



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:30 pm BST

PDB ID : 1TB3  
Title : Crystal Structure Analysis of Recombinant Rat Kidney Long-chain Hydroxy Acid Oxidase  
Authors : Cunane, L.M.; Barton, J.D.; Chen, Z.W.; Le, K.H.D.; Amar, D.; Lederer, F.; Mathews, F.S.  
Deposited on : 2004-05-19  
Resolution : 2.30 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.

---

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

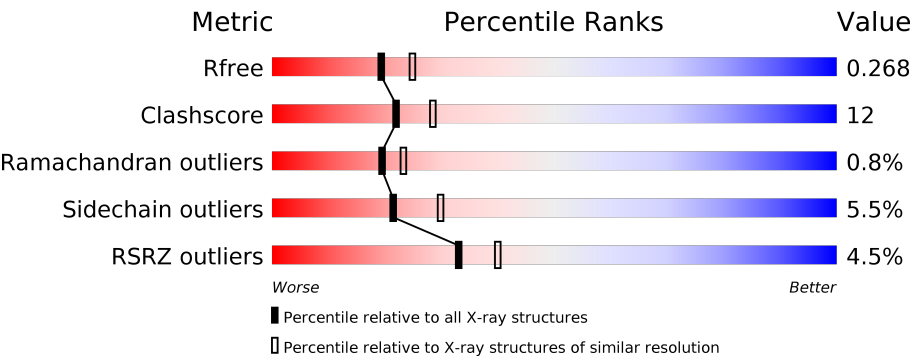
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	352	<div><div>3%</div><div><div></div><div>73%</div><div>18%</div><div>• 6%</div></div></div>
1	B	352	<div><div>4%</div><div><div></div><div>71%</div><div>19%</div><div>• 7%</div></div></div>
1	C	352	<div><div>6%</div><div><div></div><div>72%</div><div>20%</div><div>• 6%</div></div></div>
1	D	352	<div><div>3%</div><div><div></div><div>70%</div><div>20%</div><div>• 7%</div></div></div>
1	E	352	<div><div>6%</div><div><div></div><div>71%</div><div>19%</div><div>• 8%</div></div></div>
1	F	352	<div><div>3%</div><div><div></div><div>70%</div><div>21%</div><div>• 6%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	352	<div><div></div><div>4%</div><div></div><div>71%</div><div></div><div>20%</div><div></div><div>•</div><div>7%</div></div>
1	H	352	<div><div></div><div>5%</div><div></div><div>71%</div><div></div><div>20%</div><div></div><div>•</div><div>6%</div></div>

## 2 Entry composition

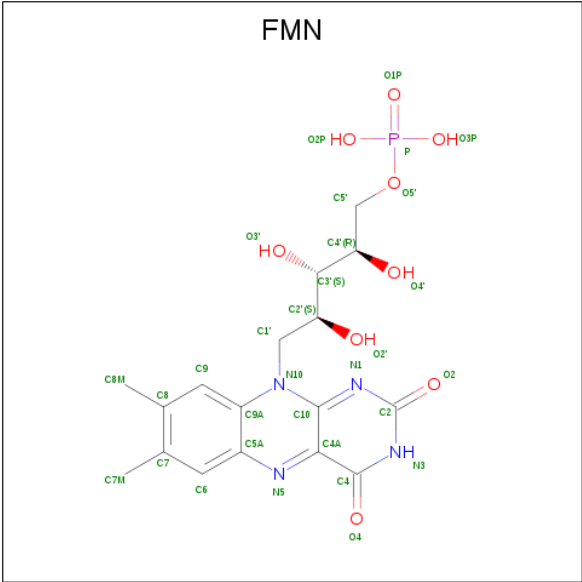
There are 4 unique types of molecules in this entry. The entry contains 21605 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hydroxyacid oxidase 3.

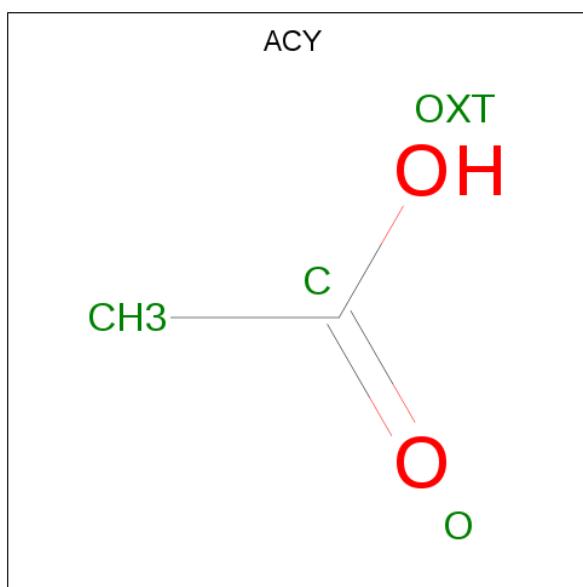
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			
1	B	327	Total	C	N	O	S	0	0	0
			2537	1605	444	474	14			
1	C	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			
1	D	329	Total	C	N	O	S	0	0	0
			2550	1614	446	476	14			
1	E	324	Total	C	N	O	S	0	0	0
			2519	1593	441	471	14			
1	F	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			
1	G	329	Total	C	N	O	S	0	0	0
			2547	1611	446	476	14			
1	H	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	130	Total O 130 130	0	0
4	B	75	Total O 75 75	0	0
4	C	106	Total O 106 106	0	0
4	D	115	Total O 115 115	0	0

*Continued on next page...*

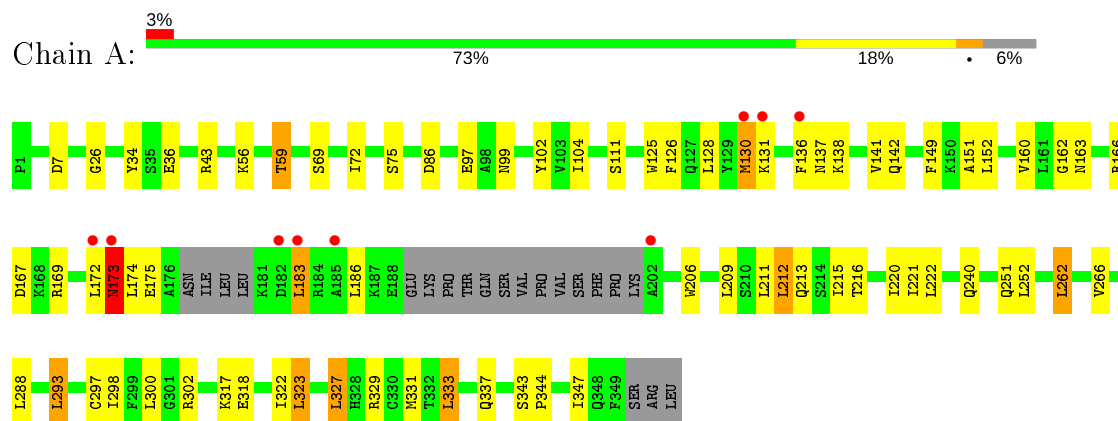
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	71	Total 71	O 71	0	0
4	F	166	Total 166	O 166	0	0
4	G	109	Total 109	O 109	0	0
4	H	128	Total 128	O 128	0	0

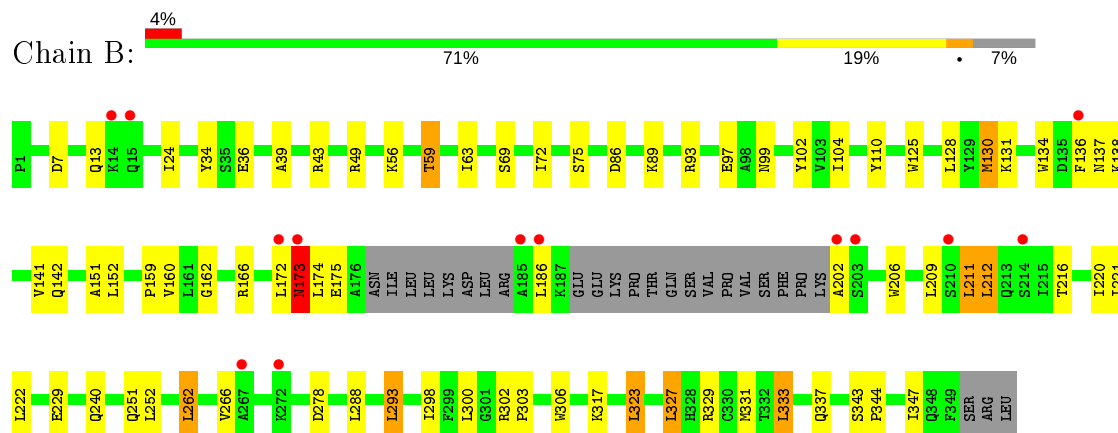
### 3 Residue-property plots [i](#)

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.

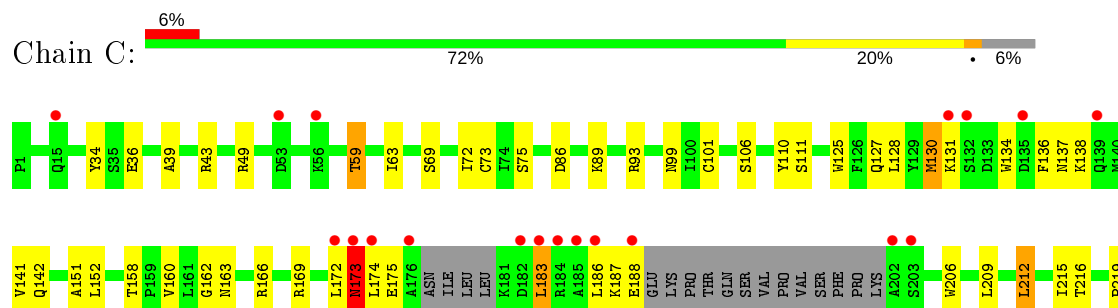
#### • Molecule 1: Hydroxyacid oxidase 3



#### • Molecule 1: Hydroxyacid oxidase 3

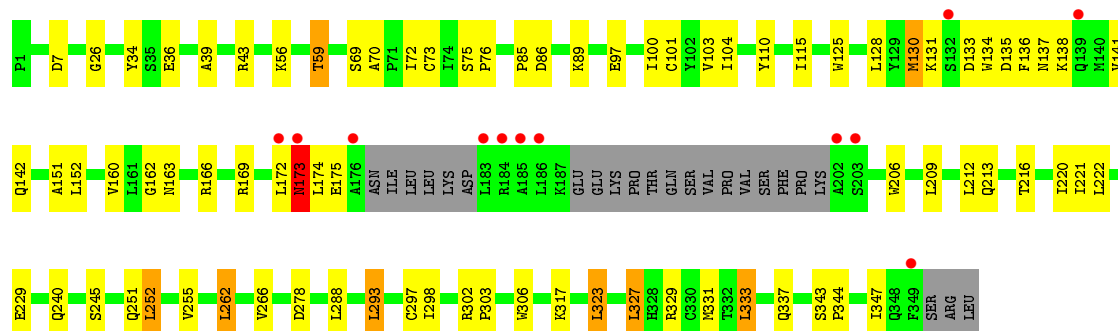


#### • Molecule 1: Hydroxyacid oxidase 3

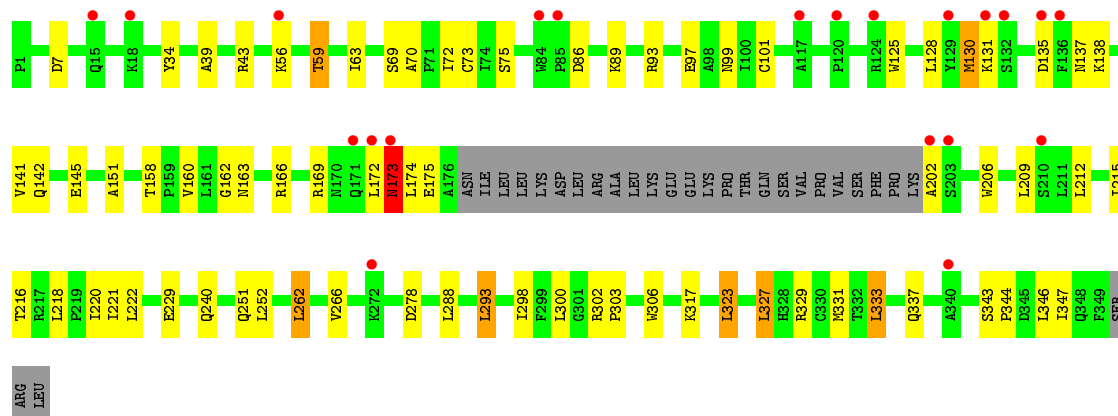




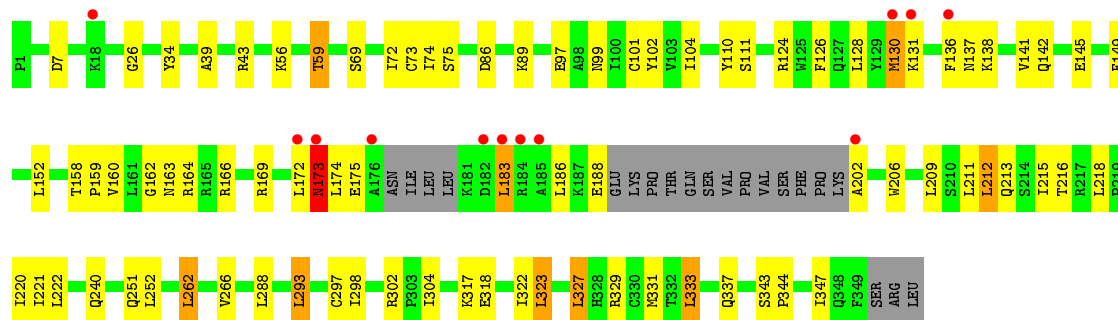
• Molecule 1: Hydroxyacid oxidase 3



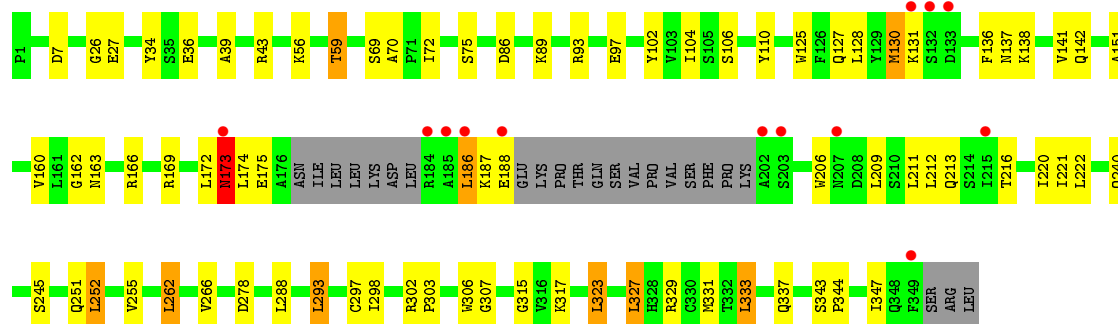
• Molecule 1: Hydroxyacid oxidase 3



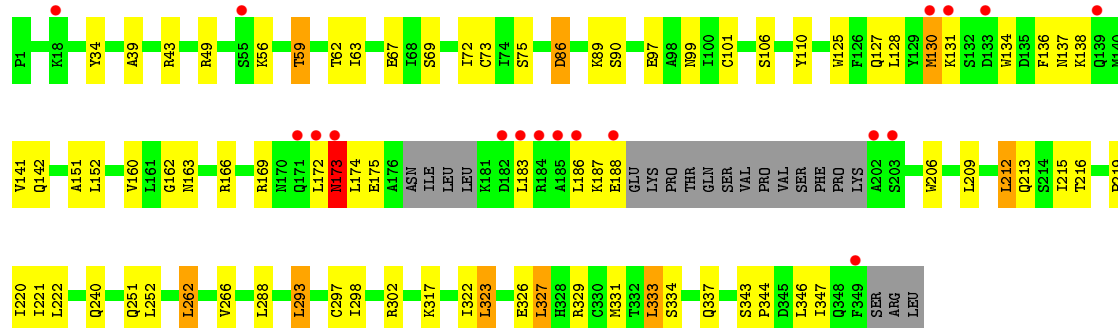
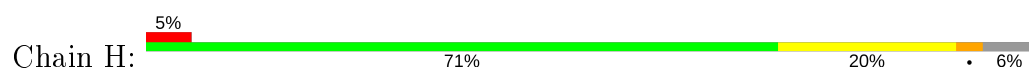
• Molecule 1: Hydroxyacid oxidase 3



• Molecule 1: Hydroxyacid oxidase 3



• Molecule 1: Hydroxyacid oxidase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.84Å 151.10Å 222.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 39.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.1 (40.00-2.30) 83.2 (39.99-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239 , 0.269 0.236 , 0.268	Depositor DCC
$R_{free}$ test set	8006 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 90.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6809e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.35	0/2610	0.62	0/3528
1	B	0.34	0/2579	0.60	0/3485
1	C	0.34	0/2610	0.60	0/3528
1	D	0.35	0/2592	0.60	0/3503
1	E	0.34	0/2562	0.59	0/3463
1	F	0.36	0/2610	0.62	0/3528
1	G	0.36	0/2589	0.60	0/3499
1	H	0.35	0/2610	0.61	0/3528
All	All	0.35	0/20762	0.60	0/28062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2568	0	2584	58	0
1	B	2537	0	2563	64	0
1	C	2568	0	2584	63	0
1	D	2550	0	2576	66	0
1	E	2519	0	2546	61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2568	0	2584	64	0
1	G	2547	0	2567	70	0
1	H	2568	0	2584	69	0
2	A	31	0	19	0	0
2	B	31	0	19	1	0
2	C	31	0	19	1	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	0	0
3	H	4	0	3	0	0
4	A	130	0	0	4	0
4	B	75	0	0	2	0
4	C	106	0	0	2	0
4	D	115	0	0	2	0
4	E	71	0	0	3	0
4	F	166	0	0	6	0
4	G	109	0	0	2	0
4	H	128	0	0	4	0
All	All	21605	0	20764	489	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 12.

