4	D	45	THR
4	D	46	LEU
4	D	54	LEU
4	D	57	PHE
4	D	58	PHE
4	D	62	ILE
4	D	63	ARG
4	D	71	ARG

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Mol	Chain	Res	Type
4	D	84	ILE
4	D	87	ASP
4	D	113	ILE
4	D	128	ILE
4	D	132	ILE
4	D	133	ASP
4	D	139	LEU
4	D	155	LEU
4	D	163	LEU
4	D	166	LEU
4	D	178	ASN
4	D	181	MET
4	D	182	LEU
4	D	190	LEU
4	D	191	ILE
4	D	194	MET
4	D	195	ILE
4	D	200	THR
4	D	204	GLU
5	E	4	TYR
5	E	12	ILE
5	E	22	PHE
5	E	23	LEU
5	E	32	SER
5	E	38	SER
5	E	53	VAL
5	E	54	PRO
5	E	58	LEU
5	E	61	ASN
5	E	77	PHE
5	E	82	THR
5	E	90	LEU
5	E	92	GLN
5	E	95	GLU
5	E	96	MET
5	E	98	LEU
5	E	113	LEU
5	E	120	CYS
5	E	122	ILE
5	E	129	MET
5	E	134	TYR
5	E	151	MET

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Mol	Chain	Res	Type
5	E	152	LEU
5	E	154	ILE
5	E	173	LEU
5	E	176	LEU
5	E	178	ILE
5	E	181	ILE
5	E	191	MET
5	E	192	SER
6	F	13	LEU
6	F	16	LEU
6	F	29	LEU
6	F	34	ASP
6	F	66	VAL
6	F	89	ASP
6	F	99	SER
6	F	102	GLU
6	F	104	ARG
6	F	119	MET
6	F	122	GLU
6	F	266	GLU
6	F	382	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	209	HIS
2	B	85	HIS
2	B	313	ASN
2	B	354	ASN
3	C	37	GLN
3	C	40	ASN
3	C	90	ASN
3	C	110	GLN
4	D	24	GLN
5	E	61	ASN
5	E	92	GLN
6	F	227	ASN
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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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$
11	FES	F	501	6	0,4,4	0.00	-	-		
7	FMN	B	600	2	28,32,33	1.49	4 (14%)	32,47,50	1.87	6 (18%)
12	FAD	F	502	-	51,58,58	3.82	24 (47%)	60,89,89	2.10	13 (21%)
7	FMN	C	301	3	28,32,33	1.48	4 (14%)	32,47,50	1.65	5 (15%)
10	RBF	E	201	-	27,29,29	1.64	6 (22%)	33,43,43	2.84	8 (24%)

