



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:20 pm BST

PDB ID : 3HR4  
Title : Human iNOS Reductase and Calmodulin Complex  
Authors : Xia, C.; Misra, I.; Iyanaki, T.; Kim, J.J.K.  
Deposited on : 2009-06-08  
Resolution : 2.50 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.

---

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

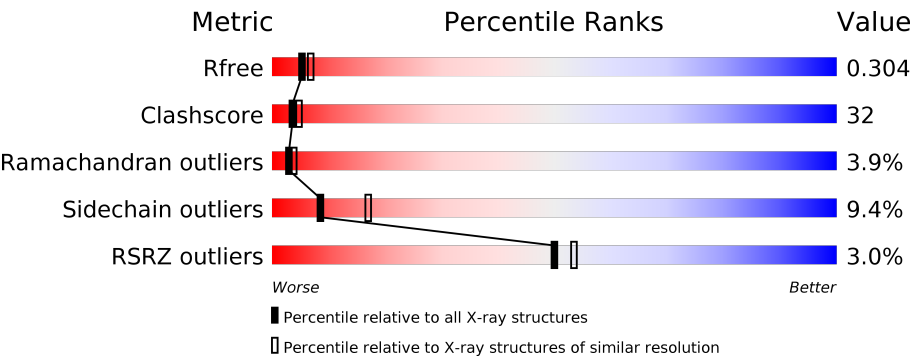
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


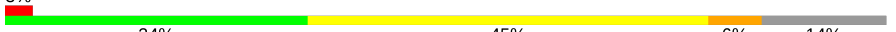


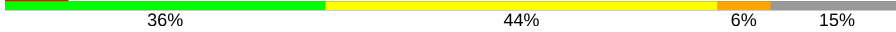

The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	219	
1	C	219	
1	E	219	
1	G	219	
2	B	149	
2	D	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	149	<div><div></div><div>52%40%6%</div></div>
2	H	149	<div><div>7%</div><div>49%43%5%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10594 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 Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1470	943	250	263	14			
1	C	188	Total	C	N	O	S	0	0	0
			1455	931	248	262	14			
1	E	189	Total	C	N	O	S	0	0	0
			1463	937	249	263	14			
1	G	187	Total	C	N	O	S	0	0	0
			1449	931	246	258	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	497	HIS	-	EXPRESSION TAG	UNP P35228
A	498	HIS	-	EXPRESSION TAG	UNP P35228
A	499	HIS	-	EXPRESSION TAG	UNP P35228
A	500	HIS	-	EXPRESSION TAG	UNP P35228
A	501	HIS	-	EXPRESSION TAG	UNP P35228
A	502	HIS	-	EXPRESSION TAG	UNP P35228
C	497	HIS	-	EXPRESSION TAG	UNP P35228
C	498	HIS	-	EXPRESSION TAG	UNP P35228
C	499	HIS	-	EXPRESSION TAG	UNP P35228
C	500	HIS	-	EXPRESSION TAG	UNP P35228
C	501	HIS	-	EXPRESSION TAG	UNP P35228
C	502	HIS	-	EXPRESSION TAG	UNP P35228
E	497	HIS	-	EXPRESSION TAG	UNP P35228
E	498	HIS	-	EXPRESSION TAG	UNP P35228
E	499	HIS	-	EXPRESSION TAG	UNP P35228
E	500	HIS	-	EXPRESSION TAG	UNP P35228
E	501	HIS	-	EXPRESSION TAG	UNP P35228
E	502	HIS	-	EXPRESSION TAG	UNP P35228
G	497	HIS	-	EXPRESSION TAG	UNP P35228
G	498	HIS	-	EXPRESSION TAG	UNP P35228
G	499	HIS	-	EXPRESSION TAG	UNP P35228

*Continued on next page...*

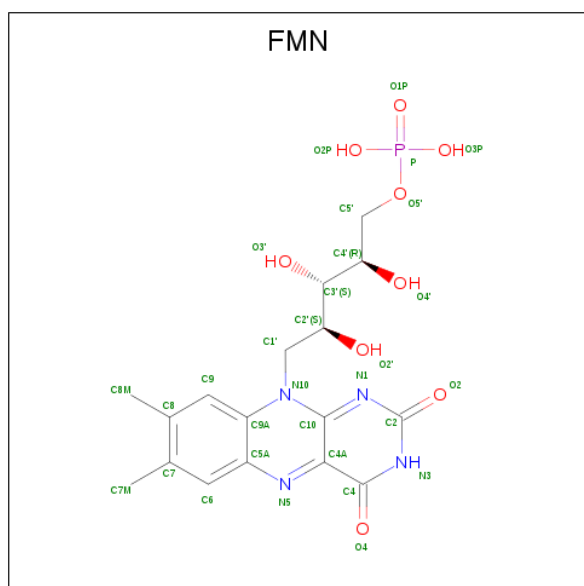
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	500	HIS	-	EXPRESSION TAG	UNP P35228
G	501	HIS	-	EXPRESSION TAG	UNP P35228
G	502	HIS	-	EXPRESSION TAG	UNP P35228

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1143	701	184	249	9			
2	D	145	Total	C	N	O	S	0	0	0
			1136	696	183	248	9			
2	F	145	Total	C	N	O	S	0	0	0
			1143	701	184	249	9			
2	H	145	Total	C	N	O	S	0	0	0
			1124	689	181	245	9			

- Molecule 3 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).



- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total 4	Ca 4	0	0
4	B	4	Total 4	Ca 4	0	0
4	D	4	Total 4	Ca 4	0	0
4	F	4	Total 4	Ca 4	0	0


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	7	Total 7	O 7	0	0
5	C	5	Total 5	O 5	0	0
5	D	23	Total 23	O 23	0	0
5	E	2	Total 2	O 2	0	0
5	F	15	Total 15	O 15	0	0
5	G	5	Total 5	O 5	0	0
5	H	3	Total 3	O 3	0	0


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.