All (489) 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)
1:B:220:ILE:H	1:B:240:GLN:HE21	1.13	0.96
1:F:220:ILE:H	1:F:240:GLN:HE21	1.12	0.94
1:G:220:ILE:H	1:G:240:GLN:HE21	1.16	0.94
1:D:220:ILE:H	1:D:240:GLN:HE21	1.16	0.93
1:E:220:ILE:H	1:E:240:GLN:HE21	1.18	0.91
1:A:220:ILE:H	1:A:240:GLN:HE21	1.14	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ILE:H	1:C:240:GLN:HE21	1.19	0.88
1:H:220:ILE:H	1:H:240:GLN:HE21	1.19	0.85
1:F:130:MET:HA	1:F:130:MET:HE2	1.61	0.83
1:A:130:MET:HA	1:A:130:MET:HE3	1.64	0.79
1:E:130:MET:HE2	1:E:130:MET:HA	1.65	0.79
1:B:130:MET:HE3	1:B:130:MET:HA	1.66	0.77
1:H:130:MET:HA	1:H:130:MET:HE3	1.68	0.76
1:C:130:MET:HE3	1:C:130:MET:HA	1.70	0.74
1:C:141:VAL:HG11	1:C:216:THR:HB	1.70	0.73
1:F:213:GLN:HG2	1:F:220:ILE:HD12	1.70	0.73
1:A:220:ILE:H	1:A:240:GLN:NE2	1.87	0.73
1:H:220:ILE:H	1:H:240:GLN:NE2	1.87	0.72
1:C:220:ILE:H	1:C:240:GLN:NE2	1.87	0.72
1:H:141:VAL:HG11	1:H:216:THR:HB	1.72	0.71
1:F:220:ILE:H	1:F:240:GLN:NE2	1.86	0.71
1:B:220:ILE:H	1:B:240:GLN:NE2	1.86	0.70
1:E:220:ILE:H	1:E:240:GLN:NE2	1.89	0.70
1:H:138:LYS:HA	1:H:215:ILE:HD12	1.72	0.70
1:G:130:MET:HA	1:G:130:MET:HE3	1.74	0.70
1:G:220:ILE:H	1:G:240:GLN:NE2	1.89	0.68
1:D:220:ILE:H	1:D:240:GLN:NE2	1.90	0.67
1:B:141:VAL:HG11	1:B:216:THR:HB	1.76	0.67
1:F:169:ARG:NH2	4:F:6537:HOH:O	2.27	0.66
1:F:164:ARG:HD3	4:F:6507:HOH:O	1.96	0.66
1:E:162:GLY:H	1:E:251:GLN:HE22	1.43	0.65
1:F:173:ASN:O	1:F:175:GLU:HG2	1.96	0.65
1:F:131:LYS:H	1:F:137:ASN:HD21	1.43	0.65
1:F:172:LEU:HD13	4:F:6514:HOH:O	1.95	0.64
1:A:213:GLN:HG2	1:A:220:ILE:HD12	1.79	0.63
1:B:211:LEU:HD12	1:B:211:LEU:C	2.18	0.63
1:D:130:MET:HA	1:D:130:MET:HE2	1.80	0.63
1:H:128:LEU:HG	1:H:130:MET:HE1	1.80	0.63
1:A:131:LYS:H	1:A:137:ASN:HD21	1.47	0.63
1:C:128:LEU:HG	1:C:130:MET:HE1	1.81	0.63
1:A:212:LEU:O	1:A:215:ILE:HG12	2.00	0.62
1:B:131:LYS:H	1:B:137:ASN:HD21	1.45	0.62
1:B:220:ILE:N	1:B:240:GLN:HE21	1.93	0.62
1:B:298:ILE:C	1:B:298:ILE:HD12	2.19	0.61
1:G:212:LEU:O	1:G:216:THR:HG22	2.01	0.61
1:F:128:LEU:HG	1:F:130:MET:HE3	1.83	0.61
1:D:125:TRP:CD1	1:D:151:ALA:HB3	2.36	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:LYS:HE2	1:H:136:PHE:CE1	2.37	0.60
1:H:220:ILE:N	1:H:240:GLN:HE21	1.97	0.60
1:E:131:LYS:H	1:E:137:ASN:HD21	1.46	0.60
1:E:141:VAL:HG11	1:E:216:THR:HB	1.84	0.60
1:A:220:ILE:N	1:A:240:GLN:HE21	1.94	0.60
1:D:173:ASN:O	1:D:175:GLU:HG2	2.02	0.59
1:G:162:GLY:H	1:G:251:GLN:HE22	1.48	0.59
1:C:220:ILE:N	1:C:240:GLN:HE21	1.96	0.59
1:A:128:LEU:HG	1:A:130:MET:HE1	1.84	0.59
1:G:262:LEU:HD22	1:G:266:VAL:HG23	1.85	0.59
1:F:212:LEU:O	1:F:215:ILE:HG12	2.02	0.59
1:G:298:ILE:HD12	1:G:298:ILE:C	2.23	0.59
1:A:160:VAL:HG12	1:D:333:LEU:HD13	1.84	0.59
1:E:298:ILE:C	1:E:298:ILE:HD12	2.24	0.59
1:H:298:ILE:HD12	1:H:298:ILE:C	2.23	0.59
1:A:173:ASN:HA	4:A:1507:HOH:O	2.02	0.59
1:F:141:VAL:HG11	1:F:216:THR:HB	1.84	0.59
1:G:131:LYS:HE2	1:G:136:PHE:CE1	2.38	0.59
1:A:262:LEU:HD22	1:A:266:VAL:HG23	1.85	0.58
1:H:162:GLY:H	1:H:251:GLN:HE22	1.52	0.58
1:G:128:LEU:HG	1:G:130:MET:HE1	1.86	0.58
1:C:298:ILE:C	1:C:298:ILE:HD12	2.24	0.58
1:D:298:ILE:C	1:D:298:ILE:HD12	2.24	0.57
1:G:162:GLY:H	1:G:251:GLN:NE2	2.02	0.57
1:B:162:GLY:H	1:B:251:GLN:HE22	1.50	0.57
1:F:131:LYS:HE2	1:F:136:PHE:CE1	2.39	0.57
1:A:343:SER:HB2	1:A:344:PRO:HD2	1.86	0.57
1:B:343:SER:HB2	1:B:344:PRO:HD2	1.87	0.57
1:D:131:LYS:HE2	1:D:136:PHE:CE1	2.40	0.56
1:D:343:SER:HB2	1:D:344:PRO:HD2	1.86	0.56
1:D:128:LEU:HG	1:D:130:MET:HE3	1.87	0.56
1:D:166:ARG:HG2	1:D:166:ARG:HH11	1.71	0.56
1:D:262:LEU:HD22	1:D:266:VAL:HG23	1.86	0.56
1:H:128:LEU:CD2	1:H:130:MET:HE1	2.36	0.56
1:E:162:GLY:H	1:E:251:GLN:NE2	2.04	0.56
1:H:169:ARG:NH2	4:H:8440:HOH:O	2.38	0.56
1:C:173:ASN:O	1:C:175:GLU:HG2	2.05	0.56
1:A:169:ARG:NH1	1:D:7:ASP:OD1	2.38	0.56
1:F:124:ARG:NH1	4:F:6516:HOH:O	2.38	0.56
1:E:72:ILE:HD13	1:E:323:LEU:HB3	1.88	0.56
1:F:188:GLU:HA	4:F:6553:HOH:O	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ALA:HA	4:E:5470:HOH:O	2.04	0.55
1:F:343:SER:HB2	1:F:344:PRO:HD2	1.87	0.55
1:A:173:ASN:O	1:A:175:GLU:HG2	2.07	0.55
1:D:162:GLY:H	1:D:251:GLN:HE22	1.55	0.55
1:A:162:GLY:H	1:A:251:GLN:HE22	1.54	0.55
1:A:141:VAL:HG11	1:A:216:THR:HB	1.88	0.55
1:C:343:SER:HB2	1:C:344:PRO:HD2	1.88	0.55
1:C:162:GLY:H	1:C:251:GLN:HE22	1.55	0.55
1:E:220:ILE:N	1:E:240:GLN:HE21	1.97	0.55
1:F:220:ILE:N	1:F:240:GLN:HE21	1.92	0.55
1:F:59:THR:HG23	1:F:69:SER:O	2.06	0.55
1:F:298:ILE:HD12	1:F:298:ILE:C	2.27	0.54
1:B:128:LEU:HG	1:B:130:MET:HE1	1.89	0.54
1:A:298:ILE:C	1:A:298:ILE:HD12	2.27	0.54
1:G:343:SER:HB2	1:G:344:PRO:HD2	1.89	0.54
1:D:293:LEU:HD13	1:D:347:ILE:HG13	1.90	0.54
1:E:343:SER:HB2	1:E:344:PRO:HD2	1.90	0.54
1:H:343:SER:HB2	1:H:344:PRO:HD2	1.88	0.54
1:B:293:LEU:HD13	1:B:347:ILE:HG13	1.90	0.54
1:E:128:LEU:HG	1:E:130:MET:HE3	1.90	0.54
1:G:128:LEU:CD2	1:G:130:MET:HE1	2.37	0.54
1:B:160:VAL:HG12	1:C:333:LEU:HD13	1.90	0.54
1:E:293:LEU:HD13	1:E:347:ILE:HG13	1.88	0.54
1:F:162:GLY:H	1:F:251:GLN:HE22	1.55	0.54
1:C:293:LEU:HD13	1:C:347:ILE:HG13	1.90	0.54
1:A:293:LEU:HD13	1:A:347:ILE:HG13	1.89	0.54
1:G:89:LYS:HE2	1:G:110:TYR:CE2	2.42	0.54
1:A:131:LYS:HE2	1:A:136:PHE:CE1	2.43	0.54
1:G:166:ARG:HH11	1:G:166:ARG:HG2	1.71	0.54
1:G:220:ILE:N	1:G:240:GLN:HE21	1.97	0.53
1:F:160:VAL:HG12	1:G:333:LEU:HD13	1.89	0.53
1:B:138:LYS:O	1:B:142:GLN:HG3	2.08	0.53
1:F:145:GLU:HG3	1:F:218:LEU:HD11	1.90	0.53
1:C:59:THR:HG23	1:C:69:SER:O	2.09	0.53
1:H:39:ALA:O	1:H:43:ARG:HG3	2.08	0.53
1:B:262:LEU:HD22	1:B:266:VAL:HG23	1.90	0.53
1:B:7:ASP:OD1	1:D:169:ARG:NH1	2.42	0.53
1:G:293:LEU:HD13	1:G:347:ILE:HG13	1.90	0.53
1:H:293:LEU:HD13	1:H:347:ILE:HG13	1.90	0.53
1:D:327:LEU:HD22	1:D:331:MET:HG3	1.91	0.53
1:E:130:MET:HG3	1:E:137:ASN:OD1	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:LEU:HD22	1:F:266:VAL:HG23	1.90	0.53
1:F:293:LEU:HD13	1:F:347:ILE:HG13	1.91	0.53
1:G:173:ASN:O	1:G:175:GLU:HG2	2.09	0.53
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.74	0.53
1:G:136:PHE:HD1	1:G:137:ASN:HD22	1.55	0.52
1:H:131:LYS:HE2	1:H:136:PHE:CD1	2.45	0.52
1:B:134:TRP:CD2	1:B:211:LEU:HD21	2.44	0.52
1:C:130:MET:CE	1:C:130:MET:HA	2.40	0.52
1:D:26:GLY:HA2	4:D:4437:HOH:O	2.09	0.52
1:F:221:ILE:N	1:F:221:ILE:HD12	2.24	0.52
1:H:72:ILE:HD13	1:H:323:LEU:HB3	1.91	0.52
1:C:246:ASN:HA	4:C:3410:HOH:O	2.09	0.52
1:B:72:ILE:HD13	1:B:323:LEU:HB3	1.91	0.52
1:H:130:MET:CE	1:H:130:MET:HA	2.38	0.52
1:D:162:GLY:H	1:D:251:GLN:NE2	2.07	0.52
1:E:138:LYS:O	1:E:142:GLN:HG3	2.10	0.52
1:G:186:LEU:C	1:G:188:GLU:H	2.13	0.52
1:H:221:ILE:N	1:H:221:ILE:HD12	2.25	0.51
1:A:221:ILE:HD12	1:A:221:ILE:N	2.26	0.51
1:D:89:LYS:HE2	1:D:110:TYR:CE2	2.45	0.51
1:A:111:SER:HA	1:A:183:LEU:HD11	1.92	0.51
1:G:59:THR:HG23	1:G:69:SER:O	2.11	0.51
1:B:162:GLY:H	1:B:251:GLN:NE2	2.08	0.51
1:E:125:TRP:CD1	1:E:151:ALA:HB3	2.45	0.51
1:G:131:LYS:H	1:G:137:ASN:HD21	1.57	0.51
1:C:138:LYS:O	1:C:142:GLN:HG3	2.11	0.51
1:E:160:VAL:HG12	1:H:333:LEU:HD13	1.92	0.51
1:A:172:LEU:O	1:A:173:ASN:HB3	2.11	0.51
1:H:166:ARG:HB2	4:H:8470:HOH:O	2.10	0.51
1:C:131:LYS:HE2	1:C:136:PHE:CE1	2.46	0.51
1:C:72:ILE:HD13	1:C:323:LEU:HB3	1.92	0.51
1:D:136:PHE:HD1	1:D:137:ASN:ND2	2.09	0.51
1:F:130:MET:HA	1:F:130:MET:CE	2.39	0.51
1:H:166:ARG:HH11	1:H:166:ARG:HG2	1.75	0.51
1:C:186:LEU:C	1:C:188:GLU:H	2.12	0.51
1:F:131:LYS:HE2	1:F:136:PHE:CZ	2.45	0.51
1:H:34:TYR:HE1	1:H:302:ARG:CZ	2.24	0.51
1:C:106:SER:HB2	1:C:127:GLN:O	2.11	0.50
1:C:128:LEU:CD2	1:C:130:MET:HE1	2.40	0.50
1:H:138:LYS:O	1:H:142:GLN:HG3	2.12	0.50
1:H:138:LYS:CA	1:H:215:ILE:HD12	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:TRP:CD1	1:B:151:ALA:HB3	2.47	0.50
1:C:221:ILE:N	1:C:221:ILE:HD12	2.27	0.50
1:C:34:TYR:HE1	1:C:302:ARG:CZ	2.25	0.50
1:B:173:ASN:O	1:B:175:GLU:HG2	2.11	0.50
1:C:39:ALA:O	1:C:43:ARG:HG3	2.12	0.50
1:D:125:TRP:CG	1:D:151:ALA:HB3	2.47	0.50
1:G:125:TRP:CD1	1:G:151:ALA:HB3	2.47	0.50
1:G:141:VAL:HG11	1:G:216:THR:HB	1.93	0.50
1:H:173:ASN:O	1:H:175:GLU:HG2	2.12	0.50
1:A:166:ARG:HH11	1:A:166:ARG:HG2	1.77	0.50
1:B:59:THR:HG23	1:B:69:SER:O	2.11	0.50
1:A:59:THR:HG23	1:A:69:SER:O	2.12	0.50
1:B:221:ILE:N	1:B:221:ILE:HD12	2.27	0.50
1:C:172:LEU:O	1:C:173:ASN:HB3	2.10	0.50
1:B:211:LEU:O	1:B:211:LEU:HD12	2.11	0.50
1:C:187:LYS:O	1:C:188:GLU:CB	2.59	0.50
1:E:69:SER:OG	1:E:99:ASN:HB3	2.12	0.50
1:F:163:ASN:HB2	1:G:329:ARG:NE	2.27	0.49
1:F:172:LEU:O	1:F:173:ASN:HB3	2.12	0.49
1:H:187:LYS:O	1:H:188:GLU:CB	2.59	0.49
1:F:169:ARG:NH1	1:G:7:ASP:OD1	2.45	0.49
1:B:130:MET:HG3	1:B:137:ASN:OD1	2.12	0.49
1:H:128:LEU:CG	1:H:130:MET:HE1	2.43	0.49
1:H:186:LEU:C	1:H:188:GLU:H	2.14	0.49
1:A:130:MET:HA	1:A:130:MET:CE	2.40	0.49
1:A:7:ASP:OD1	1:C:169:ARG:NH1	2.46	0.49
1:F:34:TYR:HE1	1:F:302:ARG:CZ	2.24	0.49
1:F:97:GLU:HG2	1:F:317:LYS:HE3	1.94	0.49
1:D:220:ILE:N	1:D:240:GLN:HE21	1.97	0.49
4:A:1468:HOH:O	1:D:329:ARG:HD3	2.12	0.49
1:E:135:ASP:O	1:E:138:LYS:HG2	2.12	0.49
1:E:327:LEU:HD22	1:E:331:MET:SD	2.52	0.49
1:F:333:LEU:HD13	1:H:160:VAL:HG12	1.95	0.49
1:G:136:PHE:HD1	1:G:137:ASN:ND2	2.10	0.49
1:A:128:LEU:CD2	1:A:130:MET:HE1	2.43	0.49
1:B:125:TRP:CG	1:B:151:ALA:HB3	2.47	0.49
1:C:262:LEU:HD22	1:C:266:VAL:HG23	1.95	0.49
1:E:262:LEU:HD22	1:E:266:VAL:HG23	1.95	0.49
1:A:162:GLY:H	1:A:251:GLN:NE2	2.10	0.49
1:F:329:ARG:HD3	4:H:8476:HOH:O	2.12	0.49
1:G:138:LYS:O	1:G:142:GLN:HG3	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:ALA:O	1:G:43:ARG:HG3	2.13	0.49
1:C:212:LEU:O	1:C:215:ILE:HG12	2.13	0.49
1:E:166:ARG:HG2	1:E:166:ARG:HH11	1.78	0.48
1:E:59:THR:HG23	1:E:69:SER:O	2.13	0.48
1:F:162:GLY:H	1:F:251:GLN:NE2	2.11	0.48
1:A:59:THR:CG2	1:A:69:SER:O	2.62	0.48
1:B:97:GLU:HG2	1:B:317:LYS:HE3	1.96	0.48
1:F:59:THR:CG2	1:F:69:SER:O	2.60	0.48
1:B:202:ALA:HA	4:B:2453:HOH:O	2.13	0.48
1:G:221:ILE:N	1:G:221:ILE:HD12	2.28	0.48
1:D:39:ALA:O	1:D:43:ARG:HG3	2.13	0.48
1:E:130:MET:HA	1:E:130:MET:CE	2.42	0.48
1:F:327:LEU:HD22	1:F:331:MET:HG3	1.95	0.48
1:B:333:LEU:HD13	1:D:160:VAL:HG12	1.95	0.48
1:A:163:ASN:HB2	1:D:329:ARG:NE	2.29	0.48
1:C:89:LYS:HE2	1:C:110:TYR:CE2	2.49	0.48
1:E:145:GLU:HG2	1:E:218:LEU:HG	1.96	0.48
1:E:173:ASN:O	1:E:175:GLU:HG2	2.14	0.48
1:B:13:GLN:HG3	4:B:2477:HOH:O	2.13	0.48
1:C:131:LYS:H	1:C:137:ASN:HD21	1.60	0.48
1:D:72:ILE:HD13	1:D:323:LEU:HB3	1.96	0.48
1:E:7:ASP:OD1	1:G:169:ARG:NH1	2.47	0.48
1:H:262:LEU:HD22	1:H:266:VAL:HG23	1.95	0.48
1:A:131:LYS:HE2	1:A:136:PHE:CZ	2.49	0.47
1:D:131:LYS:H	1:D:137:ASN:HD21	1.61	0.47
1:D:136:PHE:HD1	1:D:137:ASN:HD22	1.61	0.47
1:F:166:ARG:HG2	1:F:166:ARG:HH11	1.78	0.47
1:F:206:TRP:O	1:F:209:LEU:HB2	2.14	0.47
1:G:327:LEU:HD22	1:G:331:MET:HG3	1.96	0.47
1:A:206:TRP:O	1:A:209:LEU:HB2	2.14	0.47
1:E:89:LYS:O	1:E:93:ARG:HG3	2.15	0.47
1:C:173:ASN:HA	4:C:3468:HOH:O	2.13	0.47
1:H:89:LYS:HE2	1:H:110:TYR:CE2	2.50	0.47
1:A:97:GLU:HG2	1:A:317:LYS:HE3	1.95	0.47
1:A:333:LEU:HD13	1:C:160:VAL:HG12	1.94	0.47
1:A:211:LEU:O	1:A:215:ILE:HG23	2.14	0.47
1:C:166:ARG:HH11	1:C:166:ARG:HG2	1.79	0.47