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
11	FES	F	501	6	-	-	0/1/1/1
10	RBF	E	201	-	-	7/14/14/14	0/3/3/3
7	FMN	B	600	2	-	9/15/17/18	0/3/3/3
7	FMN	C	301	3	-	0/15/17/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FAD	F	502	-	-	5/30/50/50	0/6/6/6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	502	FAD	C2B-C3B	-10.52	1.24	1.53
12	F	502	FAD	C10-N1	8.37	1.44	1.33
12	F	502	FAD	O4B-C1B	8.23	1.52	1.41
12	F	502	FAD	C5X-N5	7.85	1.48	1.35
12	F	502	FAD	C4X-C10	6.99	1.45	1.38
12	F	502	FAD	O4B-C4B	-6.68	1.30	1.45
12	F	502	FAD	C9A-N10	6.21	1.46	1.38
12	F	502	FAD	C4-C4X	5.66	1.51	1.41
12	F	502	FAD	C3B-C4B	5.54	1.67	1.53
12	F	502	FAD	C2B-C1B	5.53	1.62	1.53
12	F	502	FAD	C4X-N5	5.48	1.41	1.33
12	F	502	FAD	C2-N3	4.82	1.47	1.38
12	F	502	FAD	C4-N3	4.70	1.41	1.33
12	F	502	FAD	C2-N1	4.48	1.47	1.38
7	C	301	FMN	C10-N1	4.38	1.38	1.33
10	E	201	RBF	C4A-N5	4.18	1.39	1.33
7	B	600	FMN	C10-N1	4.15	1.38	1.33
12	F	502	FAD	C2A-N3A	3.93	1.38	1.32
12	F	502	FAD	O2B-C2B	3.31	1.50	1.43
7	C	301	FMN	C4A-N5	3.18	1.37	1.33
12	F	502	FAD	O2'-C2'	-3.12	1.36	1.43
7	B	600	FMN	C1'-N10	3.08	1.51	1.48
7	B	600	FMN	C4A-N5	3.07	1.37	1.33
7	B	600	FMN	C4-N3	2.91	1.38	1.33
10	E	201	RBF	C2'-C3'	-2.88	1.48	1.53
7	C	301	FMN	C4-N3	2.88	1.38	1.33
12	F	502	FAD	C1'-N10	2.87	1.51	1.48
10	E	201	RBF	C10-N1	2.86	1.36	1.33
12	F	502	FAD	O3B-C3B	2.83	1.49	1.43
10	E	201	RBF	O4'-C4'	-2.74	1.37	1.43
12	F	502	FAD	C6A-N6A	2.72	1.44	1.34
7	C	301	FMN	C1'-N10	2.63	1.50	1.48
12	F	502	FAD	C7M-C7	2.42	1.55	1.51
12	F	502	FAD	PA-O1A	2.24	1.58	1.50
12	F	502	FAD	C4A-N3A	2.21	1.38	1.35
10	E	201	RBF	C9A-C5A	-2.14	1.38	1.42
10	E	201	RBF	C1'-N10	-2.06	1.46	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	502	FAD	C8A-N7A	2.05	1.38	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	201	RBF	C1'-N10-C9A	11.16	127.08	118.29
12	F	502	FAD	C1B-N9A-C4A	-8.75	111.27	126.64
10	E	201	RBF	C1'-N10-C10	-6.54	112.56	118.41
7	B	600	FMN	C4-N3-C2	6.02	120.22	115.14
12	F	502	FAD	C4-N3-C2	5.85	120.08	115.14
10	E	201	RBF	C4-N3-C2	5.63	119.89	115.14
12	F	502	FAD	N3A-C2A-N1A	-5.52	120.05	128.68
7	C	301	FMN	C4-N3-C2	5.52	119.80	115.14
7	B	600	FMN	C1'-N10-C10	4.91	122.80	118.41
7	B	600	FMN	C5A-C9A-N10	4.30	120.83	117.72
12	F	502	FAD	C3B-C2B-C1B	4.05	107.08	100.98
7	C	301	FMN	C4A-N5-C5A	3.38	120.15	116.77
10	E	201	RBF	C7M-C7-C8	3.34	127.57	120.74
10	E	201	RBF	C7M-C7-C6	-3.28	112.49	120.34
10	E	201	RBF	C4A-N5-C5A	3.27	120.04	116.77
7	B	600	FMN	C4A-N5-C5A	3.25	120.02	116.77
12	F	502	FAD	C4X-N5-C5X	3.22	119.98	116.77
12	F	502	FAD	C2B-C3B-C4B	3.15	108.76	102.64
7	C	301	FMN	C5A-C9A-N10	2.97	119.87	117.72
7	C	301	FMN	C1'-N10-C9A	2.95	120.61	118.29
12	F	502	FAD	C5X-C9A-N10	2.93	119.84	117.72
7	B	600	FMN	C4A-C4-N3	-2.71	119.73	123.43
10	E	201	RBF	C5A-C9A-N10	2.71	119.68	117.72
12	F	502	FAD	C5A-C6A-N6A	2.69	124.44	120.35
12	F	502	FAD	C1'-N10-C9A	2.69	120.41	118.29
12	F	502	FAD	C7M-C7-C6	-2.60	114.13	120.34
12	F	502	FAD	C4X-C4-N3	-2.56	119.92	123.43
7	C	301	FMN	C4A-C4-N3	-2.44	120.09	123.43
12	F	502	FAD	P-O3P-PA	-2.44	124.47	132.83
10	E	201	RBF	C4A-C4-N3	-2.36	120.20	123.43
12	F	502	FAD	C7M-C7-C8	2.34	125.53	120.74
7	B	600	FMN	C9A-N10-C10	-2.24	118.98	121.91

There are no chirality outliers.

All (21) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
7	B	600	FMN	C2'-C1'-N10-C9A
7	B	600	FMN	N10-C1'-C2'-O2'
7	B	600	FMN	N10-C1'-C2'-C3'
7	B	600	FMN	C1'-C2'-C3'-O3'
7	B	600	FMN	C1'-C2'-C3'-C4'
7	B	600	FMN	O2'-C2'-C3'-C4'
7	B	600	FMN	C3'-C4'-C5'-O5'
7	B	600	FMN	O4'-C4'-C5'-O5'
12	F	502	FAD	C1'-C2'-C3'-C4'
10	E	201	RBF	C1'-C2'-C3'-O3'
10	E	201	RBF	C1'-C2'-C3'-C4'
7	B	600	FMN	O2'-C2'-C3'-O3'
10	E	201	RBF	O2'-C2'-C3'-O3'
10	E	201	RBF	O2'-C2'-C3'-C4'
12	F	502	FAD	O2'-C2'-C3'-C4'
10	E	201	RBF	O4'-C4'-C5'-O5'
12	F	502	FAD	C5B-O5B-PA-O1A
12	F	502	FAD	O2'-C2'-C3'-O3'
12	F	502	FAD	C5B-O5B-PA-O3P
10	E	201	RBF	C3'-C4'-C5'-O5'
10	E	201	RBF	O3'-C3'-C4'-C5'