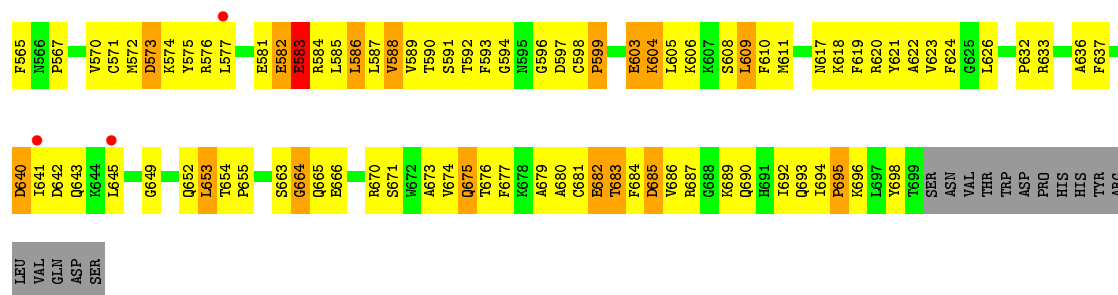
- Chain A:**

Amino Acid	SER (%)	ASP (%)	THR (%)
HIS	43%	37%	6%
HIS	43%	37%	6%
HIS	43%	37%	6%
HIS	43%	37%	6%
HIS	43%	37%	6%
GLU	43%	37%	6%
ASP	43%	37%	6%
LYS	43%	37%	6%
ARG	43%	37%	6%
ARG	43%	37%	6%
PRO	43%	37%	6%
LYS	43%	37%	6%
ARG	43%	37%	6%
RS11	43%	37%	6%
ES12	43%	37%	6%
TS12	43%	37%	6%
P514	43%	37%	6%
L515	43%	37%	6%
K516	43%	37%	6%
V517	43%	37%	6%
L518	43%	37%	6%
V519	43%	37%	6%
L523	43%	37%	6%
F524	43%	37%	6%
A525	43%	37%	6%
C526	43%	37%	6%
N527	43%	37%	6%
L528	43%	37%	6%
R529	43%	37%	6%
R530	43%	37%	6%
M531	43%	37%	6%
T532	43%	37%	6%
V537	43%	37%	6%
L542	43%	37%	6%
F543	43%	37%	6%
A544	43%	37%	6%
T545	43%	37%	6%
E546	43%	37%	6%
S550	43%	37%	6%
E551	43%	37%	6%
A552	43%	37%	6%
L553	43%	37%	6%
A554	43%	37%	6%
M555	43%	37%	6%
L560	43%	37%	6%
F565	43%	37%	6%
V570	43%	37%	6%
V571	43%	37%	6%
M572	43%	37%	6%
L577	43%	37%	6%
S578	43%	37%	6%
E581	43%	37%	6%
E582	43%	37%	6%
E583	43%	37%	6%
R584	43%	37%	6%
L586	43%	37%	6%
L587	43%	37%	6%
V588	43%	37%	6%
V589	43%	37%	6%
T590	43%	37%	6%
S591	43%	37%	6%
T592	43%	37%	6%
F593	43%	37%	6%
G596	43%	37%	6%
D597	43%	37%	6%
C598	43%	37%	6%
P599	43%	37%	6%
G600	43%	37%	6%
N601	43%	37%	6%
G602	43%	37%	6%
E603	43%	37%	6%
K604	43%	37%	6%
L605	43%	37%	6%
K606	43%	37%	6%
L609	43%	37%	6%
F610	43%	37%	6%
M611	43%	37%	6%
N617	43%	37%	6%
K618	43%	37%	6%
F619	43%	37%	6%
R620	43%	37%	6%
I621	43%	37%	6%
A622	43%	37%	6%
F623	43%	37%	6%
V624	43%	37%	6%
G625	43%	37%	6%
L626	43%	37%	6%
G627	43%	37%	6%
S628	43%	37%	6%
R629	43%	37%	6%
R633	43%	37%	6%
F634	43%	37%	6%
C635	43%	37%	6%
G636	43%	37%	6%
F637	43%	37%	6%
I641	43%	37%	6%
D642	43%	37%	6%
Q643	43%	37%	6%
L653	43%	37%	6%
T654	43%	37%	6%
G659	43%	37%	6%
D660	43%	37%	6%
L662	43%	37%	6%
Q665	43%	37%	6%
B666	43%	37%	6%
D667	43%	37%	6%
A668	43%	37%	6%
F669	43%	37%	6%
R670	43%	37%	6%
S671	43%	37%	6%
w672	43%	37%	6%
k673	43%	37%	6%
w674	43%	37%	6%
Q675	43%	37%	6%
Q676	43%	37%	6%
T676	43%	37%	6%
T683	43%	37%	6%
F684	43%	37%	6%
D685	43%	37%	6%
K689	43%	37%	6%
Q690	43%	37%	

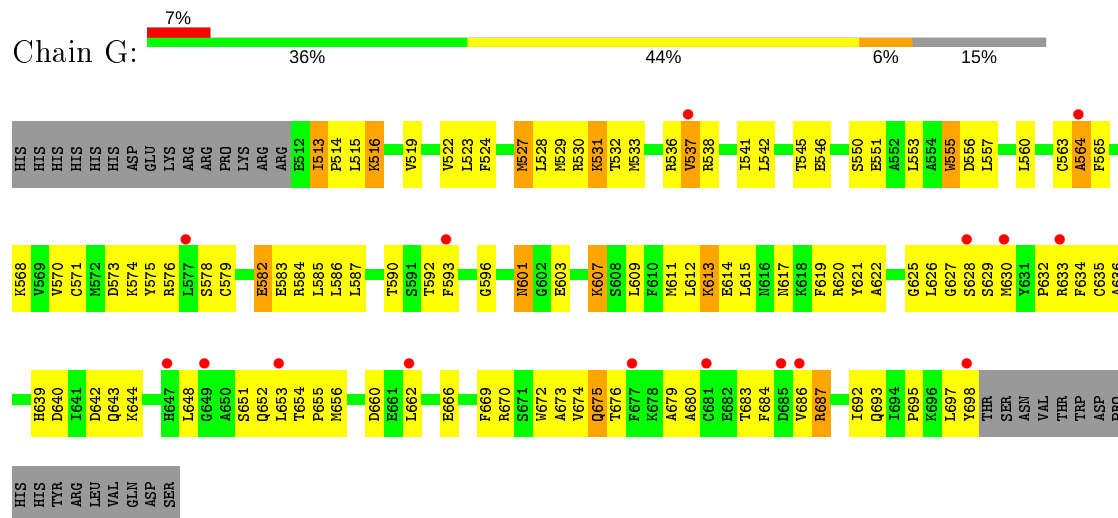
- Chain C: 