1:C:172:LEU:O	1:C:173:ASN:CB	2.62	0.47
1:E:327:LEU:HD22	1:E:331:MET:HG3	1.97	0.47
1:G:125:TRP:CG	1:G:151:ALA:HB3	2.50	0.47
1:H:125:TRP:CD1	1:H:151:ALA:HB3	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:GLU:HG2	1:E:317:LYS:HE3	1.96	0.47
1:F:138:LYS:O	1:F:142:GLN:HG3	2.14	0.47
1:B:39:ALA:O	1:B:43:ARG:HG3	2.14	0.47
1:D:131:LYS:HE2	1:D:136:PHE:CD1	2.49	0.47
1:H:162:GLY:H	1:H:251:GLN:NE2	2.12	0.47
1:F:213:GLN:CG	1:F:220:ILE:HD12	2.44	0.47
1:C:59:THR:CG2	1:C:69:SER:O	2.63	0.47
1:E:333:LEU:HD13	1:G:160:VAL:HG12	1.96	0.47
1:A:138:LYS:O	1:A:142:GLN:HG3	2.14	0.46
1:A:69:SER:OG	1:A:99:ASN:HB3	2.16	0.46
1:B:327:LEU:HD22	1:B:331:MET:SD	2.55	0.46
1:C:125:TRP:CD1	1:C:151:ALA:HB3	2.50	0.46
1:F:211:LEU:O	1:F:215:ILE:HG23	2.14	0.46
1:A:34:TYR:HE1	1:A:302:ARG:CZ	2.28	0.46
1:B:206:TRP:O	1:B:209:LEU:HB2	2.16	0.46
1:E:39:ALA:O	1:E:43:ARG:HG3	2.15	0.46
1:F:102:TYR:CZ	1:F:104:ILE:HG12	2.50	0.46
1:F:158:THR:HG22	1:F:158:THR:O	2.15	0.46
1:B:128:LEU:CD2	1:B:130:MET:HE1	2.46	0.46
1:B:212:LEU:O	1:B:216:THR:HG22	2.14	0.46
1:D:166:ARG:HG2	1:D:166:ARG:NH1	2.30	0.46
1:B:300:LEU:HD11	1:B:323:LEU:HD12	1.97	0.46
1:C:125:TRP:CG	1:C:151:ALA:HB3	2.51	0.46
1:D:59:THR:HG23	1:D:69:SER:O	2.15	0.46
1:E:128:LEU:CD2	1:E:130:MET:HE3	2.46	0.46
1:A:172:LEU:O	1:A:173:ASN:CB	2.63	0.46
1:F:39:ALA:O	1:F:43:ARG:HG3	2.16	0.46
1:H:136:PHE:HD1	1:H:137:ASN:HD22	1.64	0.46
1:H:59:THR:CG2	1:H:69:SER:O	2.64	0.46
1:B:278:ASP:OD2	1:B:278:ASP:C	2.54	0.46
1:C:111:SER:HA	1:C:183:LEU:HD11	1.98	0.46
1:C:69:SER:OG	1:C:99:ASN:HB3	2.16	0.46
1:D:133:ASP:OD2	1:D:135:ASP:HB2	2.16	0.46
1:D:245:SER:HB2	1:D:278:ASP:OD2	2.15	0.46
1:H:59:THR:HG23	1:H:69:SER:O	2.15	0.46
1:E:206:TRP:O	1:E:209:LEU:HB2	2.16	0.46
1:E:278:ASP:C	1:E:278:ASP:OD2	2.53	0.46
1:E:172:LEU:O	1:E:173:ASN:OD1	2.33	0.46
1:A:327:LEU:HD22	1:A:331:MET:HG3	1.97	0.45
1:F:172:LEU:O	1:F:173:ASN:CB	2.64	0.45
1:G:166:ARG:HG2	1:G:166:ARG:NH1	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LYS:HE2	1:B:110:TYR:CE2	2.51	0.45
1:D:128:LEU:CD2	1:D:130:MET:HE3	2.47	0.45
1:F:26:GLY:HA2	4:F:6458:HOH:O	2.16	0.45
1:G:327:LEU:HD22	1:G:331:MET:SD	2.56	0.45
1:A:72:ILE:HD13	1:A:323:LEU:HB3	1.98	0.45
1:B:329:ARG:NE	1:D:163:ASN:HB2	2.31	0.45
1:D:278:ASP:OD2	1:D:278:ASP:C	2.54	0.45
1:F:128:LEU:CD2	1:F:130:MET:HE3	2.46	0.45
1:G:172:LEU:O	1:G:173:ASN:HB3	2.16	0.45
1:G:323:LEU:HD23	1:G:323:LEU:HA	1.86	0.45
1:H:209:LEU:O	1:H:213:GLN:HG3	2.17	0.45
1:D:138:LYS:O	1:D:142:GLN:HG3	2.17	0.45
1:D:172:LEU:O	1:D:173:ASN:HB3	2.16	0.45
1:G:26:GLY:HA2	4:G:7444:HOH:O	2.16	0.45
1:G:240:GLN:N	1:G:240:GLN:CD	2.70	0.45
1:F:7:ASP:OD1	1:H:169:ARG:NH1	2.50	0.45
1:H:327:LEU:HD22	1:H:331:MET:HG3	1.98	0.45
1:A:102:TYR:CZ	1:A:104:ILE:HG12	2.51	0.45
1:B:49:ARG:NH2	1:D:229:GLU:HB3	2.31	0.45
1:C:186:LEU:C	1:C:188:GLU:N	2.70	0.45
1:A:26:GLY:HA2	4:A:1445:HOH:O	2.17	0.45
1:G:206:TRP:O	1:G:209:LEU:HB2	2.17	0.45
1:H:106:SER:HB2	1:H:127:GLN:O	2.17	0.45
1:B:56:LYS:O	1:B:337:GLN:HG2	2.17	0.45
1:B:102:TYR:CZ	1:B:104:ILE:HG12	2.52	0.45
1:C:162:GLY:H	1:C:251:GLN:NE2	2.14	0.45
1:D:221:ILE:HD12	1:D:221:ILE:N	2.32	0.45
1:E:221:ILE:N	1:E:221:ILE:HD12	2.31	0.45
1:G:172:LEU:O	1:G:173:ASN:CB	2.65	0.45
1:B:240:GLN:N	1:B:240:GLN:CD	2.69	0.44
1:E:212:LEU:O	1:E:216:THR:HG22	2.17	0.44
1:E:329:ARG:NE	1:G:163:ASN:HB2	2.31	0.44
1:E:125:TRP:CG	1:E:151:ALA:HB3	2.52	0.44
1:H:334:SER:HB2	1:H:346:LEU:HD11	1.99	0.44
1:H:73:CYS:HB3	1:H:101:CYS:O	2.17	0.44
1:E:303:PRO:HA	1:E:306:TRP:CE3	2.53	0.44
1:B:160:VAL:HG12	1:C:333:LEU:CD1	2.47	0.44
1:E:137:ASN:O	1:E:141:VAL:HG23	2.17	0.44
1:B:69:SER:OG	1:B:99:ASN:HB3	2.18	0.44
1:D:172:LEU:O	1:D:173:ASN:CB	2.65	0.44
1:F:111:SER:HA	1:F:183:LEU:HD11	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TRP:CD1	1:A:151:ALA:HB3	2.52	0.44
1:F:72:ILE:HD13	1:F:323:LEU:HB3	1.98	0.44
1:G:102:TYR:CZ	1:G:104:ILE:HG12	2.53	0.44
1:A:136:PHE:HD1	1:A:137:ASN:HD22	1.66	0.44
1:G:89:LYS:O	1:G:93:ARG:HG3	2.17	0.44
1:H:172:LEU:O	1:H:173:ASN:CB	2.64	0.44
1:E:63:ILE:O	1:E:63:ILE:HG13	2.18	0.44
1:G:59:THR:O	1:G:70:ALA:HA	2.18	0.44
1:H:56:LYS:O	1:H:337:GLN:HG2	2.18	0.44
1:E:169:ARG:NH2	4:E:5462:HOH:O	2.51	0.44
1:G:27:GLU:CD	1:G:27:GLU:H	2.21	0.44
1:H:125:TRP:CG	1:H:151:ALA:HB3	2.53	0.44
1:C:63:ILE:O	1:C:63:ILE:HG13	2.18	0.43
1:D:130:MET:HG3	1:D:137:ASN:OD1	2.17	0.43
1:G:130:MET:CE	1:G:130:MET:HA	2.47	0.43
1:G:128:LEU:CG	1:G:130:MET:HE1	2.47	0.43
1:G:137:ASN:O	1:G:141:VAL:HG23	2.18	0.43
1:A:99:ASN:ND2	4:A:1517:HOH:O	2.51	0.43
1:C:206:TRP:O	1:C:209:LEU:HB2	2.17	0.43
1:E:163:ASN:HB2	1:H:329:ARG:NE	2.33	0.43
1:G:34:TYR:HE1	1:G:302:ARG:CZ	2.31	0.43
1:F:74:ILE:HG23	1:F:304:ILE:HG13	2.00	0.43
1:H:172:LEU:O	1:H:173:ASN:HB3	2.18	0.43
1:B:172:LEU:O	1:B:173:ASN:CB	2.66	0.43
1:B:63:ILE:HG13	1:B:63:ILE:O	2.18	0.43
1:C:128:LEU:CG	1:C:130:MET:HE1	2.46	0.43
1:C:131:LYS:HE2	1:C:136:PHE:CD1	2.53	0.43
1:E:329:ARG:HD3	4:E:5461:HOH:O	2.18	0.43
1:G:245:SER:HB2	1:G:278:ASP:OD2	2.19	0.43
1:H:131:LYS:H	1:H:137:ASN:HD21	1.66	0.43
1:A:130:MET:HG3	1:A:137:ASN:OD1	2.19	0.43
1:B:172:LEU:O	1:B:173:ASN:HB3	2.18	0.43
1:B:89:LYS:O	1:B:93:ARG:HG3	2.19	0.43
1:F:56:LYS:O	1:F:337:GLN:HG2	2.19	0.43
1:A:167:ASP:HB3	1:A:172:LEU:HD23	2.01	0.43
1:E:212:LEU:O	1:E:212:LEU:HD23	2.18	0.43
1:G:131:LYS:HE2	1:G:136:PHE:CD1	2.53	0.43
1:G:131:LYS:HE2	1:G:136:PHE:CZ	2.53	0.43
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.88	0.43
1:C:318:GLU:O	1:C:322:ILE:HG13	2.18	0.43
1:A:56:LYS:O	1:A:337:GLN:HG2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:TRP:HA	1:C:137:ASN:HB2	2.00	0.43
1:D:252:LEU:HD13	1:D:255:VAL:CG1	2.48	0.43
1:H:206:TRP:O	1:H:209:LEU:HB2	2.19	0.43
1:A:126:PHE:HB2	1:A:149:PHE:CD2	2.53	0.43
1:D:76:PRO:HD3	1:D:103:VAL:HG11	2.01	0.43
1:D:141:VAL:HG11	1:D:216:THR:HB	2.00	0.43
1:D:206:TRP:O	1:D:209:LEU:HB2	2.18	0.43
1:E:56:LYS:O	1:E:337:GLN:HG2	2.19	0.43
1:A:141:VAL:HG22	1:A:152:LEU:HD21	2.01	0.42
1:F:318:GLU:O	1:F:322:ILE:HG13	2.19	0.42
1:G:106:SER:HB2	1:G:127:GLN:O	2.19	0.42
1:D:73:CYS:HB3	1:D:101:CYS:O	2.19	0.42
1:D:36:GLU:CD	1:D:43:ARG:HH22	2.22	0.42
1:E:172:LEU:O	1:E:173:ASN:CB	2.67	0.42
1:H:138:LYS:CB	1:H:215:ILE:HD12	2.49	0.42
1:H:323:LEU:HA	1:H:323:LEU:HD23	1.90	0.42
1:H:63:ILE:O	1:H:63:ILE:HG13	2.20	0.42
1:B:141:VAL:HG22	1:B:152:LEU:HD21	2.01	0.42
1:G:262:LEU:HD22	1:G:266:VAL:CG2	2.49	0.42
1:H:131:LYS:HE2	1:H:136:PHE:CZ	2.54	0.42
1:E:229:GLU:HB3	1:H:49:ARG:NH2	2.34	0.42
1:B:131:LYS:HE2	1:B:136:PHE:CE1	2.54	0.42
1:B:24:ILE:HA	2:B:2401:FMN:HM71	2.01	0.42
1:C:334:SER:HB2	1:C:346:LEU:HD11	2.00	0.42
1:D:59:THR:CG2	1:D:69:SER:O	2.68	0.42
1:E:138:LYS:HB3	1:E:215:ILE:HD12	2.00	0.42
1:G:187:LYS:O	1:G:188:GLU:CB	2.67	0.42
1:H:97:GLU:HG2	1:H:317:LYS:HE3	2.01	0.42
1:D:59:THR:O	1:D:70:ALA:HA	2.20	0.42
1:E:300:LEU:HD11	1:E:323:LEU:HD12	2.01	0.42
1:F:130:MET:HG3	1:F:137:ASN:OD1	2.18	0.42
1:F:186:LEU:C	1:F:188:GLU:H	2.22	0.42
1:F:159:PRO:HA	1:F:202:ALA:HB3	2.02	0.42
1:G:252:LEU:HD13	1:G:255:VAL:CG1	2.50	0.42
1:G:278:ASP:OD2	1:G:278:ASP:C	2.58	0.42
1:A:300:LEU:HD11	1:A:323:LEU:HD12	2.01	0.42
1:D:104:ILE:HD13	1:D:115:ILE:HG21	2.01	0.42
1:E:240:GLN:N	1:E:240:GLN:CD	2.73	0.42
1:F:89:LYS:HE2	1:F:110:TYR:CE2	2.54	0.42
1:G:56:LYS:O	1:G:337:GLN:HG2	2.19	0.42
1:C:141:VAL:HG22	1:C:152:LEU:HD21	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:HG2	1:D:317:LYS:HE3	2.01	0.42
1:G:36:GLU:CD	1:G:43:ARG:HH22	2.23	0.42
1:G:97:GLU:HG2	1:G:317:LYS:HE3	2.02	0.42
1:H:322:ILE:O	1:H:326:GLU:HG3	2.20	0.42
1:E:160:VAL:HG12	1:H:333:LEU:CD1	2.50	0.42
1:D:100:ILE:C	1:D:100:ILE:HD12	2.40	0.42
1:D:130:MET:HA	1:D:130:MET:CE	2.47	0.42
1:D:303:PRO:HA	1:D:306:TRP:CE3	2.55	0.42
1:E:323:LEU:HA	1:E:323:LEU:HD23	1.90	0.42
1:F:329:ARG:NE	1:H:163:ASN:HB2	2.35	0.42
1:F:69:SER:OG	1:F:99:ASN:HB3	2.20	0.42
1:G:303:PRO:HA	1:G:306:TRP:CE3	2.53	0.42
1:G:302:ARG:HG3	2:G:7401:FMN:O2P	2.20	0.42
1:H:166:ARG:NH1	1:H:166:ARG:HG2	2.35	0.42
1:E:158:THR:HG22	1:E:158:THR:O	2.19	0.42
1:H:134:TRP:HA	1:H:137:ASN:HB2	2.01	0.42
1:B:229:GLU:HB3	1:C:49:ARG:NH2	2.35	0.41
1:C:219:PRO:HA	1:C:240:GLN:HE21	1.84	0.41
1:D:85:PRO:HB2	4:D:4491:HOH:O	2.18	0.41
1:F:128:LEU:CG	1:F:130:MET:HE3	2.49	0.41
1:G:307:GLY:O	1:G:315:GLY:HA3	2.20	0.41
1:H:69:SER:OG	1:H:99:ASN:HB3	2.20	0.41
1:A:36:GLU:CD	1:A:43:ARG:HH22	2.22	0.41
1:B:34:TYR:HE1	1:B:302:ARG:CZ	2.33	0.41
1:C:158:THR:O	1:C:158:THR:HG22	2.20	0.41
1:D:262:LEU:HD22	1:D:266:VAL:CG2	2.51	0.41
1:D:56:LYS:O	1:D:337:GLN:HG2	2.20	0.41
1:E:73:CYS:HB3	1:E:101:CYS:O	2.20	0.41
1:A:138:LYS:HE3	1:A:138:LYS:HB2	1.90	0.41
1:A:329:ARG:NE	1:C:163:ASN:HB2	2.34	0.41
1:B:212:LEU:O	1:B:212:LEU:HD23	2.21	0.41
1:C:36:GLU:CD	1:C:43:ARG:HH22	2.23	0.41
1:E:34:TYR:HE1	1:E:302:ARG:CZ	2.33	0.41
1:C:278:ASP:OD2	1:C:278:ASP:C	2.59	0.41
1:C:73:CYS:HB3	1:C:101:CYS:O	2.21	0.41
1:F:73:CYS:HB3	1:F:101:CYS:O	2.20	0.41
1:A:128:LEU:CG	1:A:130:MET:HE1	2.48	0.41
1:B:303:PRO:HA	1:B:306:TRP:CE3	2.55	0.41
1:F:126:PHE:HB2	1:F:149:PHE:CD2	2.56	0.41
1:H:212:LEU:O	1:H:216:THR:HG22	2.21	0.41
1:A:318:GLU:O	1:A:322:ILE:HG13	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:PHE:HD1	1:C:137:ASN:HD22	1.67	0.41
1:F:141:VAL:HG22	1:F:152:LEU:HD21	2.02	0.41
1:A:166:ARG:NH1	1:A:166:ARG:HG2	2.36	0.41
1:C:89:LYS:O	1:C:93:ARG:HG3	2.20	0.41
1:B:211:LEU:CD1	1:B:211:LEU:C	2.87	0.41
1:C:136:PHE:C	1:C:136:PHE:CD1	2.93	0.41
1:D:141:VAL:HG22	1:D:152:LEU:HD21	2.02	0.41
1:B:36:GLU:CD	1:B:43:ARG:HH22	2.21	0.41
1:D:213:GLN:HG2	1:D:220:ILE:HD12	2.03	0.41
1:G:211:LEU:HG	1:G:212:LEU:N	2.36	0.41
1:H:62:THR:HG22	1:H:67:GLU:HA	2.02	0.41
1:B:130:MET:CE	1:B:130:MET:HA	2.42	0.41
1:H:186:LEU:HB2	4:H:8521:HOH:O	2.21	0.41
1:H:86:ASP:HB3	1:H:90:SER:OG	2.21	0.41
1:C:250:ARG:NH1	2:C:3401:FMN:HM82	2.36	0.40
1:H:34:TYR:CE1	1:H:302:ARG:CZ	3.04	0.40
1:B:134:TRP:CZ3	1:B:211:LEU:HG	2.55	0.40
1:D:240:GLN:CD	1:D:240:GLN:N	2.75	0.40
1:E:59:THR:O	1:E:70:ALA:HA	2.21	0.40
1:G:329:ARG:NH2	4:G:7440:HOH:O	2.40	0.40
1:G:72:ILE:HD13	1:G:323:LEU:HB3	2.03	0.40
1:H:141:VAL:HG22	1:H:152:LEU:HD21	2.02	0.40
1:B:159:PRO:HA	1:B:202:ALA:HB3	2.02	0.40
1:C:138:LYS:HA	1:C:215:ILE:HD12	2.03	0.40
1:D:327:LEU:HD22	1:D:331:MET:SD	2.62	0.40
1:D:34:TYR:HE1	1:D:302:ARG:CZ	2.34	0.40
1:G:186:LEU:C	1:G:188:GLU:N	2.75	0.40
1:H:219:PRO:HA	1:H:240:GLN:HE21	1.86	0.40
1:B:327:LEU:HD22	1:B:331:MET:HG3	2.03	0.40
1:E:343:SER:O	1:E:346:LEU:HB2	2.22	0.40
1:G:213:GLN:HG2	1:G:220:ILE:HD12	2.04	0.40
1:D:134:TRP:HA	1:D:137:ASN:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	326/352 (93%)	310 (95%)	13 (4%)	3 (1%)	17	20
1	B	321/352 (91%)	308 (96%)	11 (3%)	2 (1%)	25	31
1	C	326/352 (93%)	309 (95%)	14 (4%)	3 (1%)	17	20
1	D	323/352 (92%)	310 (96%)	11 (3%)	2 (1%)	25	31
1	E	320/352 (91%)	306 (96%)	12 (4%)	2 (1%)	25	31
1	F	326/352 (93%)	311 (95%)	12 (4%)	3 (1%)	17	20
1	G	323/352 (92%)	309 (96%)	12 (4%)	2 (1%)	25	31
1	H	326/352 (93%)	311 (95%)	12 (4%)	3 (1%)	17	20
All	All	2591/2816 (92%)	2474 (96%)	97 (4%)	20 (1%)	19	23