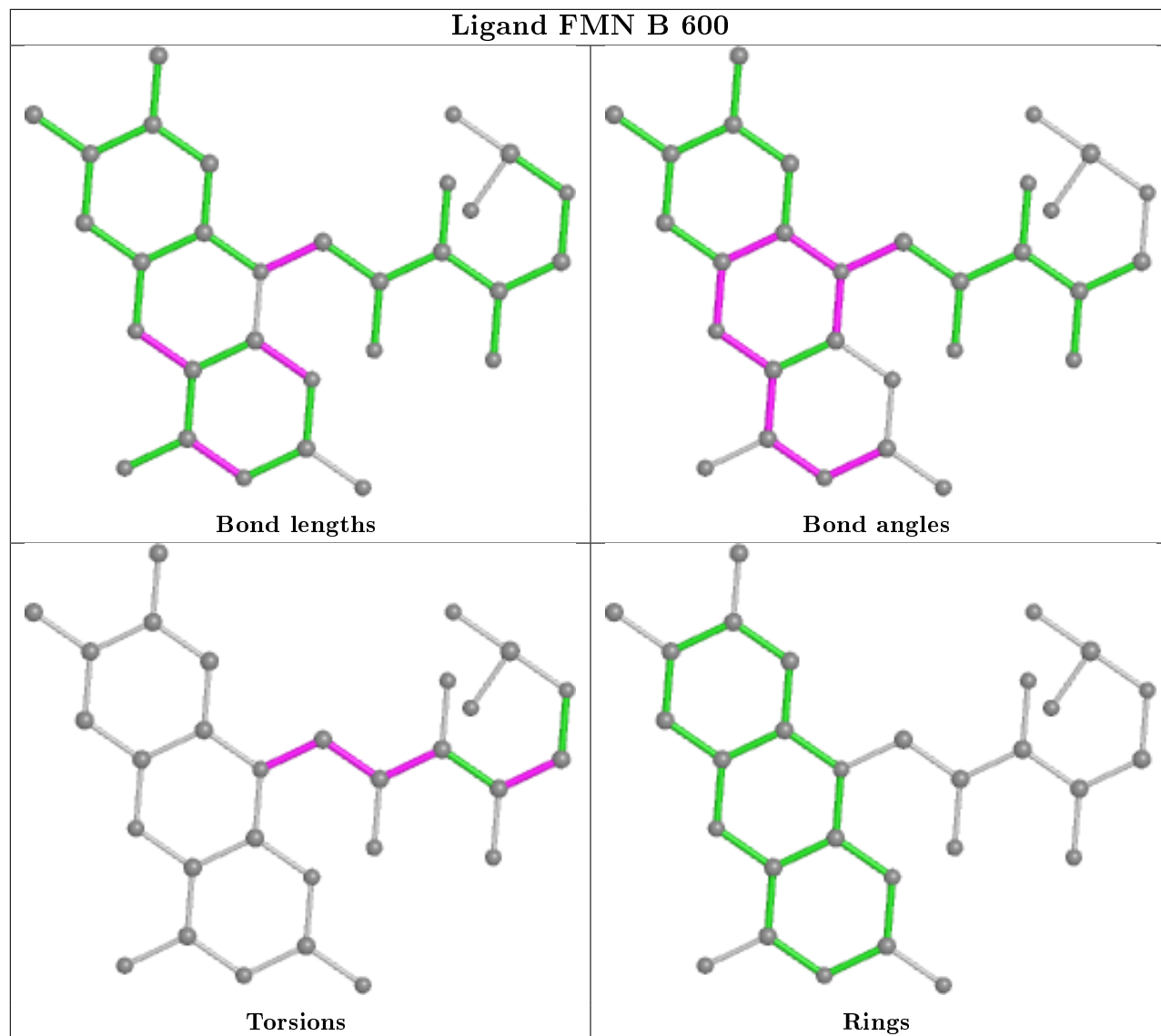
There are no ring outliers.