Residue	Category	Residue	Category	Residue	Category	Residue	Category
HIS	Grey	S562	Yellow	W630	Yellow	THR	Grey
HIS	Green	S563	Yellow	Y631	Yellow	TRP	Yellow
HIS	Green	A564	Yellow	P632	Yellow	ASP	Yellow
HIS	Green	F565	Yellow	P633	Yellow	PRO	Yellow
HIS	Green	I566	Yellow	F634	Yellow	HIS	Yellow
ASP	Green	F567	Yellow	Q635	Green	HIS	Yellow
GLU	Green	M572	Yellow	A636	Yellow	TYR	Yellow
LYS	Green	D573	Yellow	A638	Yellow	ARG	Yellow
ARG	Grey	K574	Yellow			LEU	Yellow
ARG	Grey	W575	Yellow			VAL	Yellow
PRO	Grey	S576	Yellow			GLN	Yellow
LYS	Green	L577	Yellow			ASP	Yellow
ARG	Grey	S578	Yellow			SER	Grey
ARG	Grey	C579	Yellow				
E512	Yellow	L580	Yellow				
L513	Yellow	E581	Yellow				
F514	Green	E582	Yellow				
L515	Yellow	E583	Yellow				
K516	Yellow	R584	Yellow				
V517	Yellow	L585	Yellow				
L518	Yellow	L586	Yellow				
V519	Orange	L587	Yellow				
		S588	Yellow				
		V589	Yellow				
		T590	Yellow				
		S591	Yellow				
		T592	Yellow				
		F593	Yellow				
		G594	Yellow				
		I595	Yellow				
		G596	Yellow				
		D597	Yellow				
		C598	Yellow				
		P599	Yellow				
		L605	Yellow				
		R606	Yellow				
		K607	Yellow				
		S608	Yellow				
		L609	Yellow				
		F610	Yellow				
		M611	Yellow				
		L612	Yellow				
		K613	Yellow				
		E614	Yellow				
		L615	Yellow				
		L616	Yellow				
		K617	Yellow				
		F618	Yellow				
		F619	Yellow				
		R620	Yellow				
		W621	Yellow				
		F624	Yellow				
		G625	Yellow				
		L626	Yellow				
		G627	Yellow				
		S628	Yellow				
		W629	Yellow				
		L553	Yellow				
		A554	Yellow				
		V555	Yellow				
		D556	Yellow				
		L560	Yellow				
		F561	Yellow				

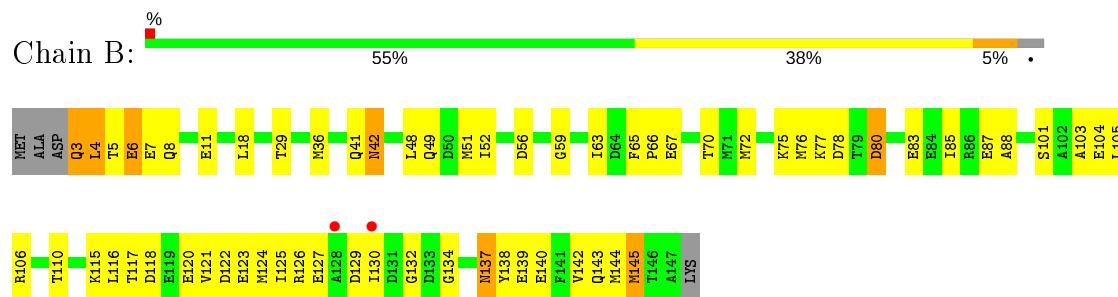
- Chain E: 



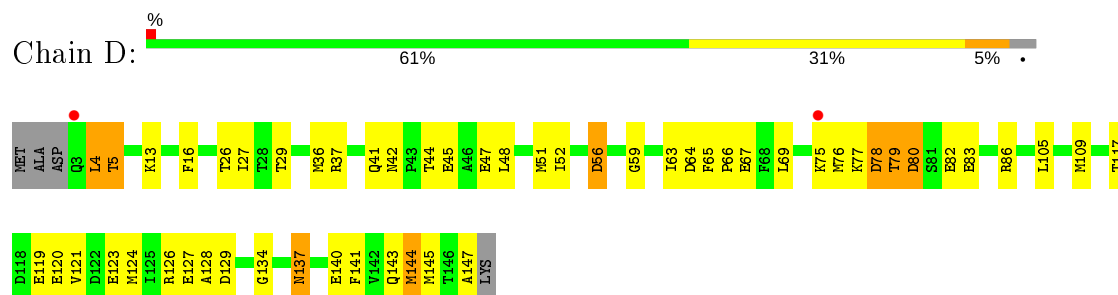
- Molecule 1: Nitric oxide synthase, inducible



- Molecule 2: Calmodulin



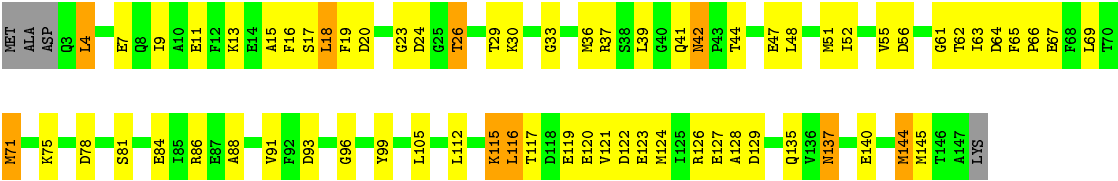
- Molecule 2: Calmodulin



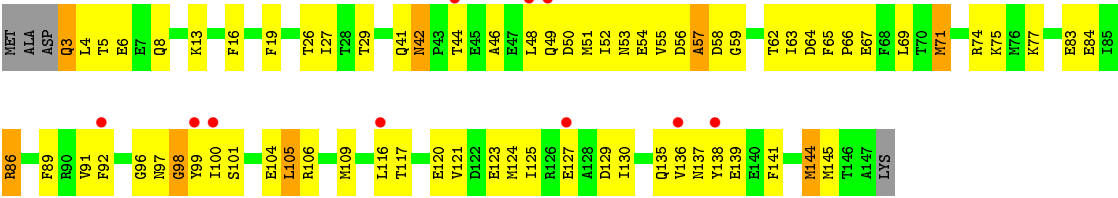
- Molecule 2: Calmodulin







• Molecule 2: Calmodulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.60 Å 160.84 Å 127.77 Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	29.69 – 2.50 36.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.69-2.50) 86.8 (36.60-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.51 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.237 , 0.309 0.230 , 0.304	Depositor DCC
$R_{free}$ test set	2213 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.051 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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 [i](#)