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	B	173	ASN
1	C	173	ASN
1	D	173	ASN
1	E	173	ASN
1	F	173	ASN
1	G	173	ASN
1	H	173	ASN
1	A	174	LEU
1	A	183	LEU
1	B	174	LEU
1	D	174	LEU
1	F	174	LEU
1	F	183	LEU
1	G	174	LEU
1	H	174	LEU
1	C	174	LEU
1	C	183	LEU
1	E	174	LEU
1	H	183	LEU

### 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	272/296 (92%)	256 (94%)	16 (6%)	19	27
1	B	270/296 (91%)	254 (94%)	16 (6%)	19	27
1	C	272/296 (92%)	257 (94%)	15 (6%)	21	30
1	D	271/296 (92%)	256 (94%)	15 (6%)	21	30
1	E	269/296 (91%)	256 (95%)	13 (5%)	25	36
1	F	272/296 (92%)	257 (94%)	15 (6%)	21	30
1	G	270/296 (91%)	255 (94%)	15 (6%)	21	29
1	H	272/296 (92%)	257 (94%)	15 (6%)	21	30
All	All	2168/2368 (92%)	2048 (94%)	120 (6%)	21	30

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	THR
1	A	75	SER
1	A	86	ASP
1	A	130	MET
1	A	173	ASN
1	A	186	LEU
1	A	212	LEU
1	A	222	LEU
1	A	252	LEU
1	A	262	LEU
1	A	288	LEU
1	A	293	LEU
1	A	297	CYS
1	A	323	LEU
1	A	327	LEU
1	A	333	LEU
1	B	59	THR
1	B	75	SER
1	B	86	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	130	MET
1	B	173	ASN
1	B	186	LEU
1	B	211	LEU
1	B	212	LEU
1	B	222	LEU
1	B	252	LEU
1	B	262	LEU
1	B	288	LEU
1	B	293	LEU
1	B	323	LEU
1	B	327	LEU
1	B	333	LEU
1	C	59	THR
1	C	75	SER
1	C	86	ASP
1	C	130	MET
1	C	173	ASN
1	C	212	LEU
1	C	222	LEU
1	C	252	LEU
1	C	262	LEU
1	C	288	LEU
1	C	293	LEU
1	C	297	CYS
1	C	323	LEU
1	C	327	LEU
1	C	333	LEU
1	D	59	THR
1	D	75	SER
1	D	86	ASP
1	D	130	MET
1	D	173	ASN
1	D	212	LEU
1	D	222	LEU
1	D	252	LEU
1	D	262	LEU
1	D	288	LEU
1	D	293	LEU
1	D	297	CYS
1	D	323	LEU
1	D	327	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	333	LEU
1	E	59	THR
1	E	75	SER
1	E	86	ASP
1	E	130	MET
1	E	173	ASN
1	E	222	LEU
1	E	252	LEU
1	E	262	LEU
1	E	288	LEU
1	E	293	LEU
1	E	323	LEU
1	E	327	LEU
1	E	333	LEU
1	F	59	THR
1	F	75	SER
1	F	86	ASP
1	F	130	MET
1	F	173	ASN
1	F	212	LEU
1	F	222	LEU
1	F	252	LEU
1	F	262	LEU
1	F	288	LEU
1	F	293	LEU
1	F	297	CYS
1	F	323	LEU
1	F	327	LEU
1	F	333	LEU
1	G	59	THR
1	G	75	SER
1	G	86	ASP
1	G	130	MET
1	G	173	ASN
1	G	186	LEU
1	G	222	LEU
1	G	252	LEU
1	G	262	LEU
1	G	288	LEU
1	G	293	LEU
1	G	297	CYS
1	G	323	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	327	LEU
1	G	333	LEU
1	H	59	THR
1	H	75	SER
1	H	86	ASP
1	H	130	MET
1	H	173	ASN
1	H	212	LEU
1	H	222	LEU
1	H	252	LEU
1	H	262	LEU
1	H	288	LEU
1	H	293	LEU
1	H	297	CYS
1	H	323	LEU
1	H	327	LEU
1	H	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	99	ASN
1	A	137	ASN
1	A	163	ASN
1	A	171	GLN
1	A	237	HIS
1	A	240	GLN
1	A	251	GLN
1	B	64	GLN
1	B	99	ASN
1	B	137	ASN
1	B	163	ASN
1	B	171	GLN
1	B	173	ASN
1	B	237	HIS
1	B	240	GLN
1	B	251	GLN
1	C	64	GLN
1	C	99	ASN
1	C	137	ASN
1	C	163	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	171	GLN
1	C	237	HIS
1	C	240	GLN
1	C	251	GLN
1	D	64	GLN
1	D	99	ASN
1	D	137	ASN
1	D	163	ASN
1	D	171	GLN
1	D	173	ASN
1	D	237	HIS
1	D	240	GLN
1	D	251	GLN
1	E	64	GLN
1	E	99	ASN
1	E	137	ASN
1	E	163	ASN
1	E	171	GLN
1	E	173	ASN
1	E	237	HIS
1	E	240	GLN
1	E	251	GLN
1	F	64	GLN
1	F	99	ASN
1	F	137	ASN
1	F	163	ASN
1	F	171	GLN
1	F	237	HIS
1	F	240	GLN
1	F	251	GLN
1	G	64	GLN
1	G	99	ASN
1	G	137	ASN
1	G	163	ASN
1	G	171	GLN
1	G	173	ASN
1	G	240	GLN
1	G	251	GLN
1	H	64	GLN
1	H	99	ASN
1	H	137	ASN
1	H	163	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	171	GLN
1	H	237	HIS
1	H	240	GLN
1	H	251	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FMN	E	5401	-	31,33,33	2.96	11 (35%)	40,50,50	3.04	8 (20%)
2	FMN	D	4401	-	31,33,33	2.95	11 (35%)	40,50,50	2.97	8 (20%)
3	ACY	A	1402	-	1,3,3	3.28	1 (100%)	0,3,3	0.00	-
2	FMN	A	1401	-	31,33,33	2.90	11 (35%)	40,50,50	3.04	8 (20%)
3	ACY	H	8402	-	1,3,3	3.24	1 (100%)	0,3,3	0.00	-
2	FMN	H	8401	-	31,33,33	3.00	12 (38%)	40,50,50	2.99	8 (20%)
3	ACY	B	2402	-	1,3,3	3.13	1 (100%)	0,3,3	0.00	-
2	FMN	B	2401	-	31,33,33	2.96	12 (38%)	40,50,50	2.99	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FMN	C	3401	-	31,33,33	2.91	12 (38%)	40,50,50	2.97	8 (20%)
3	ACY	D	4402	-	1,3,3	3.10	1 (100%)	0,3,3	0.00	-
3	ACY	G	7402	-	1,3,3	3.22	1 (100%)	0,3,3	0.00	-
2	FMN	G	7401	-	31,33,33	3.01	11 (35%)	40,50,50	2.97	9 (22%)
3	ACY	E	5402	-	1,3,3	3.22	1 (100%)	0,3,3	0.00	-
3	ACY	F	6402	-	1,3,3	3.21	1 (100%)	0,3,3	0.00	-
2	FMN	F	6401	-	31,33,33	2.86	11 (35%)	40,50,50	3.07	9 (22%)
3	ACY	C	3402	-	1,3,3	3.05	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	E	5401	-	-	5/18/18/18	0/3/3/3
2	FMN	D	4401	-	-	5/18/18/18	0/3/3/3
2	FMN	A	1401	-	-	5/18/18/18	0/3/3/3
2	FMN	H	8401	-	-	5/18/18/18	0/3/3/3
2	FMN	B	2401	-	-	5/18/18/18	0/3/3/3
2	FMN	C	3401	-	-	5/18/18/18	0/3/3/3
2	FMN	G	7401	-	-	5/18/18/18	0/3/3/3
2	FMN	F	6401	-	-	5/18/18/18	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7401	FMN	C1'-N10	-11.16	1.36	1.48
2	H	8401	FMN	C1'-N10	-10.82	1.37	1.48
2	E	5401	FMN	C1'-N10	-10.79	1.37	1.48
2	D	4401	FMN	C1'-N10	-10.75	1.37	1.48
2	B	2401	FMN	C1'-N10	-10.58	1.37	1.48
2	C	3401	FMN	C1'-N10	-10.44	1.37	1.48
2	A	1401	FMN	C1'-N10	-9.89	1.38	1.48
2	F	6401	FMN	C1'-N10	-9.66	1.38	1.48
2	A	1401	FMN	C4A-N5	6.29	1.42	1.33
2	C	3401	FMN	C4A-N5	6.23	1.42	1.33
2	B	2401	FMN	C4A-N5	6.19	1.42	1.33
2	E	5401	FMN	C4A-N5	6.17	1.42	1.33