5 monomers are involved in 13 short contacts:

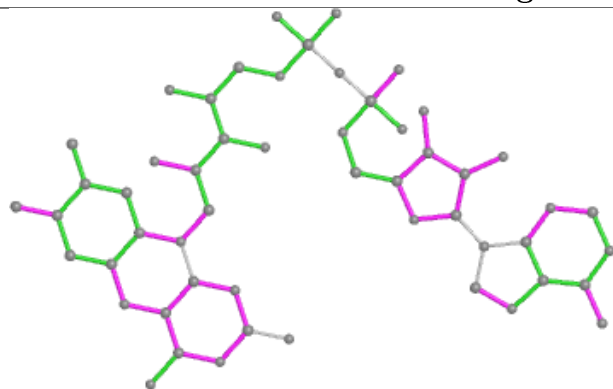
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	501	FES	1	0
7	B	600	FMN	5	0
12	F	502	FAD	3	0
7	C	301	FMN	2	0
10	E	201	RBF	2	0

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

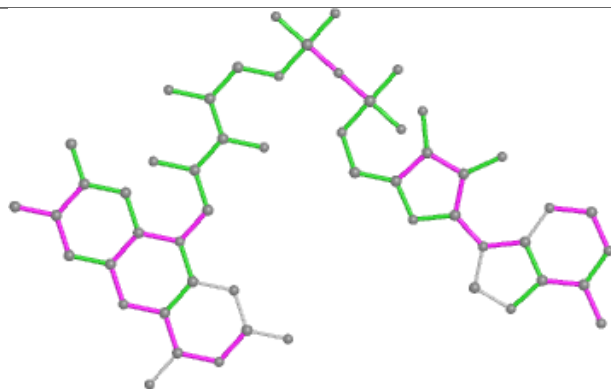
equivalents in the CSD to analyse the geometry.