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

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

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	0.44	0/1499	0.64	0/2016
1	C	0.40	0/1484	0.64	0/1997
1	E	0.40	0/1492	0.61	0/2008
1	G	0.44	1/1478 (0.1%)	0.69	2/1989 (0.1%)
2	B	0.40	0/1155	0.59	0/1551
2	D	0.46	0/1148	0.73	1/1542 (0.1%)
2	F	0.45	0/1155	0.67	0/1551
2	H	0.35	0/1136	0.58	0/1527
All	All	0.42	1/10547 (0.0%)	0.65	3/14181 (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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	613	LYS	C-O	-5.28	1.13	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	614	GLU	N-CA-CB	-10.18	92.28	110.60
1	G	613	LYS	N-CA-C	8.26	133.30	111.00
2	D	4	LEU	CB-CA-C	-6.56	97.73	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	ARG	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	1470	0	1485	81	0
1	C	1455	0	1454	119	0
1	E	1463	0	1465	115	0
1	G	1449	0	1462	118	0
2	B	1143	0	1071	79	0
2	D	1136	0	1056	62	0
2	F	1143	0	1071	72	0
2	H	1124	0	1036	83	0
3	A	31	0	18	1	0
3	C	31	0	18	5	0
3	E	31	0	18	1	0
3	G	31	0	18	1	0
4	B	4	0	0	0	0
4	D	4	0	0	0	0
4	F	4	0	0	0	0
4	H	4	0	0	0	0
5	A	11	0	0	3	0
5	B	7	0	0	0	0
5	C	5	0	0	1	0
5	D	23	0	0	1	0
5	E	2	0	0	0	0
5	F	15	0	0	0	0
5	G	5	0	0	0	0
5	H	3	0	0	0	0
All	All	10594	0	10172	656	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 32.