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8401	FMN	C4A-N5	6.16	1.42	1.33
2	G	7401	FMN	C4A-N5	6.15	1.42	1.33
2	D	4401	FMN	C4A-N5	6.13	1.42	1.33
2	F	6401	FMN	C4A-N5	6.09	1.42	1.33
2	H	8401	FMN	C10-N1	5.08	1.39	1.33
2	E	5401	FMN	C10-N1	4.87	1.39	1.33
2	G	7401	FMN	C10-N1	4.76	1.39	1.33
2	A	1401	FMN	C10-N1	4.76	1.39	1.33
2	F	6401	FMN	C10-N1	4.69	1.39	1.33
2	B	2401	FMN	C10-N1	4.66	1.39	1.33
2	H	8401	FMN	C4-N3	4.63	1.41	1.33
2	B	2401	FMN	C4-N3	4.56	1.41	1.33
2	A	1401	FMN	C4-N3	4.55	1.41	1.33
2	C	3401	FMN	C10-N1	4.54	1.39	1.33
2	D	4401	FMN	C4-N3	4.51	1.40	1.33
2	C	3401	FMN	C4-N3	4.45	1.40	1.33
2	D	4401	FMN	C10-N1	4.42	1.38	1.33
2	F	6401	FMN	C4-N3	4.41	1.40	1.33
2	E	5401	FMN	C4-N3	4.40	1.40	1.33
2	G	7401	FMN	C4-N3	4.37	1.40	1.33
2	F	6401	FMN	C9A-N10	4.27	1.44	1.38
2	A	1401	FMN	C9A-N10	4.12	1.44	1.38
2	H	8401	FMN	C9A-N10	4.06	1.44	1.38
2	G	7401	FMN	C9A-N10	3.78	1.43	1.38
2	C	3401	FMN	C9A-N10	3.73	1.43	1.38
2	D	4401	FMN	C5A-N5	3.71	1.41	1.35
2	B	2401	FMN	C9A-N10	3.66	1.43	1.38
2	D	4401	FMN	C9A-N10	3.63	1.43	1.38
2	B	2401	FMN	C5A-N5	3.60	1.41	1.35
2	G	7401	FMN	C5A-N5	3.55	1.41	1.35
2	E	5401	FMN	C5A-N5	3.52	1.41	1.35
2	E	5401	FMN	C9A-N10	3.49	1.43	1.38
2	H	8401	FMN	C5A-N5	3.42	1.41	1.35
2	C	3401	FMN	C5A-N5	3.41	1.41	1.35
2	A	1401	FMN	C4-C4A	3.33	1.47	1.41
3	A	1402	ACY	CH3-C	3.28	1.52	1.48
2	F	6401	FMN	C5A-N5	3.27	1.40	1.35
3	H	8402	ACY	CH3-C	3.24	1.52	1.48
3	G	7402	ACY	CH3-C	3.22	1.52	1.48
3	E	5402	ACY	CH3-C	3.22	1.52	1.48
3	F	6402	ACY	CH3-C	3.21	1.52	1.48
2	B	2401	FMN	C4-C4A	3.19	1.46	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5401	FMN	C4-C4A	3.16	1.46	1.41
2	G	7401	FMN	C4-C4A	3.16	1.46	1.41
3	B	2402	ACY	CH3-C	3.13	1.52	1.48
2	F	6401	FMN	C4-C4A	3.12	1.46	1.41
2	A	1401	FMN	C5A-N5	3.10	1.40	1.35
3	D	4402	ACY	CH3-C	3.10	1.52	1.48
3	C	3402	ACY	CH3-C	3.05	1.52	1.48
2	D	4401	FMN	C4-C4A	3.03	1.46	1.41
2	C	3401	FMN	C4-C4A	2.95	1.46	1.41
2	H	8401	FMN	C4A-C10	2.86	1.41	1.38
2	E	5401	FMN	C4A-C10	2.78	1.41	1.38
2	F	6401	FMN	P-O5'	-2.78	1.51	1.60
2	F	6401	FMN	C4A-C10	2.76	1.41	1.38
2	A	1401	FMN	P-O5'	-2.76	1.51	1.60
2	H	8401	FMN	C4-C4A	2.73	1.46	1.41
2	B	2401	FMN	P-O2P	-2.72	1.44	1.54
2	D	4401	FMN	C4A-C10	2.71	1.41	1.38
2	G	7401	FMN	P-O3P	-2.68	1.44	1.54
2	B	2401	FMN	P-O5'	-2.64	1.51	1.60
2	F	6401	FMN	P-O3P	-2.56	1.45	1.54
2	E	5401	FMN	P-O2P	-2.55	1.45	1.54
2	B	2401	FMN	C4A-C10	2.53	1.41	1.38
2	G	7401	FMN	C4A-C10	2.53	1.41	1.38
2	D	4401	FMN	P-O3P	-2.50	1.45	1.54
2	C	3401	FMN	P-O2P	-2.49	1.45	1.54
2	G	7401	FMN	P-O5'	-2.49	1.52	1.60
2	G	7401	FMN	P-O2P	-2.47	1.45	1.54
2	H	8401	FMN	P-O2P	-2.47	1.45	1.54
2	E	5401	FMN	P-O5'	-2.46	1.52	1.60
2	A	1401	FMN	C4A-C10	2.44	1.41	1.38
2	A	1401	FMN	P-O3P	-2.44	1.45	1.54
2	A	1401	FMN	P-O2P	-2.42	1.45	1.54
2	B	2401	FMN	P-O3P	-2.40	1.45	1.54
2	H	8401	FMN	P-O5'	-2.39	1.52	1.60
2	D	4401	FMN	P-O2P	-2.37	1.45	1.54
2	C	3401	FMN	P-O5'	-2.35	1.52	1.60
2	C	3401	FMN	C4A-C10	2.30	1.41	1.38
2	C	3401	FMN	C5'-C4'	-2.29	1.48	1.51
2	D	4401	FMN	P-O5'	-2.24	1.53	1.60
2	B	2401	FMN	C5'-C4'	-2.21	1.48	1.51
2	C	3401	FMN	P-O3P	-2.17	1.46	1.54
2	F	6401	FMN	P-O2P	-2.16	1.46	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5401	FMN	P-O3P	-2.11	1.46	1.54
2	H	8401	FMN	P-O3P	-2.04	1.47	1.54
2	H	8401	FMN	C5'-C4'	-2.03	1.48	1.51

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5401	FMN	C4-N3-C2	14.40	127.30	115.14
2	F	6401	FMN	C4-N3-C2	14.17	127.11	115.14
2	B	2401	FMN	C4-N3-C2	14.17	127.11	115.14
2	A	1401	FMN	C4-N3-C2	14.08	127.03	115.14
2	D	4401	FMN	C4-N3-C2	14.03	126.99	115.14
2	G	7401	FMN	C4-N3-C2	13.98	126.94	115.14
2	C	3401	FMN	C4-N3-C2	13.96	126.93	115.14
2	H	8401	FMN	C4-N3-C2	13.95	126.92	115.14
2	E	5401	FMN	C4A-C4-N3	-6.83	114.10	123.43
2	B	2401	FMN	C4A-C4-N3	-6.82	114.11	123.43
2	A	1401	FMN	C4A-C4-N3	-6.79	114.14	123.43
2	D	4401	FMN	C4A-C4-N3	-6.79	114.15	123.43
2	F	6401	FMN	C4A-C4-N3	-6.78	114.16	123.43
2	C	3401	FMN	C4A-C4-N3	-6.69	114.28	123.43
2	H	8401	FMN	C4A-C4-N3	-6.68	114.30	123.43
2	G	7401	FMN	C4A-C4-N3	-6.67	114.31	123.43
2	F	6401	FMN	C1'-N10-C9A	4.83	122.10	118.29
2	F	6401	FMN	C5'-C4'-C3'	-4.66	103.20	112.20
2	A	1401	FMN	C1'-N10-C9A	4.64	121.95	118.29
2	E	5401	FMN	C4-C4A-C10	4.62	123.01	119.95
2	D	4401	FMN	C1'-N10-C9A	4.59	121.90	118.29
2	F	6401	FMN	C4-C4A-C10	4.57	122.98	119.95
2	G	7401	FMN	C4-C4A-C10	4.56	122.97	119.95
2	H	8401	FMN	C4-C4A-C10	4.46	122.91	119.95
2	A	1401	FMN	C4-C4A-C10	4.46	122.90	119.95
2	A	1401	FMN	C5'-C4'-C3'	-4.44	103.62	112.20
2	H	8401	FMN	C1'-N10-C9A	4.42	121.78	118.29
2	B	2401	FMN	C4-C4A-C10	4.36	122.84	119.95
2	D	4401	FMN	C4-C4A-C10	4.25	122.77	119.95
2	C	3401	FMN	C4-C4A-C10	4.23	122.75	119.95
2	G	7401	FMN	C5'-C4'-C3'	-4.21	104.07	112.20
2	B	2401	FMN	C5'-C4'-C3'	-4.20	104.08	112.20
2	C	3401	FMN	C5'-C4'-C3'	-4.20	104.09	112.20
2	A	1401	FMN	P-O5'-C5'	4.19	129.82	118.30
2	H	8401	FMN	C5'-C4'-C3'	-4.18	104.12	112.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5401	FMN	C5'-C4'-C3'	-4.17	104.15	112.20
2	B	2401	FMN	C1'-N10-C9A	4.13	121.54	118.29
2	G	7401	FMN	C1'-N10-C9A	4.12	121.54	118.29
2	C	3401	FMN	C1'-N10-C9A	4.08	121.50	118.29
2	H	8401	FMN	P-O5'-C5'	4.04	129.43	118.30
2	C	3401	FMN	P-O5'-C5'	4.03	129.38	118.30
2	F	6401	FMN	P-O5'-C5'	3.98	129.26	118.30
2	E	5401	FMN	C1'-N10-C9A	3.91	121.37	118.29
2	D	4401	FMN	C5'-C4'-C3'	-3.87	104.72	112.20
2	D	4401	FMN	P-O5'-C5'	3.72	128.54	118.30
2	G	7401	FMN	P-O5'-C5'	3.72	128.53	118.30
2	E	5401	FMN	P-O5'-C5'	3.71	128.51	118.30
2	B	2401	FMN	P-O5'-C5'	3.59	128.19	118.30
2	B	2401	FMN	O4'-C4'-C3'	3.10	116.64	109.10
2	C	3401	FMN	O4'-C4'-C3'	3.09	116.61	109.10
2	H	8401	FMN	O4'-C4'-C3'	3.02	116.45	109.10
2	E	5401	FMN	O4'-C4'-C3'	2.98	116.33	109.10
2	G	7401	FMN	O4'-C4'-C3'	2.96	116.30	109.10
2	D	4401	FMN	O4'-C4'-C3'	2.85	116.02	109.10
2	A	1401	FMN	O4'-C4'-C3'	2.73	115.74	109.10
2	A	1401	FMN	C4A-N5-C5A	2.73	119.50	116.77
2	F	6401	FMN	O4'-C4'-C3'	2.69	115.63	109.10
2	C	3401	FMN	C4A-N5-C5A	2.68	119.45	116.77
2	F	6401	FMN	C4A-N5-C5A	2.68	119.45	116.77
2	G	7401	FMN	C4A-N5-C5A	2.67	119.44	116.77
2	E	5401	FMN	C4A-N5-C5A	2.62	119.39	116.77
2	B	2401	FMN	C4A-N5-C5A	2.59	119.36	116.77
2	H	8401	FMN	C4A-N5-C5A	2.45	119.22	116.77
2	D	4401	FMN	C4A-N5-C5A	2.39	119.16	116.77
2	F	6401	FMN	O5'-C5'-C4'	2.08	114.91	109.36
2	G	7401	FMN	O5'-C5'-C4'	2.07	114.90	109.36

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5401	FMN	C2'-C3'-C4'-O4'
2	E	5401	FMN	O3'-C3'-C4'-O4'
2	E	5401	FMN	O3'-C3'-C4'-C5'
2	D	4401	FMN	C2'-C3'-C4'-O4'
2	D	4401	FMN	C2'-C3'-C4'-C5'
2	D	4401	FMN	O3'-C3'-C4'-O4'

*Continued on next page...*

*Continued from previous page...*

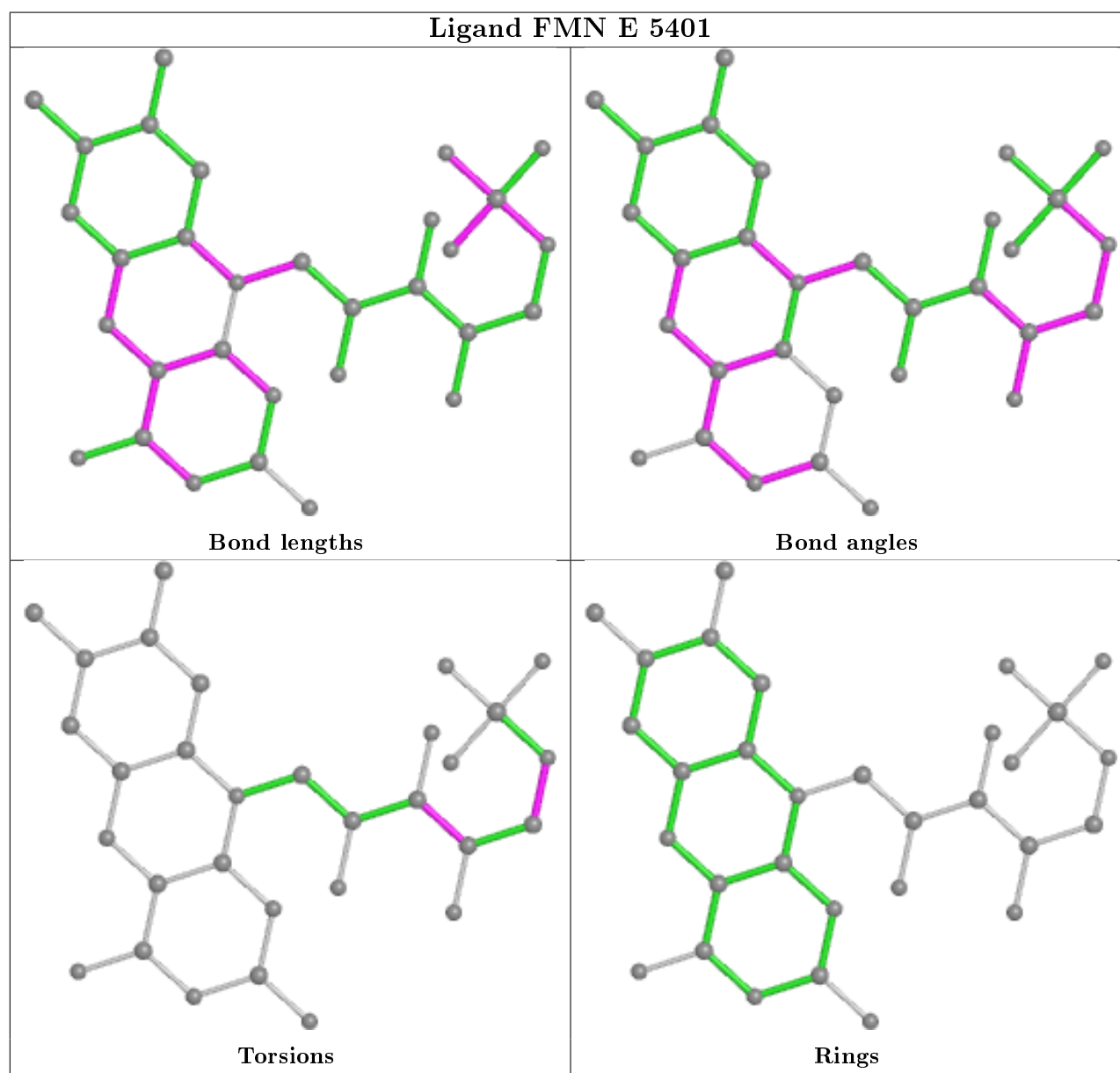
Mol	Chain	Res	Type	Atoms
2	D	4401	FMN	O3'-C3'-C4'-C5'
2	A	1401	FMN	C2'-C3'-C4'-O4'
2	A	1401	FMN	C2'-C3'-C4'-C5'
2	A	1401	FMN	O3'-C3'-C4'-O4'
2	A	1401	FMN	O3'-C3'-C4'-C5'
2	H	8401	FMN	C2'-C3'-C4'-O4'
2	H	8401	FMN	C2'-C3'-C4'-C5'
2	H	8401	FMN	O3'-C3'-C4'-O4'
2	H	8401	FMN	O3'-C3'-C4'-C5'
2	B	2401	FMN	C2'-C3'-C4'-O4'
2	B	2401	FMN	C2'-C3'-C4'-C5'
2	B	2401	FMN	O3'-C3'-C4'-O4'
2	B	2401	FMN	O3'-C3'-C4'-C5'
2	C	3401	FMN	C2'-C3'-C4'-O4'
2	C	3401	FMN	C2'-C3'-C4'-C5'
2	C	3401	FMN	O3'-C3'-C4'-O4'
2	C	3401	FMN	O3'-C3'-C4'-C5'
2	G	7401	FMN	C2'-C3'-C4'-O4'
2	G	7401	FMN	C2'-C3'-C4'-C5'
2	G	7401	FMN	O3'-C3'-C4'-O4'
2	G	7401	FMN	O3'-C3'-C4'-C5'
2	F	6401	FMN	C2'-C3'-C4'-O4'
2	F	6401	FMN	C2'-C3'-C4'-C5'
2	F	6401	FMN	O3'-C3'-C4'-O4'
2	F	6401	FMN	O3'-C3'-C4'-C5'
2	E	5401	FMN	C2'-C3'-C4'-C5'
2	G	7401	FMN	C4'-C5'-O5'-P
2	F	6401	FMN	C4'-C5'-O5'-P
2	D	4401	FMN	C4'-C5'-O5'-P
2	A	1401	FMN	C4'-C5'-O5'-P
2	E	5401	FMN	C4'-C5'-O5'-P
2	B	2401	FMN	C4'-C5'-O5'-P
2	C	3401	FMN	C4'-C5'-O5'-P
2	H	8401	FMN	C4'-C5'-O5'-P

There are no ring outliers.