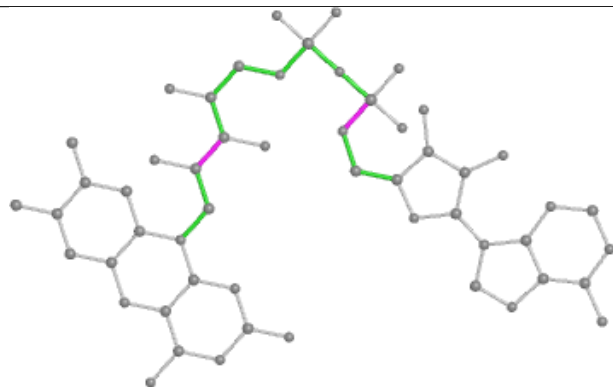
## Ligand FAD F 502



Bond lengths



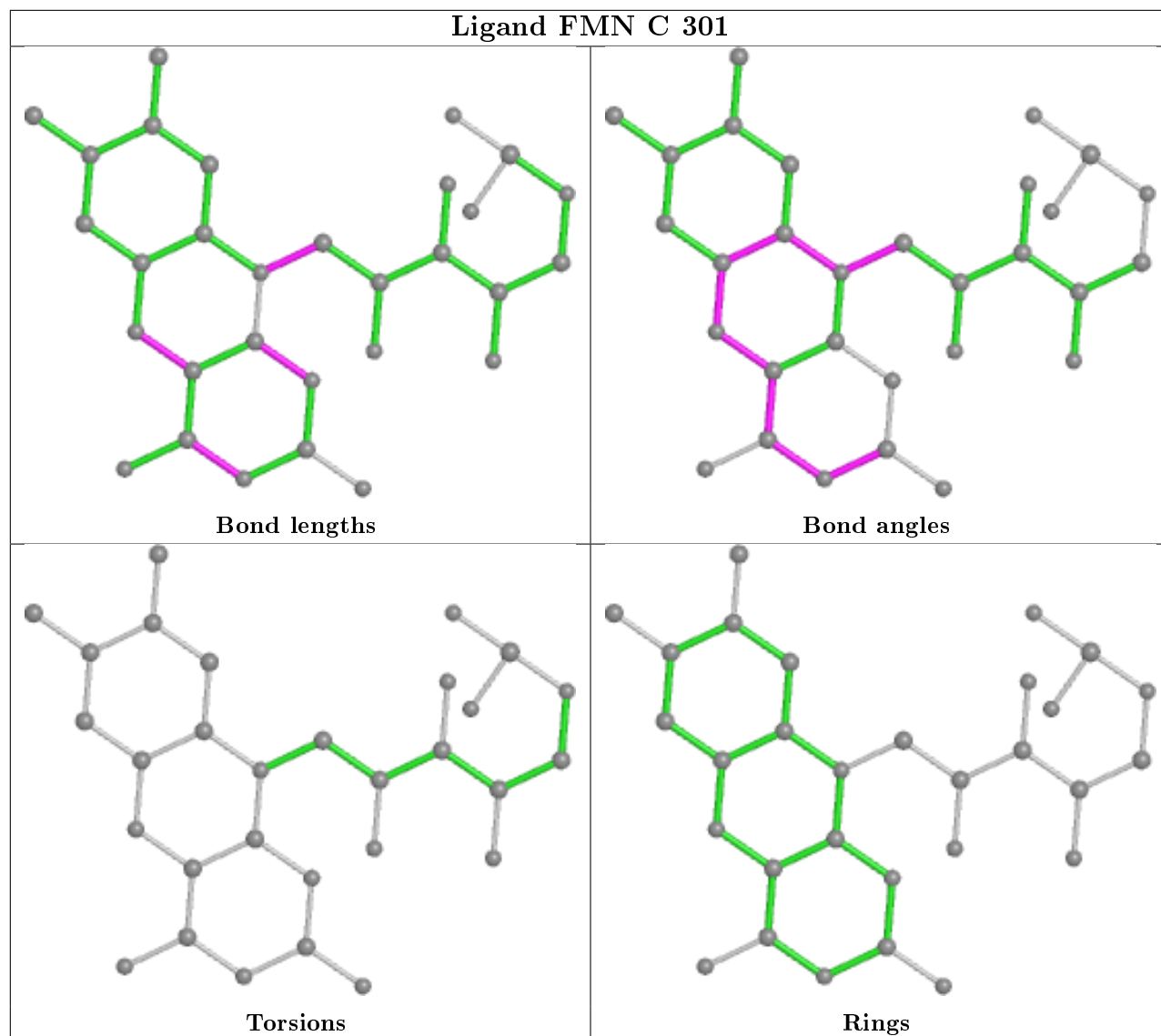
Bond angles

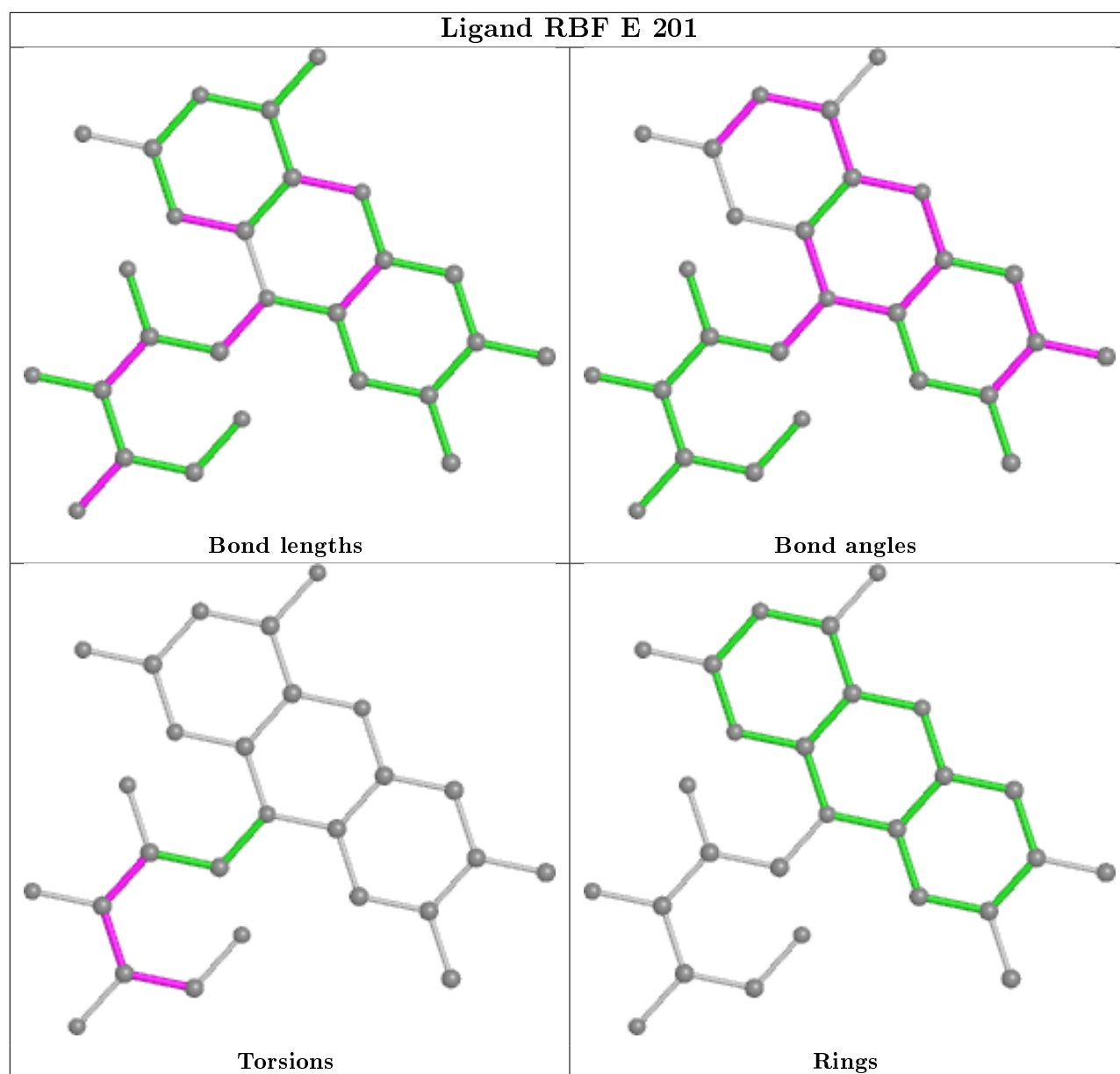


Torsions



Rings





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/449 (89%)	-0.32	3 (0%) 86 81	102, 140, 188, 226	0
2	B	348/415 (83%)	-0.34	13 (3%) 41 37	102, 149, 211, 262	0
3	C	251/257 (97%)	0.16	23 (9%) 9 9	143, 196, 252, 337	0
4	D	179/210 (85%)	-0.41	1 (0%) 89 86	103, 145, 204, 276	0
5	E	189/198 (95%)	-0.29	7 (3%) 41 37	93, 139, 211, 256	0
6	F	407/408 (99%)	0.21	31 (7%) 13 14	106, 185, 260, 329	0
All	All	1774/1937 (91%)	-0.14	78 (4%) 34 30	93, 156, 237, 337	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	408	GLY	10.3
3	C	101	SER	6.9
6	F	205	ASP	6.6
3	C	211	PRO	6.3
3	C	212	GLN	5.6
6	F	52	GLY	5.0
6	F	100	LYS	4.8
2	B	90	ASP	4.7
3	C	86	GLY	4.3
6	F	405	ASP	4.2
6	F	157	GLY	4.1
2	B	171	PRO	4.0
6	F	176	HIS	3.9
3	C	201	PRO	3.9
2	B	40	VAL	3.9
3	C	102	GLU	3.9
5	E	168	ASP	3.8
6	F	129	GLY	3.7
2	B	94	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	114	ASN	3.6
3	C	200	LYS	3.5
6	F	43	PRO	3.5
3	C	109	GLU	3.5
6	F	156	ASP	3.4
5	E	101	PHE	3.3
6	F	42	ASP	3.2