All (656) 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)
2:D:4:LEU:O	2:D:5:THR:HG23	1.24	1.31
2:B:29:THR:HG22	2:B:52:ILE:HG13	1.39	1.05
2:H:109:MET:HE2	2:H:116:LEU:HD11	1.42	1.02
1:G:633:ARG:HB3	1:G:636:ALA:HB2	1.42	1.01
2:F:42:ASN:N	2:F:42:ASN:HD22	1.55	0.99
2:F:122:ASP:HB3	2:F:126:ARG:HH22	1.25	0.97
2:D:4:LEU:O	2:D:5:THR:CG2	2.12	0.97
1:C:583:GLU:HG2	1:C:586:LEU:HD23	1.46	0.96
2:B:137:ASN:ND2	2:B:140:GLU:H	1.65	0.94
2:H:3:GLN:HG2	2:H:4:LEU:N	1.82	0.92
1:C:633:ARG:HH11	1:C:633:ARG:HG3	1.33	0.92
1:C:598:CYS:SG	1:C:606:LYS:HD2	2.10	0.91
2:F:42:ASN:H	2:F:42:ASN:HD22	1.18	0.89
2:F:137:ASN:ND2	2:F:140:GLU:H	1.72	0.87
1:E:596:GLY:HA2	1:E:636:ALA:HB3	1.56	0.87
2:H:106:ARG:HG3	2:H:121:VAL:HG21	1.57	0.86
1:A:697:LEU:HD23	1:A:697:LEU:H	1.38	0.86
2:B:137:ASN:HD21	2:B:140:GLU:H	1.21	0.86
2:D:4:LEU:C	2:D:5:THR:HG23	1.98	0.84
1:G:513:ILE:H	1:G:513:ILE:HD13	1.42	0.83
2:F:122:ASP:HB3	2:F:126:ARG:NH2	1.93	0.83
1:G:584:ARG:HD3	1:G:684:PHE:HE2	1.43	0.83
2:F:137:ASN:HD21	2:F:140:GLU:HG3	1.44	0.82
1:A:513:ILE:N	1:A:513:ILE:HD12	1.95	0.81
1:G:522:VAL:HG21	2:H:91:VAL:HG21	1.61	0.81
2:H:29:THR:HG22	2:H:52:ILE:HG13	1.60	0.81
1:C:527:MET:HE3	2:D:75:LYS:HB2	1.62	0.81
1:G:601:ASN:HD22	1:G:601:ASN:N	1.79	0.80
2:H:137:ASN:OD1	2:H:139:GLU:N	2.15	0.80
2:D:48:LEU:HA	2:D:51:MET:HE3	1.63	0.80
1:A:598:CYS:SG	1:A:603:GLU:HG2	2.22	0.80
1:E:620:ARG:HG3	1:E:620:ARG:HH11	1.47	0.79
1:A:525:ALA:HB1	2:B:41:GLN:HE22	1.48	0.79
2:F:144:MET:HE2	2:F:144:MET:HA	1.65	0.78
1:C:579:CYS:O	1:C:582:GLU:HG2	1.83	0.77
2:H:120:GLU:O	2:H:123:GLU:HB3	1.84	0.77
1:C:584:ARG:NH1	1:C:584:ARG:HB3	2.00	0.76
2:D:105:LEU:HD12	2:D:121:VAL:HG13	1.67	0.76
1:C:553:LEU:HD21	1:C:666:GLU:OE1	1.85	0.76
2:D:29:THR:HG22	2:D:52:ILE:HG13	1.67	0.76
1:E:519:VAL:HG13	2:F:145:MET:HE2	1.67	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:ASN:N	2:F:42:ASN:ND2	2.28	0.76
2:H:48:LEU:HA	2:H:51:MET:HE3	1.66	0.76
1:E:582:GLU:HG2	1:E:583:GLU:N	2.01	0.76
1:C:694:ILE:HD12	1:C:698:TYR:HB2	1.67	0.76
1:C:543:PHE:HA	1:C:589:VAL:O	1.86	0.75
2:F:115:LYS:H	2:F:115:LYS:HE2	1.51	0.75
1:E:546:GLU:HG2	1:E:599:PRO:HB3	1.68	0.74
1:G:617:ASN:HD21	1:G:619:PHE:HB3	1.53	0.74
1:C:553:LEU:HD22	1:C:669:PHE:CD2	2.23	0.73
2:H:50:ASP:O	2:H:54:GLU:HG3	1.87	0.73
1:G:644:LYS:HE3	1:G:648:LEU:HD11	1.68	0.73
1:C:519:VAL:O	2:D:145:MET:HE1	1.88	0.73
2:H:48:LEU:HD23	2:H:51:MET:CE	2.18	0.73
1:E:666:GLU:HB3	1:E:670:ARG:NH1	2.03	0.73
1:G:673:ALA:HA	1:G:676:THR:HG22	1.71	0.73
1:C:546:GLU:OE2	1:C:599:PRO:HB3	1.89	0.73
1:C:654:THR:HG21	1:C:676:THR:OG1	1.89	0.73
2:B:106:ARG:O	2:B:110:THR:HG23	1.88	0.72
1:C:637:PHE:O	1:C:641:ILE:HG22	1.90	0.72
1:G:633:ARG:HB3	1:G:636:ALA:CB	2.17	0.72
2:B:139:GLU:HG2	2:B:143:GLN:HE21	1.54	0.72
2:F:29:THR:HG22	2:F:52:ILE:HG13	1.70	0.72
2:H:48:LEU:HA	2:H:51:MET:CE	2.20	0.72
2:B:42:ASN:H	2:B:42:ASN:HD22	1.38	0.72
1:C:573:ASP:OD1	1:C:574:LYS:HG2	1.90	0.72
1:A:537:VAL:HG13	1:A:565:PHE:HD2	1.55	0.71
2:F:115:LYS:HE2	2:F:115:LYS:N	2.06	0.71
1:E:670:ARG:O	1:E:674:VAL:HG23	1.91	0.70
1:C:687:ARG:HG2	5:C:46:HOH:O	1.89	0.70
1:C:523:LEU:HB2	2:D:145:MET:HE1	1.73	0.70
1:G:557:LEU:HD21	1:G:587:LEU:HD13	1.72	0.70
1:E:542:LEU:HB2	1:E:588:VAL:HG12	1.71	0.69
1:E:544:ALA:HB3	1:E:590:THR:OG1	1.91	0.69
1:C:546:GLU:HG3	1:C:593:PHE:CD1	2.27	0.69
2:D:105:LEU:HD11	2:D:124:MET:HE3	1.74	0.69
2:F:124:MET:O	2:F:127:GLU:HB3	1.92	0.69
1:A:523:LEU:HG	2:B:145:MET:CE	2.23	0.69
1:G:630:MET:O	1:G:630:MET:HG2	1.93	0.68
2:H:51:MET:HA	2:H:54:GLU:OE2	1.93	0.68
2:H:109:MET:HE2	2:H:116:LEU:CD1	2.22	0.68
1:C:633:ARG:CG	1:C:633:ARG:HH11	2.05	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:LEU:HD23	1:C:697:LEU:O	1.94	0.68
2:B:137:ASN:HD21	2:B:140:GLU:N	1.91	0.68
2:D:105:LEU:HD11	2:D:124:MET:CE	2.24	0.68
1:E:641:ILE:HD12	1:E:642:ASP:N	2.09	0.67