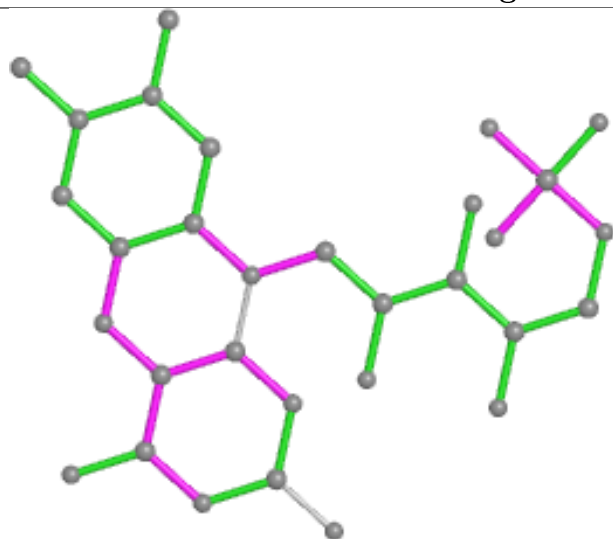
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2401	FMN	1	0
2	C	3401	FMN	1	0
2	G	7401	FMN	1	0

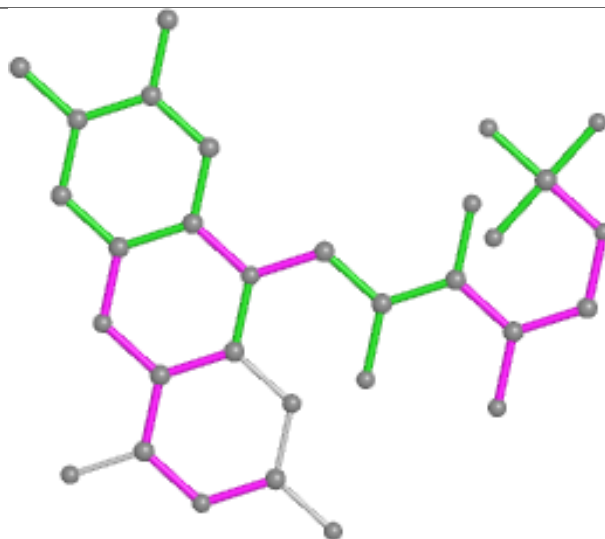
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