6	F	407	GLY	3.2
3	C	99	GLU	3.2
5	E	102	PHE	3.2
6	F	2	SER	3.1
6	F	101	GLY	3.1
2	B	97	ALA	3.1
3	C	129	ASP	3.1
6	F	302	LYS	3.1
3	C	85	GLU	3.1
4	D	10	SER	3.1
6	F	207	PRO	3.1
5	E	166	TYR	3.0
3	C	106	LEU	3.0
2	B	89	GLY	3.0
6	F	3	THR	3.0
6	F	330	ASN	2.9
6	F	255	GLY	2.9
2	B	93	ALA	2.9
1	A	116	ASP	2.9
3	C	110	GLN	2.9
6	F	301	SER	2.8
2	B	98	GLY	2.8
3	C	108	ALA	2.8
3	C	32	GLY	2.7
3	C	139	PRO	2.6
6	F	312	ARG	2.6
2	B	108	LEU	2.5
6	F	213	SER	2.5
2	B	329	TRP	2.4
6	F	328	ALA	2.4
1	A	327	ARG	2.4
5	E	196	VAL	2.4
5	E	197	GLN	2.4
6	F	344	PRO	2.4
6	F	63	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	100	ARG	2.3
6	F	99	SER	2.3
3	C	213	GLY	2.3
6	F	271	ASP	2.3
6	F	149	GLU	2.3
6	F	32	THR	2.2
6	F	181	ASP	2.2
3	C	253	ASP	2.2
3	C	196	ASP	2.1
2	B	41	THR	2.1
6	F	329	GLU	2.1
2	B	155	VAL	2.1
3	C	84	VAL	2.1
3	C	57	ALA	2.1
3	C	131	ASP	2.1
3	C	107	THR	2.0
2	B	91	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FAD	F	502	53/53	0.64	0.34	155,176,208,228	0
10	RBF	E	201	27/27	0.80	0.49	117,171,242,266	0
8	CA	C	302	1/1	0.87	0.66	170,170,170,170	0
7	FMN	B	600	30/31	0.88	0.23	129,151,190,232	0
7	FMN	C	301	30/31	0.90	0.44	148,188,217,252	0
11	FES	F	501	4/4	0.95	0.07	193,203,260,286	0