1:A:515:LEU:HD12	2:B:144:MET:HE1	1.76	0.67
1:C:542:LEU:HD12	1:C:586:LEU:HD11	1.75	0.67
1:C:572:MET:HB3	1:C:605:LEU:HD22	1.75	0.67
1:E:633:ARG:HB3	1:E:636:ALA:HB2	1.77	0.67
2:B:29:THR:CG2	2:B:52:ILE:HG13	2.21	0.67
2:F:137:ASN:HD21	2:F:140:GLU:H	1.41	0.67
1:E:537:VAL:HB	1:E:565:PHE:HD2	1.60	0.67
2:H:137:ASN:O	2:H:141:PHE:HB2	1.95	0.67
1:A:516:LYS:HG2	2:B:127:GLU:OE2	1.94	0.67
1:E:523:LEU:HB2	2:F:145:MET:HE1	1.75	0.67
1:C:527:MET:CE	2:D:75:LYS:HB2	2.25	0.66
1:C:584:ARG:HH11	1:C:584:ARG:HB3	1.60	0.66
1:E:529:MET:HG2	2:F:36:MET:CE	2.25	0.66
2:H:117:THR:O	2:H:121:VAL:HG23	1.95	0.66
1:G:584:ARG:HD3	1:G:684:PHE:CE2	2.29	0.66
1:G:529:MET:HG2	2:H:41:GLN:HG2	1.76	0.66
2:B:29:THR:HG21	2:B:49:GLN:NE2	2.11	0.65
2:B:48:LEU:HA	2:B:51:MET:HE3	1.77	0.65
2:H:109:MET:CE	2:H:116:LEU:HD11	2.24	0.65
1:G:652:GLN:NE2	1:G:655:PRO:HA	2.10	0.65
1:A:553:LEU:HD22	1:A:669:PHE:CD2	2.31	0.65
1:G:642:ASP:OD1	1:G:656:MET:HB2	1.96	0.65
2:H:49:GLN:O	2:H:53:ASN:ND2	2.30	0.65
1:G:687:ARG:HD3	1:G:687:ARG:H	1.61	0.65
2:B:85:ILE:HG12	2:B:145:MET:HE3	1.79	0.64
1:E:606:LYS:HG3	1:E:610:PHE:CE2	2.33	0.64
2:F:37:ARG:HA	2:F:41:GLN:O	1.98	0.64
2:H:105:LEU:CD1	2:H:124:MET:HE3	2.28	0.64
1:A:553:LEU:HD12	1:A:626:LEU:HD11	1.80	0.64
2:B:3:GLN:O	2:B:4:LEU:HB2	1.95	0.64
1:C:630:MET:HG2	1:C:630:MET:O	1.98	0.64
1:G:553:LEU:HD12	1:G:626:LEU:HD21	1.79	0.64
1:E:620:ARG:NH1	1:E:620:ARG:HG3	2.12	0.64
2:D:78:ASP:O	2:D:80:ASP:N	2.30	0.63
1:C:527:MET:HE3	2:D:75:LYS:CB	2.26	0.63
1:G:612:LEU:HD12	1:G:613:LYS:H	1.62	0.63
1:C:598:CYS:HB3	1:C:637:PHE:CD1	2.32	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:644:LYS:HD2	1:G:644:LYS:O	1.99	0.63
1:A:671:SER:O	1:A:675:GLN:HG2	1.98	0.63
1:E:593:PHE:O	1:E:597:ASP:HB3	1.97	0.63
1:G:530:ARG:HH22	2:H:83:GLU:HB3	1.64	0.63
2:F:37:ARG:HH11	2:F:37:ARG:HG2	1.63	0.63
1:A:673:ALA:O	1:A:676:THR:HG22	1.99	0.63
1:A:519:VAL:HG13	2:B:145:MET:SD	2.39	0.63
1:C:529:MET:HG2	2:D:36:MET:CE	2.29	0.63
1:A:553:LEU:HD22	1:A:669:PHE:CG	2.34	0.62
1:E:542:LEU:HD21	1:E:575:TYR:HB2	1.81	0.62
1:G:617:ASN:ND2	1:G:619:PHE:HB3	2.14	0.62
1:C:515:LEU:O	1:C:519:VAL:HB	1.99	0.62
2:H:92:PHE:HB3	2:H:100:ILE:HD12	1.81	0.62
1:C:627:GLY:HA2	3:C:999:FMN:H3'	1.81	0.62
2:F:44:THR:OG1	2:F:47:GLU:HG3	1.99	0.62
1:C:598:CYS:HB3	1:C:637:PHE:CE1	2.34	0.62
1:E:694:ILE:O	1:E:696:LYS:N	2.32	0.62
1:G:528:LEU:HB3	2:H:51:MET:SD	2.39	0.62
2:F:122:ASP:CB	2:F:126:ARG:HH22	2.05	0.61
2:F:15:ALA:O	2:F:18:LEU:HB2	2.00	0.61
1:G:601:ASN:ND2	1:G:601:ASN:N	2.48	0.61
1:C:697:LEU:HD22	1:C:698:TYR:CE1	2.35	0.61
2:D:79:THR:HG22	2:D:79:THR:O	1.99	0.61
1:A:666:GLU:HB3	1:A:670:ARG:NH1	2.14	0.61
2:H:3:GLN:CG	2:H:4:LEU:N	2.58	0.61
2:F:64:ASP:OD1	2:F:67:GLU:HG3	1.98	0.61
1:C:543:PHE:O	1:C:572:MET:HG3	2.00	0.61
1:E:537:VAL:HG13	1:E:584:ARG:HE	1.65	0.61
1:A:596:GLY:HA2	1:A:636:ALA:HB3	1.83	0.60
1:E:623:VAL:HG11	1:E:641:ILE:HD11	1.83	0.60
1:G:537:VAL:HG23	1:G:584:ARG:HD2	1.83	0.60
1:C:536:ARG:HD2	2:D:47:GLU:OE2	2.01	0.60
1:A:537:VAL:HG12	5:A:27:HOH:O	2.00	0.60
1:C:523:LEU:HD12	2:D:145:MET:SD	2.42	0.60
2:D:137:ASN:ND2	2:D:140:GLU:H	1.99	0.60
1:C:523:LEU:HD22	1:C:527:MET:SD	2.41	0.60
2:F:144:MET:CE	2:F:144:MET:HA	2.30	0.60
1:E:693:GLN:NE2	1:E:696:LYS:NZ	2.50	0.60
1:G:629:SER:OG	1:G:662:LEU:HD22	2.01	0.60
1:G:570:VAL:HG12	1:G:571:CYS:O	2.02	0.59
2:D:109:MET:HG3	2:D:124:MET:HE1	1.83	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:ILE:O	2:H:129:ASP:HB2	2.01	0.59
2:F:7:GLU:O	2:F:11:GLU:HG3	2.02	0.59
1:G:644:LYS:CE	1:G:648:LEU:HD11	2.33	0.59
1:G:620:ARG:HG2	1:G:651:SER:HB2	1.84	0.59
1:A:591:SER:HA	1:A:626:LEU:O	2.02	0.59
1:E:673:ALA:HA	1:E:676:THR:HG22	1.84	0.59
1:E:674:VAL:HG22	1:E:698:TYR:HB3	1.84	0.59
1:A:530:ARG:HG3	1:A:530:ARG:HH11	1.67	0.59
2:B:125:ILE:C	2:B:127:GLU:H	2.06	0.59