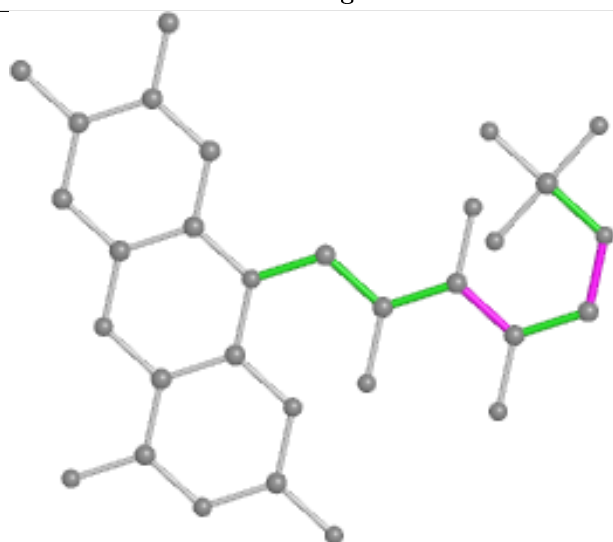
## Ligand FMN D 4401



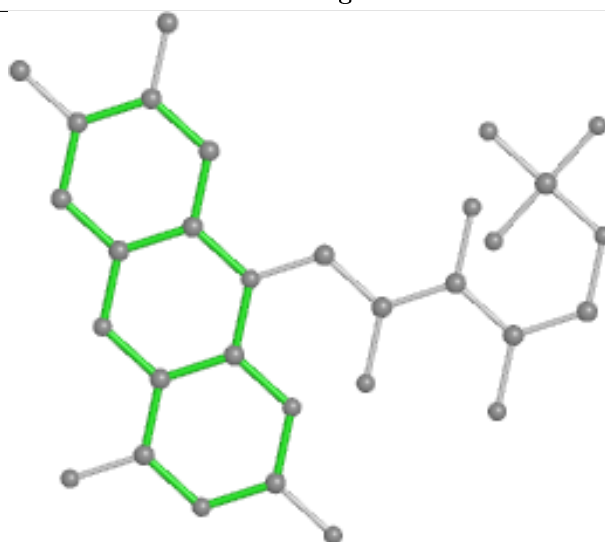
Bond lengths



Bond angles

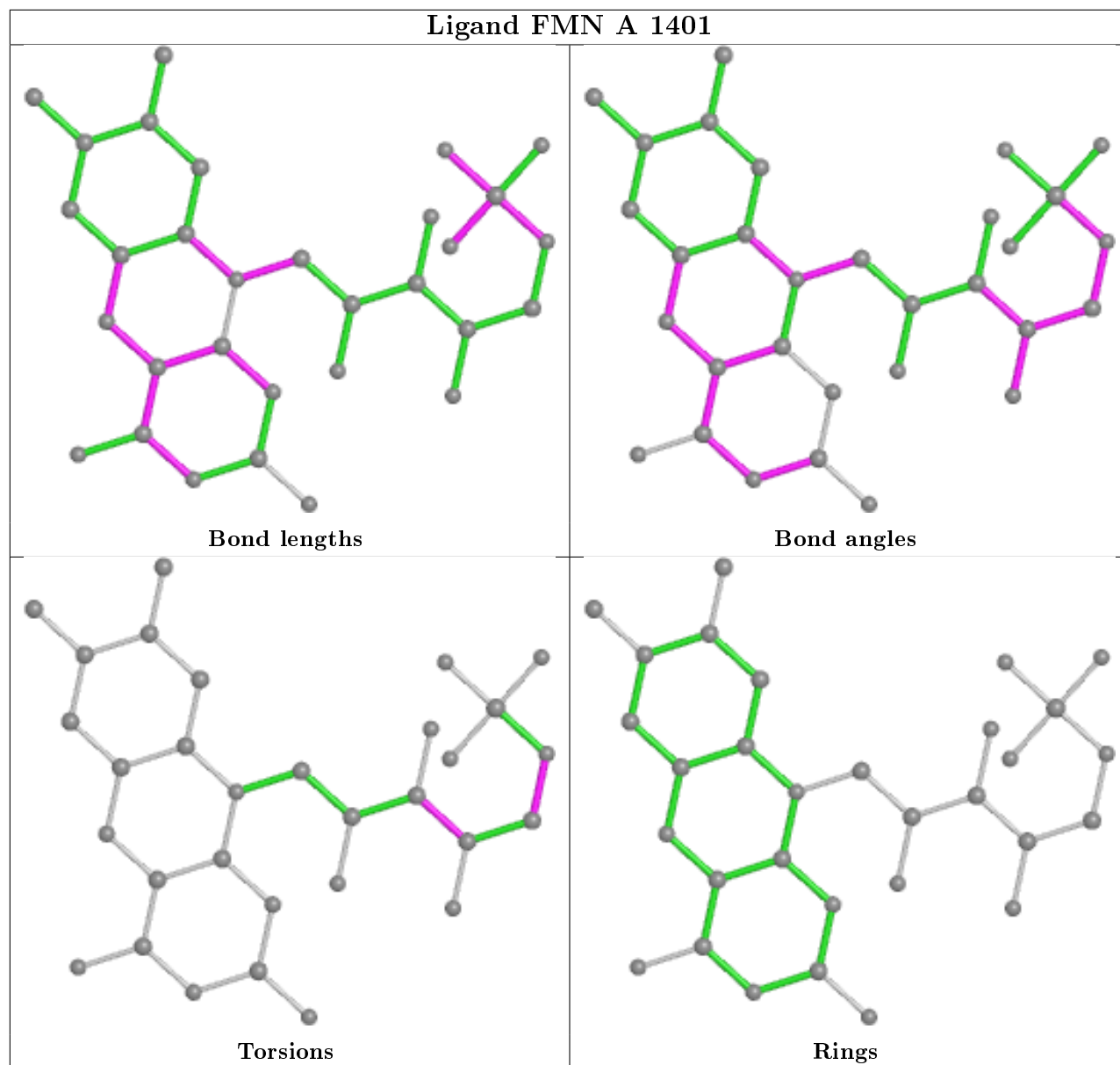


Torsions

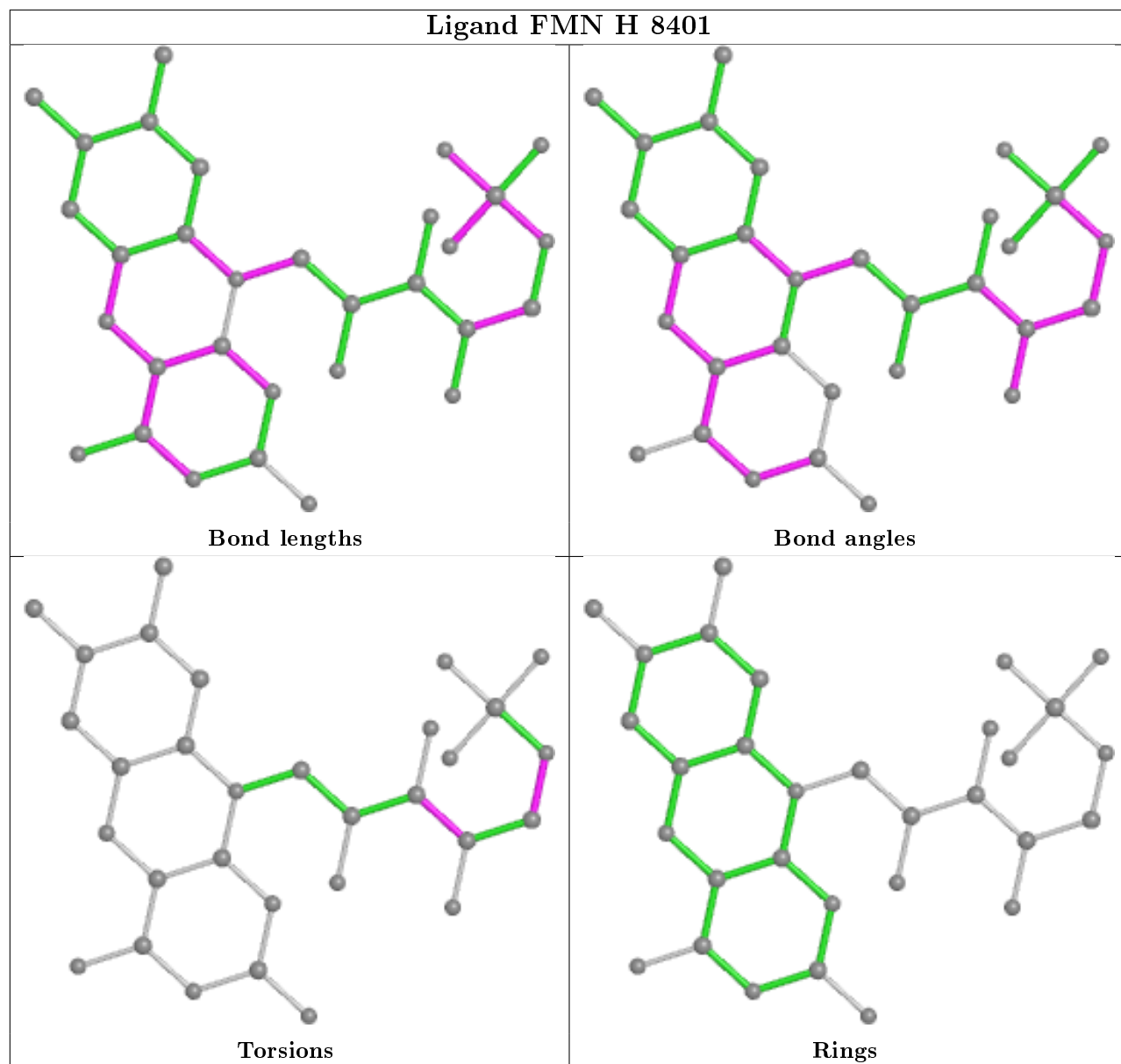


Rings

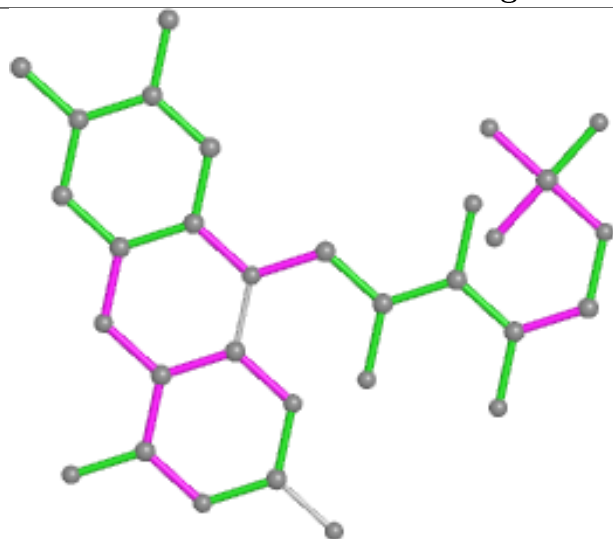
## Ligand FMN A 1401



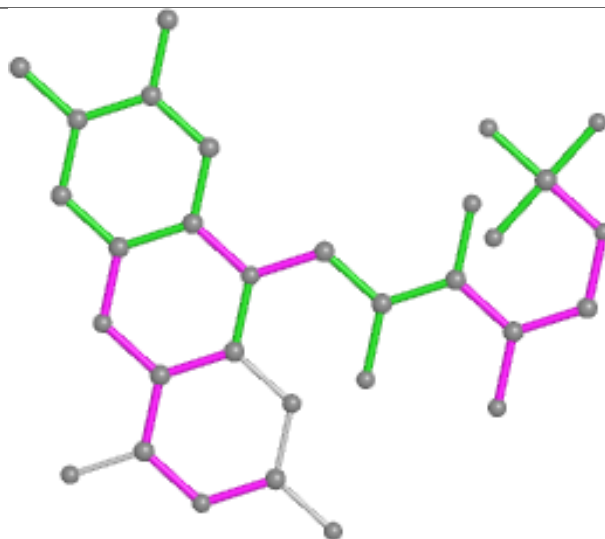
## Ligand FMN H 8401



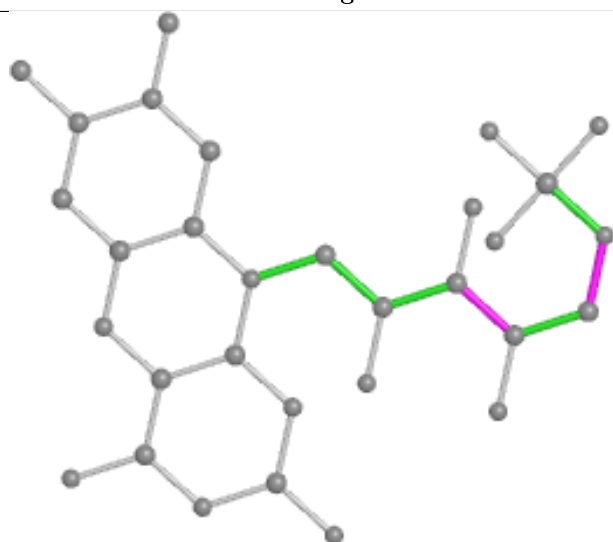
## Ligand FMN B 2401



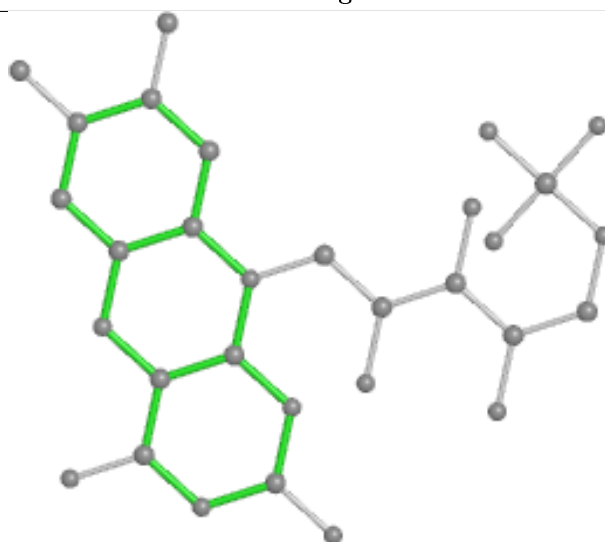
Bond lengths



Bond angles

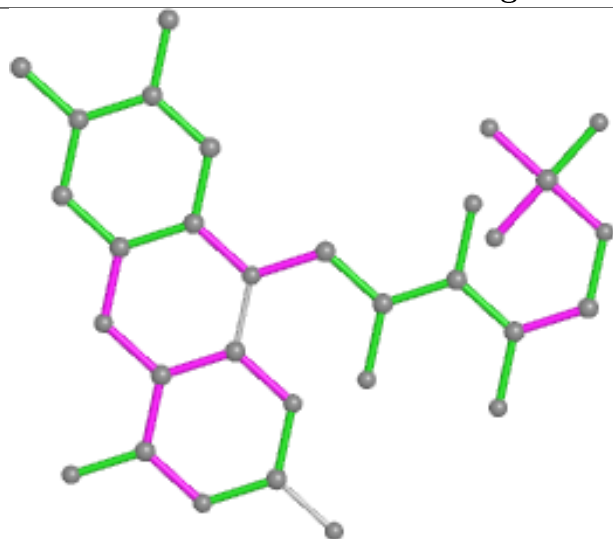


Torsions

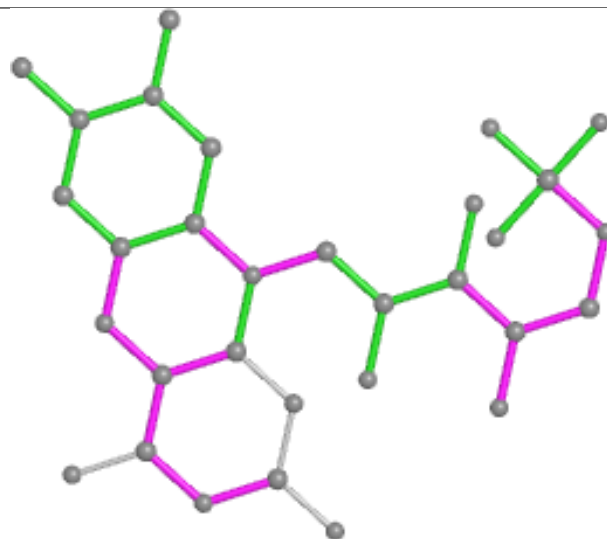


Rings

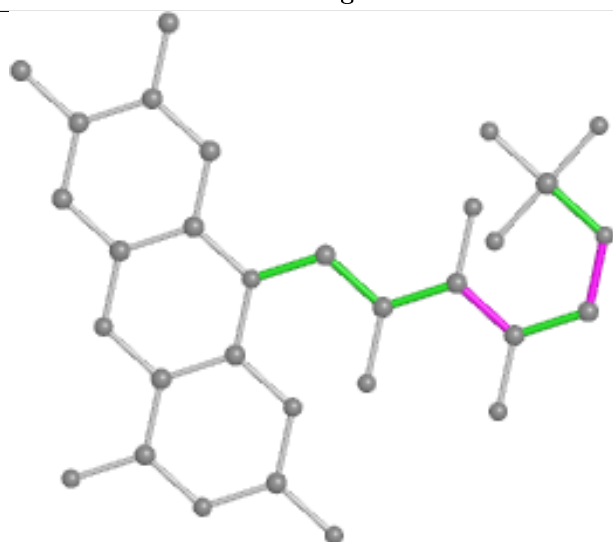
## Ligand FMN C 3401



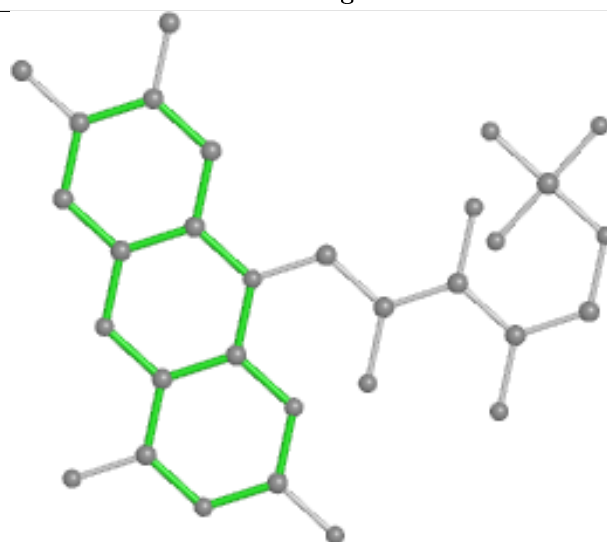
Bond lengths



Bond angles

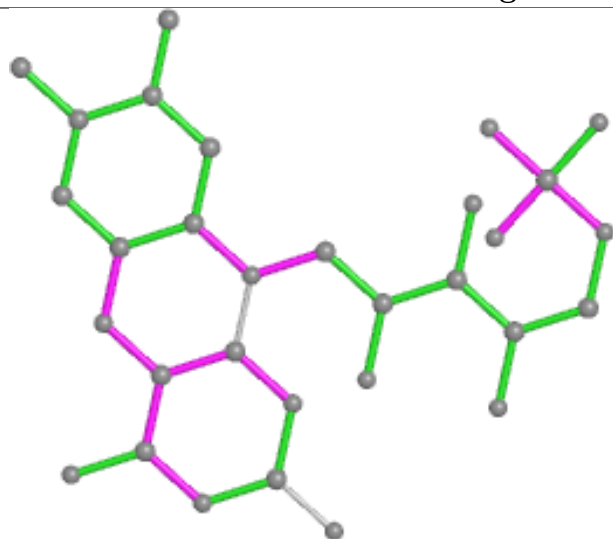


Torsions

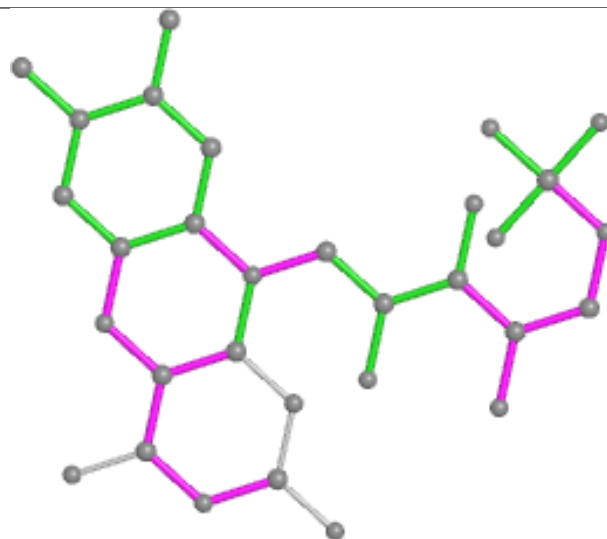


Rings

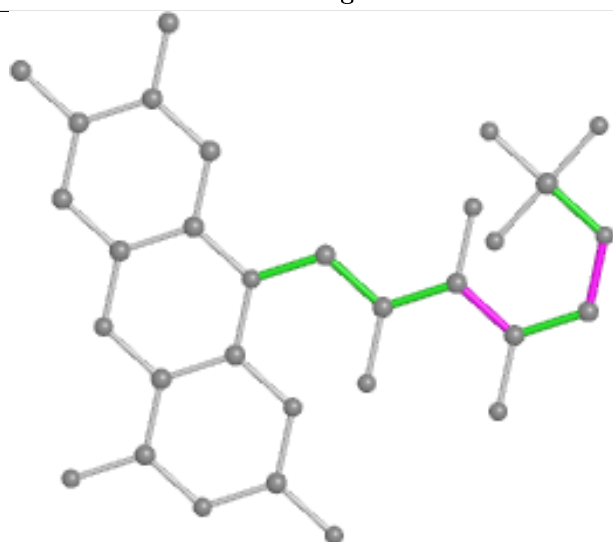
## Ligand FMN G 7401



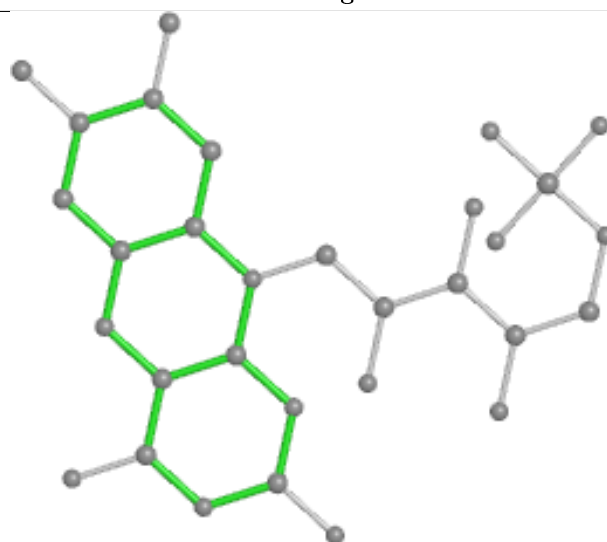
Bond lengths



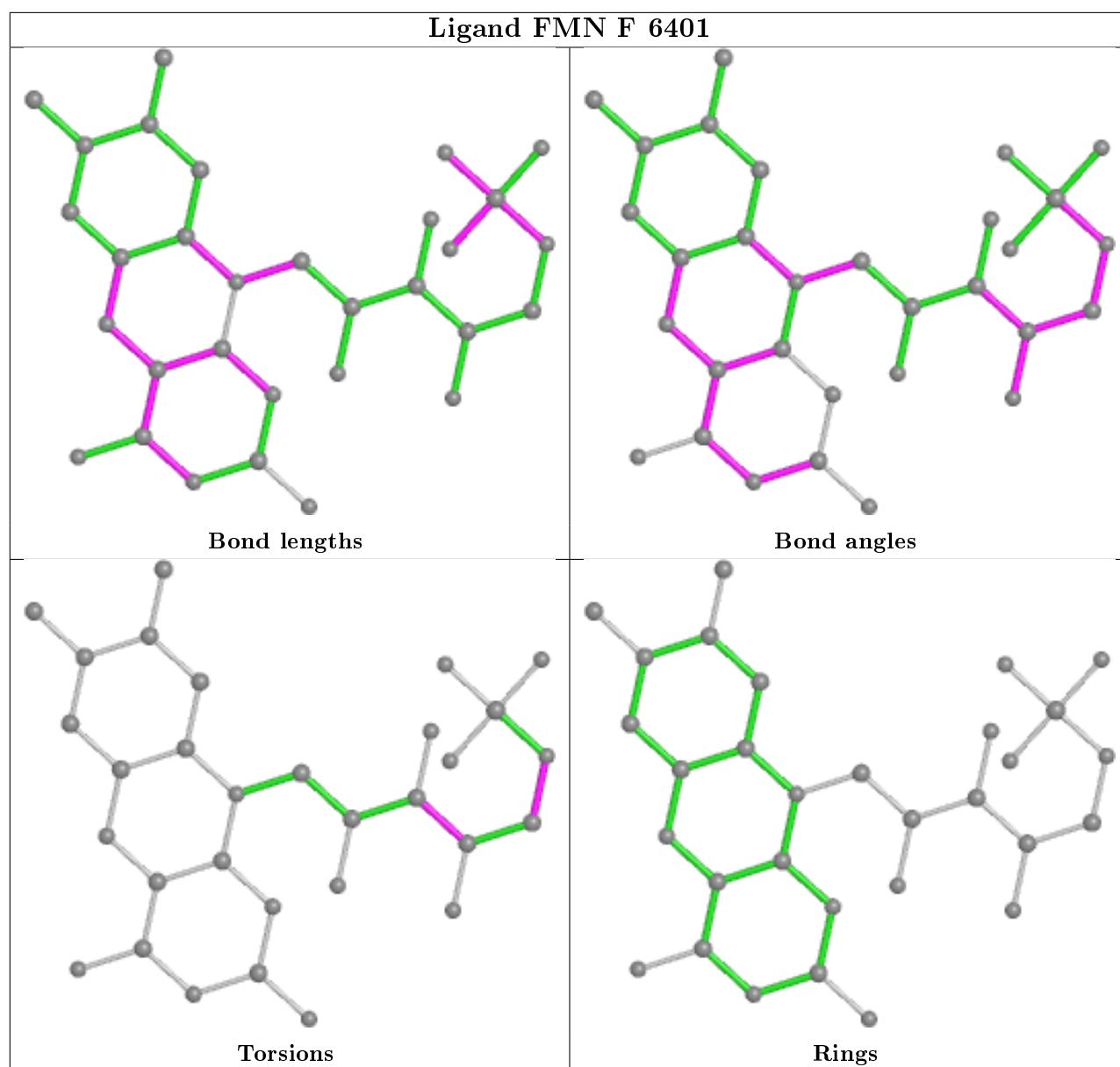
Bond angles



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	332/352 (94%)	-0.19	9 (2%) 54 62	16, 31, 73, 98	0
1	B	327/352 (92%)	0.06	13 (3%) 38 45	22, 39, 73, 96	0
1	C	332/352 (94%)	-0.04	20 (6%) 21 28	21, 35, 78, 99	0
1	D	329/352 (93%)	-0.11	12 (3%) 42 49	20, 36, 76, 96	0
1	E	324/352 (92%)	0.22	21 (6%) 18 24	22, 40, 73, 95	0
1	F	332/352 (94%)	-0.18	12 (3%) 42 49	13, 28, 72, 97	0
1	G	329/352 (93%)	-0.00	13 (3%) 38 45	18, 35, 77, 99	0
1	H	332/352 (94%)	-0.05	18 (5%) 25 32	19, 34, 76, 99	0
All	All	2637/2816 (93%)	-0.04	118 (4%) 33 40	13, 35, 76, 99	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	8.7
1	E	202	ALA	6.8
1	C	182	ASP	6.3
1	A	182	ASP	6.2
1	C	183	LEU	6.1
1	C	185	ALA	5.8
1	B	202	ALA	5.8
1	C	202	ALA	5.7
1	F	182	ASP	5.4
1	G	188	GLU	5.4
1	H	173	ASN	5.3
1	C	173	ASN	5.2
1	D	183	LEU	5.1
1	D	202	ALA	5.1
1	E	173	ASN	4.9
1	H	183	LEU	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	185	ALA	4.8
1	G	203	SER	4.8
1	E	132	SER	4.7
1	H	185	ALA	4.7
1	H	182	ASP	4.7
1	F	173	ASN	4.5
1	C	131	LYS	4.4
1	B	173	ASN	4.4
1	D	185	ALA	4.2
1	D	203	SER	4.2
1	C	139	GLN	4.0
1	F	183	LEU	4.0
1	H	172	LEU	4.0
1	A	202	ALA	4.0
1	H	139	GLN	3.7
1	C	186	LEU	3.6
1	E	203	SER	3.6
1	A	173	ASN	3.6
1	A	183	LEU	3.6
1	G	202	ALA	3.6
1	B	186	LEU	3.6
1	G	173	ASN	3.6
1	E	85	PRO	3.5
1	B	15	GLN	3.5
1	G	186	LEU	3.5
1	A	136	PHE	3.5
1	F	172	LEU	3.5
1	E	136	PHE	3.5
1	D	184	ARG	3.4
1	D	349	PHE	3.4
1	G	132	SER	3.4
1	E	56	LYS	3.4
1	F	202	ALA	3.4
1	C	188	GLU	3.4
1	E	272	LYS	3.3
1	A	172	LEU	3.3
1	H	186	LEU	3.3
1	E	172	LEU	3.2
1	G	207	ASN	3.2
1	H	131	LYS	3.1
1	D	173	ASN	3.1
1	B	136	PHE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	176	ALA	2.9
1	F	185	ALA	2.9
1	H	188	GLU	2.9
1	C	172	LEU	2.9
1	E	120	PRO	2.8
1	B	203	SER	2.8
1	H	202	ALA	2.7
1	G	349	PHE	2.7
1	B	272	LYS	2.7
1	A	185	ALA	2.7
1	C	184	ARG	2.7
1	G	133	ASP	2.6
1	E	131	LYS	2.6
1	F	184	ARG	2.6
1	D	172	LEU	2.6
1	G	215	ILE	2.5
1	H	55	SER	2.5
1	F	131	LYS	2.5
1	H	171	GLN	2.5
1	H	18	LYS	2.5
1	F	130	MET	2.5
1	H	203	SER	2.5
1	D	186	LEU	2.5
1	F	18	LYS	2.4
1	D	132	SER	2.4
1	C	56	LYS	2.4
1	H	184	ARG	2.4
1	D	139	GLN	2.4
1	H	130	MET	2.4
1	F	136	PHE	2.4
1	A	131	LYS	2.3
1	E	171	GLN	2.3
1	F	176	ALA	2.3
1	C	349	PHE	2.3
1	E	210	SER	2.3
1	G	131	LYS	2.2
1	H	349	PHE	2.2
1	B	14	LYS	2.2
1	C	53	ASP	2.2
1	G	184	ARG	2.2
1	B	172	LEU	2.2
1	E	124	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	18	LYS	2.2
1	B	210	SER	2.2
1	E	135	ASP	2.2
1	H	133	ASP	2.2
1	E	129	TYR	2.2
1	E	15	GLN	2.2
1	E	117	ALA	2.2
1	C	15	GLN	2.2
1	C	135	ASP	2.1
1	A	130	MET	2.1
1	E	84	TRP	2.1
1	E	340	ALA	2.1
1	C	174	LEU	2.1
1	B	214	SER	2.1
1	C	176	ALA	2.0
1	C	132	SER	2.0
1	C	203	SER	2.0
1	B	267	ALA	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 carbohydrates 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, 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( $\text{\AA}^2$ )	Q<0.9
3	ACY	B	2402	4/4	0.81	0.35	57,58,63,64	0
3	ACY	E	5402	4/4	0.84	0.20	59,62,64,64	0
3	ACY	A	1402	4/4	0.88	0.24	36,39,41,45	0
3	ACY	F	6402	4/4	0.89	0.27	35,36,38,42	0
3	ACY	C	3402	4/4	0.89	0.31	46,48,49,50	0