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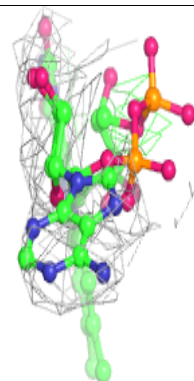
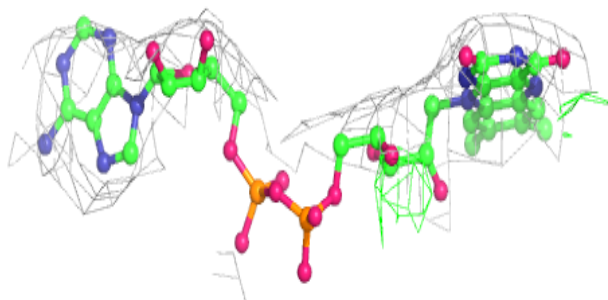
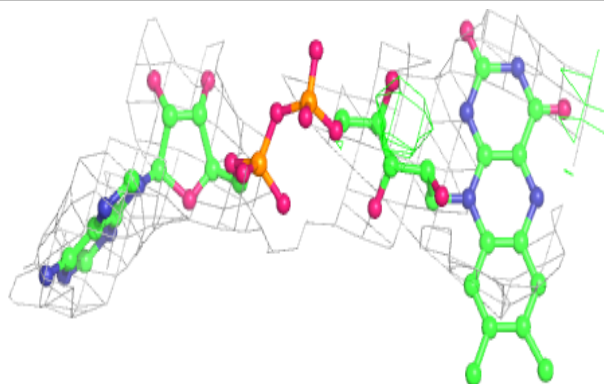
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	FE	D	301	1/1	0.99	0.20	118,118,118,118	0

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

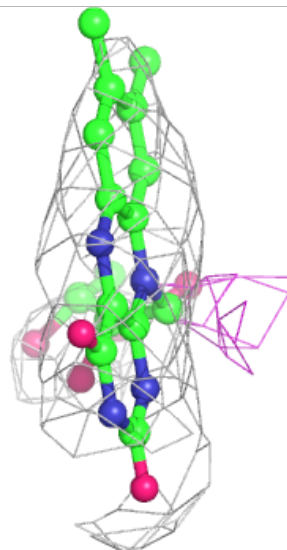
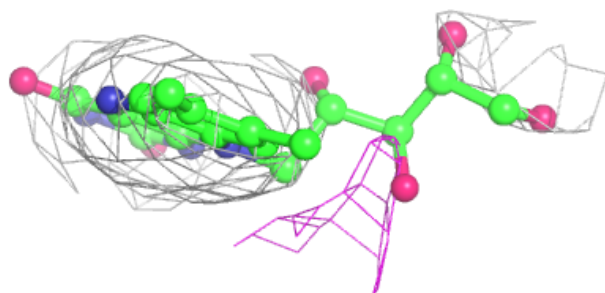
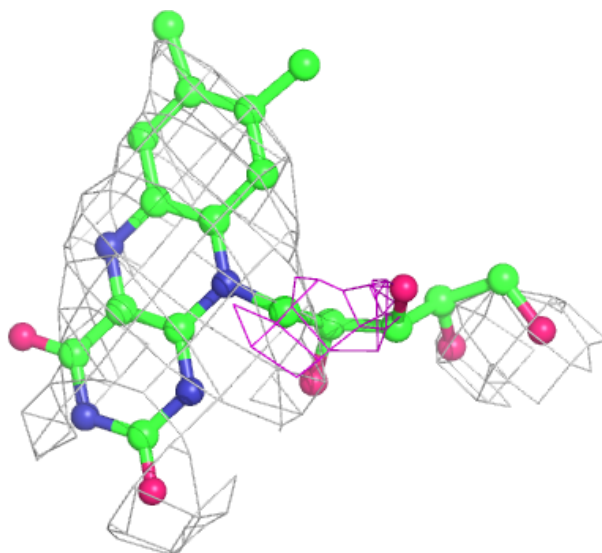
**Electron density around FAD F 502:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