1:A:523:LEU:HG	2:B:145:MET:HE3	1.84	0.59
2:B:137:ASN:HD22	2:B:137:ASN:C	2.06	0.59
1:C:577:LEU:HG	1:C:608:SER:HB3	1.84	0.59
1:G:531:LYS:C	1:G:533:MET:H	2.05	0.59
2:H:52:ILE:HD13	2:H:63:ILE:HD11	1.85	0.59
1:C:614:GLU:HA	1:C:648:LEU:HD22	1.85	0.59
1:E:513:ILE:N	1:E:513:ILE:HD12	2.18	0.58
1:G:628:SER:N	1:G:634:PHE:HE1	2.01	0.58
2:H:4:LEU:O	2:H:4:LEU:HD23	2.02	0.58
2:F:33:GLY:O	2:F:37:ARG:HG3	2.04	0.58
1:G:519:VAL:HA	1:G:522:VAL:HG12	1.85	0.58
1:G:516:LYS:HA	1:G:519:VAL:HG12	1.85	0.58
1:C:523:LEU:HB2	2:D:145:MET:CE	2.33	0.58
1:E:588:VAL:CG2	1:E:623:VAL:HG22	2.33	0.58
1:A:515:LEU:HD12	2:B:144:MET:CE	2.34	0.58
1:C:621:TYR:CD1	1:C:650:ALA:HB1	2.39	0.58
1:E:641:ILE:C	1:E:641:ILE:HD12	2.24	0.57
1:G:670:ARG:O	1:G:674:VAL:HG23	2.04	0.57
2:H:141:PHE:O	2:H:144:MET:HB3	2.04	0.57
1:E:587:LEU:CD2	1:E:622:ALA:HB3	2.34	0.57
2:B:137:ASN:HD21	2:B:140:GLU:CB	2.17	0.57
2:B:137:ASN:HD21	2:B:140:GLU:CG	2.17	0.57
1:C:633:ARG:HG3	1:C:633:ARG:NH1	2.12	0.57
1:G:692:ILE:HD12	2:H:44:THR:HG22	1.87	0.57
2:B:121:VAL:O	2:B:125:ILE:HG13	2.03	0.57
2:D:64:ASP:OD2	2:D:67:GLU:HG3	2.05	0.57
1:G:592:THR:HG21	1:G:596:GLY:HA2	1.87	0.57
2:H:89:PHE:HB2	2:H:141:PHE:CE1	2.40	0.57
1:E:618:LYS:HD2	1:E:649:GLY:O	2.05	0.57
1:G:537:VAL:HG22	1:G:565:PHE:HD2	1.69	0.57
1:A:545:THR:HB	1:A:550:SER:HB2	1.85	0.57
2:B:103:ALA:O	2:B:106:ARG:HB3	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:666:GLU:HB3	1:E:670:ARG:HH12	1.69	0.56
2:H:16:PHE:CE1	2:H:27:ILE:HD11	2.39	0.56
1:E:542:LEU:HB2	1:E:588:VAL:CG1	2.35	0.56
1:E:547:THR:HB	3:E:999:FMN:O3P	2.05	0.56
1:G:653:LEU:HD21	1:G:679:ALA:O	2.06	0.56
1:G:622:ALA:HB1	1:G:672:TRP:HZ2	1.71	0.56
2:B:42:ASN:N	2:B:42:ASN:HD22	1.99	0.56
1:G:513:ILE:HG12	1:G:513:ILE:O	2.04	0.56
2:B:72:MET:O	2:B:76:MET:HG2	2.06	0.56
1:C:644:LYS:HE3	1:C:648:LEU:HD11	1.86	0.56
1:G:530:ARG:HH11	2:H:84:GLU:CD	2.09	0.56
1:G:687:ARG:CD	1:G:687:ARG:H	2.19	0.56
1:E:581:GLU:OE2	1:E:617:ASN:HB3	2.06	0.56
1:G:523:LEU:HD12	2:H:145:MET:CE	2.36	0.56
1:A:513:ILE:CD1	1:A:513:ILE:N	2.66	0.56
2:D:83:GLU:O	2:D:86:ARG:HB3	2.06	0.55
2:F:81:SER:HA	2:F:84:GLU:HG3	1.87	0.55
2:F:48:LEU:HA	2:F:51:MET:CE	2.36	0.55
2:H:48:LEU:HD23	2:H:51:MET:HE1	1.89	0.55
1:E:582:GLU:CG	1:E:583:GLU:N	2.69	0.55
2:B:139:GLU:O	2:B:143:GLN:HG3	2.07	0.55
1:C:628:SER:C	1:C:630:MET:H	2.10	0.55
1:C:633:ARG:HB3	1:C:636:ALA:HB2	1.89	0.55
2:F:137:ASN:ND2	2:F:140:GLU:HG3	2.17	0.55
1:E:528:LEU:HB3	2:F:51:MET:SD	2.46	0.55
1:E:576:ARG:HH12	1:E:604:LYS:NZ	2.04	0.55
1:E:515:LEU:HD12	2:F:144:MET:SD	2.47	0.55
1:C:513:ILE:HD11	1:C:517:VAL:HG12	1.89	0.55
1:C:690:GLN:HG2	1:C:691:HIS:CD2	2.43	0.55
1:G:584:ARG:O	1:G:619:PHE:HB2	2.07	0.55
1:G:673:ALA:HA	1:G:676:THR:CG2	2.35	0.55
1:E:547:THR:O	1:E:547:THR:HG22	2.07	0.54
1:G:673:ALA:CA	1:G:676:THR:HG22	2.35	0.54
1:G:516:LYS:HG3	2:H:144:MET:CE	2.37	0.54
1:C:579:CYS:HB2	1:C:582:GLU:CD	2.27	0.54
1:C:690:GLN:N	1:C:690:GLN:CD	2.60	0.54
2:D:75:LYS:C	2:D:77:LYS:H	2.11	0.54
2:B:56:ASP:OD2	2:B:59:GLY:HA2	2.08	0.54
2:D:137:ASN:HD21	2:D:140:GLU:HG3	1.72	0.54
1:G:513:ILE:N	1:G:513:ILE:HD13	2.18	0.54
2:H:105:LEU:HD11	2:H:124:MET:HE3	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD12	2:B:144:MET:SD	2.48	0.54
1:C:529:MET:HG3	2:D:41:GLN:HB3	1.90	0.54
2:F:48:LEU:HA	2:F:51:MET:HE3	1.89	0.54
1:C:529:MET:HG2	2:D:36:MET:HE2	1.87	0.54
1:C:633:ARG:CG	1:C:633:ARG:NH1	2.67	0.54
2:F:93:ASP:OD2	2:F:96:GLY:HA2	2.07	0.54
2:F:99:TYR:HB3	2:F:135:GLN:HE21	1.72	0.54
2:H:137:ASN:OD1	2:H:138:TYR:N	2.40	0.54
1:E:537:VAL:HB	1:E:565:PHE:CD2	2.42	0.54
2:D:128:ALA:HB2	2:D:144:MET:SD	2.48	0.54
1:G:538:ARG:HH11	1:G:538:ARG:HG3	1.71	0.54
1:G:551:GLU:OE2	1:G:555:TRP:HZ3	1.90	0.54
2:F:115:LYS:CA	2:F:115:LYS:HE2	2.38	0.54
2:B:139:GLU:HG2	2:B:143:GLN:NE2	2.23	0.53
2:B:29:THR:HG22	2:B:52:ILE:CG1	2.25	0.53
1:E:570:VAL:HG12	1:E:571:CYS:O	2.09	0.53
1:E:654:THR:HG21	1:E:676:THR:CB	2.37	0.53
1:E:525:ALA:HB1	2:F:41:GLN:HE22	1.72	0.53
2:B:36:MET:HG2	2:B:41:GLN:NE2	2.23	0.53
1:C:686:VAL:O	1:C:689:LYS:HG3	2.08	0.53
2:H:69:LEU:HD13	2:H:69:LEU:O	2.08	0.53
1:A:519:VAL:HG11	2:B:145:MET:HG2	1.89	0.53
1:C:537:VAL:HB	1:C:565:PHE:HD2	1.72	0.53
2:B:63:ILE:HA	2:B:67:GLU:OE1	2.08	0.53
1:C:541:ILE:HA	1:C:587:LEU:O	2.09	0.53
2:B:137:ASN:HD21	2:B:140:GLU:HG3	1.74	0.53
2:B:83:GLU:O	2:B:87:GLU:HG3	2.09	0.53
1:A:527:MET:HE3	2:B:75:LYS:HG2	1.91	0.53
2:H:64:ASP:OD1	2:H:67:GLU:HG3	2.09	0.53
1:A:611:MET:CE	1:A:611:MET:HA	2.39	0.53
1:C:579:CYS:HB2	1:C:582:GLU:OE1	2.09	0.53
2:D:4:LEU:C	2:D:5:THR:CG2	2.68	0.53
1:E:528:LEU:O	1:E:532:THR:HG23	2.09	0.53
1:E:539:VAL:HG22	1:E:585:LEU:HB3	1.91	0.53
1:E:673:ALA:O	1:E:676:THR:HG22	2.09	0.53
1:A:585:LEU:HA	1:A:620:ARG:O	2.09	0.53
2:B:48:LEU:HD23	2:B:51:MET:HE3	1.91	0.53
1:E:533:MET:C	1:E:535:SER:H	2.11	0.53
2:F:117:THR:HG22	2:F:120:GLU:H	1.74	0.53
1:G:530:ARG:O	1:G:533:MET:HB3	2.09	0.53
2:H:100:ILE:HG12	2:H:136:VAL:O	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ILE:HG13	1:A:642:ASP:N	2.22	0.52
1:E:588:VAL:HG23	1:E:623:VAL:HG22	1.90	0.52
1:A:528:LEU:O	1:A:532:THR:HG23	2.08	0.52
2:B:137:ASN:ND2	2:B:140:GLU:HB2	2.23	0.52
1:C:573:ASP:OD1	1:C:574:LYS:N	2.43	0.52
2:F:123:GLU:O	2:F:127:GLU:HB2	2.09	0.52
1:C:577:LEU:H	1:C:577:LEU:HD22	1.73	0.52
1:E:654:THR:HG21	1:E:676:THR:HB	1.90	0.52
2:F:137:ASN:HD22	2:F:137:ASN:C	2.13	0.52
2:H:101:SER:OG	2:H:104:GLU:HG3	2.09	0.52
1:G:619:PHE:HE1	1:G:621:TYR:HB3	1.73	0.52
1:E:519:VAL:HG13	2:F:145:MET:CE	2.37	0.52
1:E:581:GLU:OE2	1:E:617:ASN:N	2.29	0.52
1:A:589:VAL:HA	1:A:624:PHE:O	2.10	0.52
1:A:670:ARG:O	1:A:674:VAL:HG23	2.09	0.52
2:B:42:ASN:H	2:B:42:ASN:ND2	2.03	0.52
1:G:553:LEU:HD22	1:G:669:PHE:CD2	2.45	0.52
2:H:5:THR:HG23	2:H:8:GLN:HE21	1.74	0.52
1:C:553:LEU:HD12	1:C:626:LEU:HD21	1.91	0.52
2:D:137:ASN:HD22	2:D:137:ASN:C	2.13	0.52
1:E:529:MET:O	1:E:533:MET:HB2	2.09	0.52
1:E:606:LYS:HD2	1:E:637:PHE:CE1	2.45	0.52
1:A:529:MET:HG2	2:B:36:MET:CE	2.40	0.51
1:C:592:THR:CG2	1:C:596:GLY:HA2	2.40	0.51
2:D:117:THR:OG1	2:D:120:GLU:HG3	2.11	0.51
1:C:516:LYS:HG2	2:D:127:GLU:OE2	2.11	0.51
2:F:56:ASP:OD2	2:F:61:GLY:N	2.42	0.51
1:G:680:ALA:O	1:G:684:PHE:HD1	1.93	0.51
1:E:542:LEU:HA	1:E:570:VAL:O	2.11	0.51
1:E:679:ALA:O	1:E:683:THR:HG23	2.10	0.51
1:G:634:PHE:HZ	1:G:660:ASP:HA	1.74	0.51
1:A:628:SER:N	1:A:634:PHE:HE1	2.08	0.51
2:B:116:LEU:HB3	2:B:120:GLU:HG3	1.91	0.51
1:A:519:VAL:CG1	2:B:145:MET:SD	2.98	0.51
1:C:519:VAL:HG13	2:D:145:MET:CE	2.40	0.51
1:C:689:LYS:O	1:C:692:ILE:HG12	2.10	0.51
1:C:596:GLY:HA2	1:C:636:ALA:HB3	1.93	0.51
1:C:519:VAL:HG13	2:D:145:MET:HE2	1.91	0.51
1:G:607:LYS:O	1:G:607:LYS:HE3	2.11	0.51
1:G:620:ARG:HA	1:G:651:SER:O	2.11	0.51
2:B:65:PHE:HB3	2:B:66:PRO:HD3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:532:THR:O	1:E:535:SER:HB2	2.10	0.51
1:E:606:LYS:HG3	1:E:610:PHE:CD2	2.46	0.51
1:E:563:CYS:O	1:E:692:ILE:HD11	2.10	0.51
1:G:592:THR:CG2	1:G:596:GLY:HA2	2.41	0.51
2:B:42:ASN:ND2	2:B:42:ASN:N	2.57	0.51
1:C:682:GLU:C	1:C:684:PHE:H	2.14	0.51
2:F:39:LEU:HD21	2:F:112:LEU:HD21	1.92	0.51
1:A:606:LYS:HG3	1:A:610:PHE:HE2	1.76	0.50
1:A:690:GLN:NE2	1:A:691:HIS:ND1	2.59	0.50
1:E:619:PHE:HD1	1:E:620:ARG:O	1.94	0.50
2:F:4:LEU:HD22	2:F:9:ILE:HG13	1.93	0.50
2:H:99:TYR:HB3	2:H:135:GLN:HB3	1.94	0.50
1:A:544:ALA:HB2	1:A:572:MET:SD	2.51	0.50
1:C:533:MET:SD	1:C:566:ASN:HB2	2.51	0.50
2:H:117:THR:O	2:H:120:GLU:HG2	2.12	0.50
1:A:546:GLU:HB2	1:A:593:PHE:CZ	2.47	0.50
1:C:529:MET:HG2	2:D:36:MET:HE1	1.94	0.50
1:C:648:LEU:N	1:C:648:LEU:HD23	2.26	0.50
1:G:516:LYS:HD2	1:G:516:LYS:H	1.76	0.50
1:G:550:SER:OG	1:G:626:LEU:HD22	2.11	0.50
2:B:7:GLU:O	2:B:11:GLU:HG3	2.11	0.50
2:D:126:