*Continued on next page...*

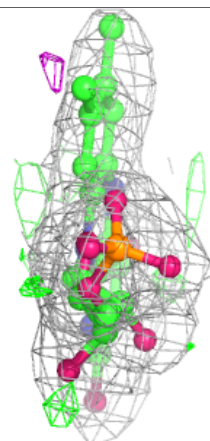
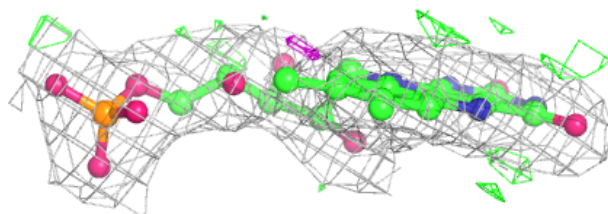
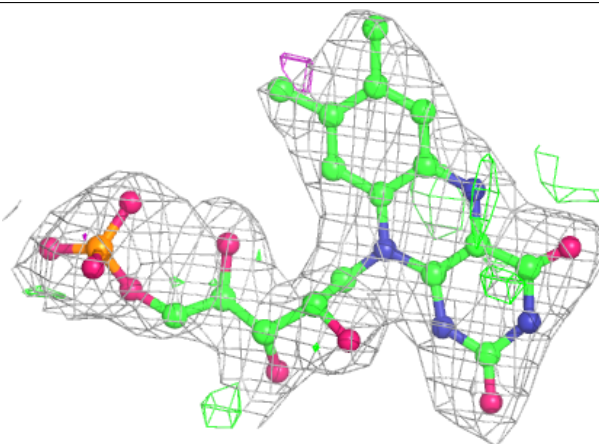
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACY	G	7402	4/4	0.91	0.15	57,60,63,64	0
3	ACY	H	8402	4/4	0.93	0.30	45,47,48,51	0
2	FMN	B	2401	31/31	0.95	0.16	21,36,43,45	0
3	ACY	D	4402	4/4	0.95	0.18	41,51,51,52	0
2	FMN	E	5401	31/31	0.95	0.15	19,37,43,45	0
2	FMN	G	7401	31/31	0.96	0.13	17,37,43,46	0
2	FMN	C	3401	31/31	0.96	0.15	18,33,37,40	0
2	FMN	D	4401	31/31	0.96	0.14	22,33,37,41	0
2	FMN	H	8401	31/31	0.96	0.15	11,29,34,36	0
2	FMN	F	6401	31/31	0.97	0.15	11,21,28,30	0
2	FMN	A	1401	31/31	0.97	0.13	15,25,36,37	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.

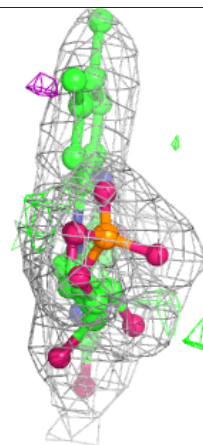
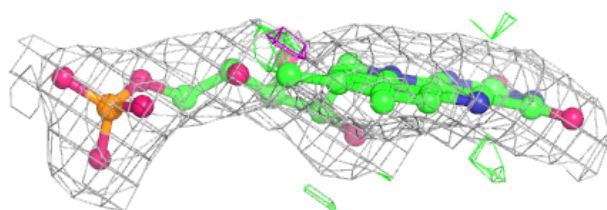
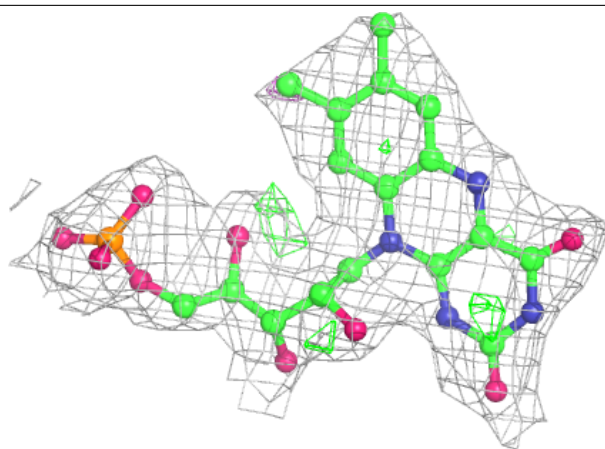
**Electron density around FMN B 2401:**

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)



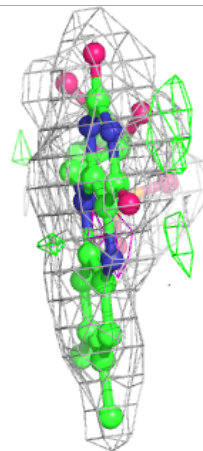
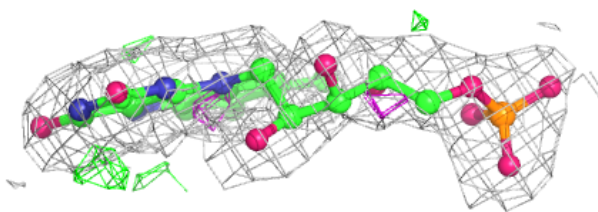
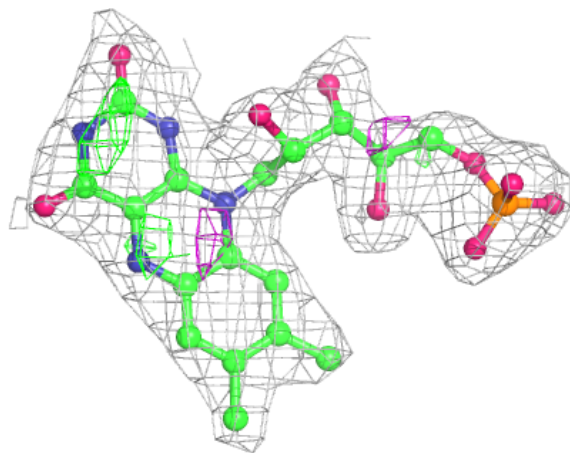
**Electron density around FMN E 5401:**

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



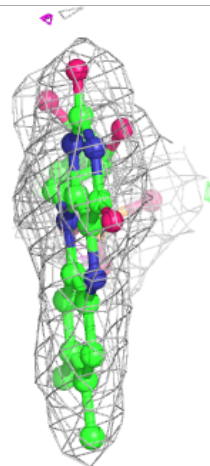
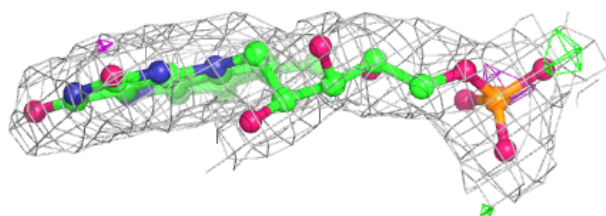
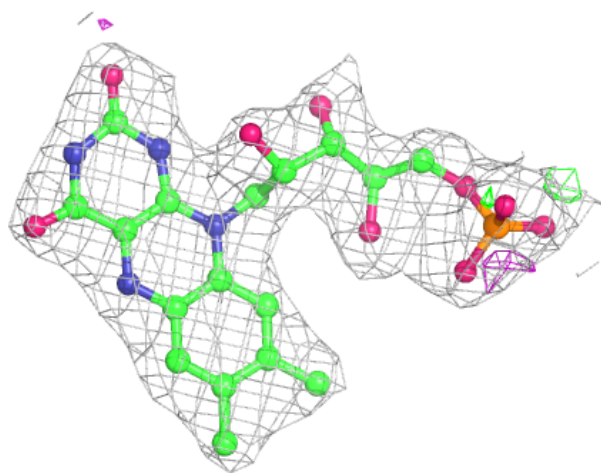
**Electron density around FMN G 7401:**

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



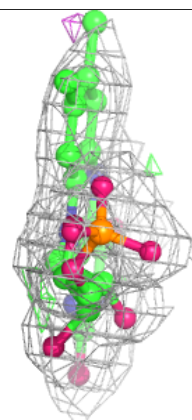
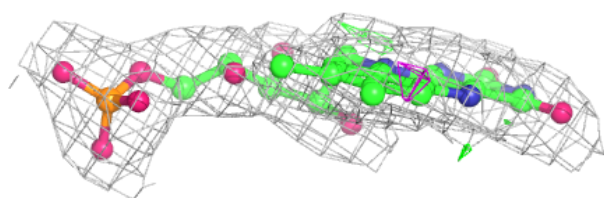
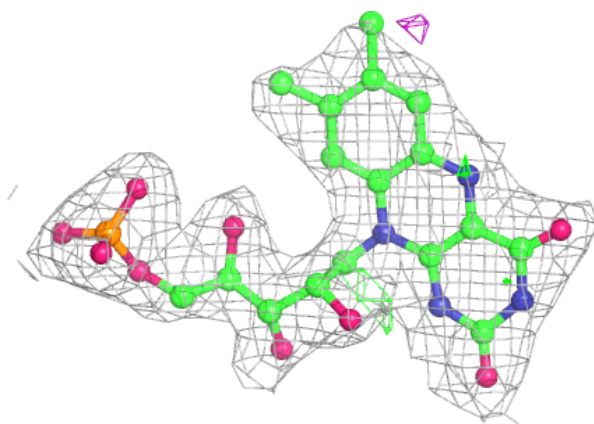
**Electron density around FMN C 3401:**

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



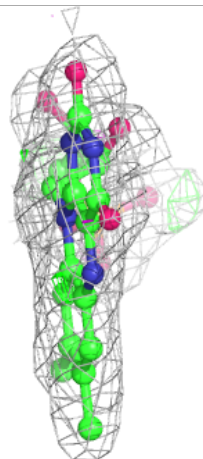
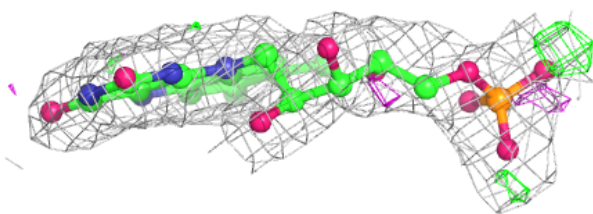
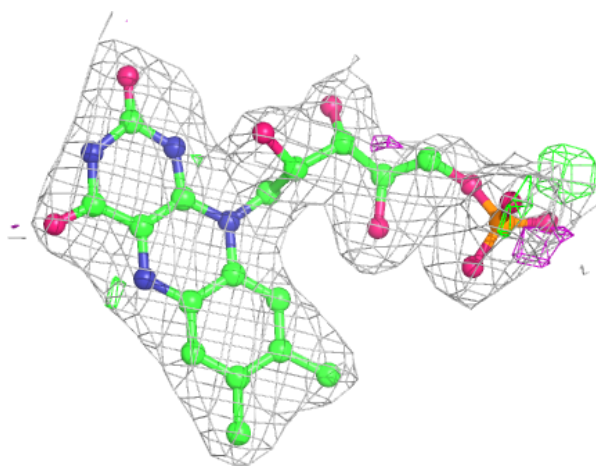
**Electron density around FMN D 4401:**

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



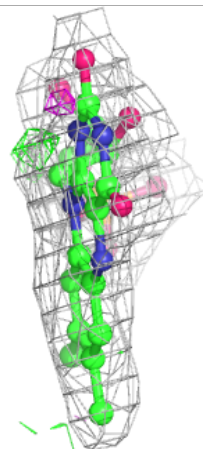
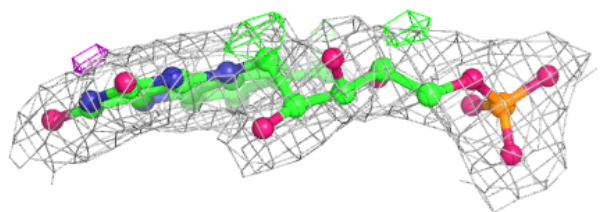
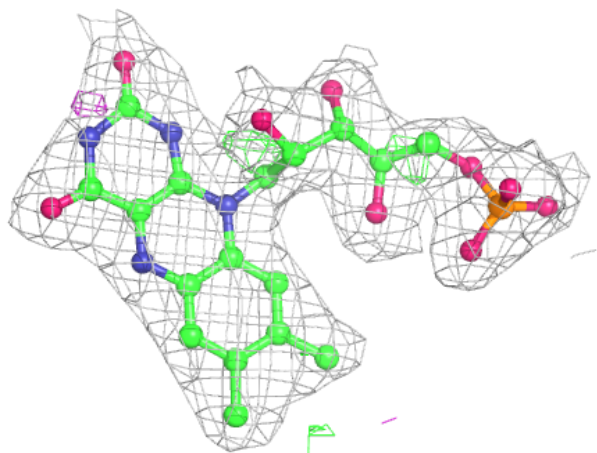
**Electron density around FMN H 8401:**

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



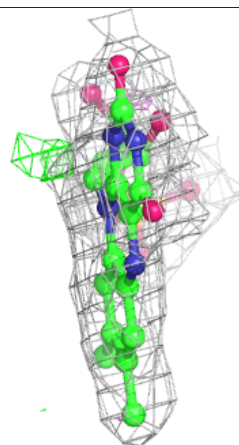
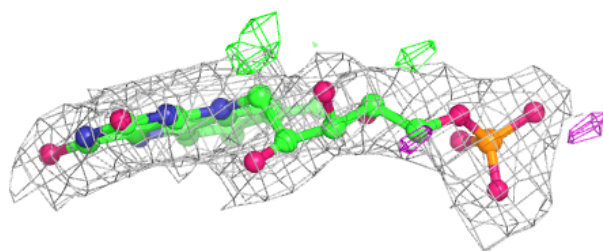
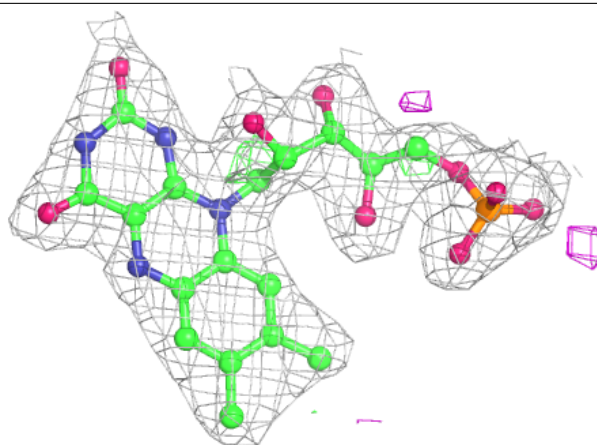
**Electron density around FMN F 6401:**

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



**Electron density around FMN A 1401:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.