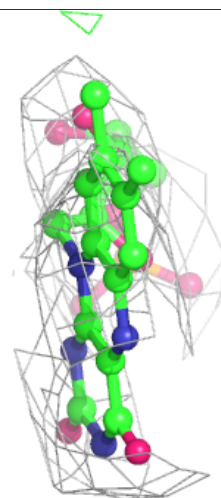
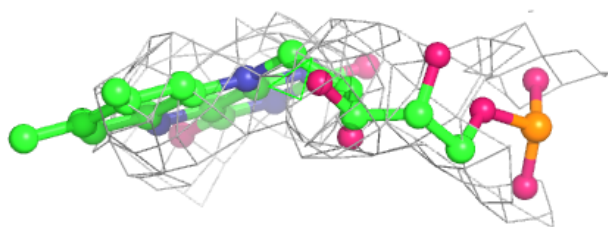
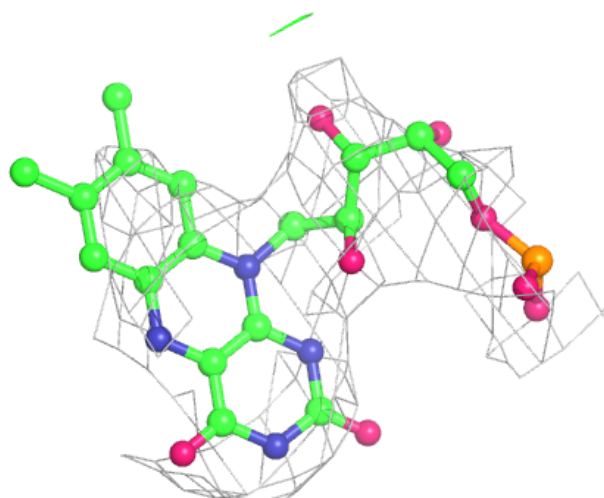
**Electron density around RBF E 201:**

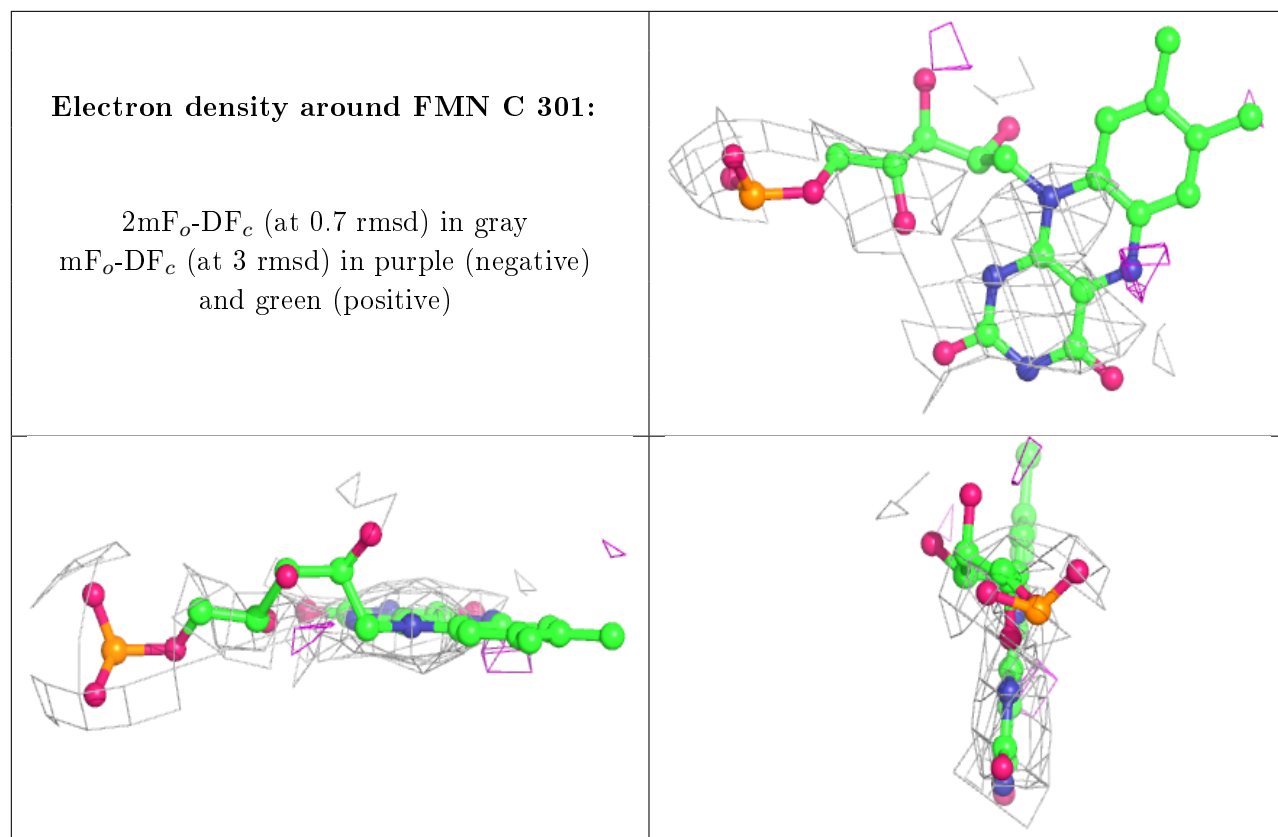
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN B 600:**

$2mF_o-DF_c$  (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.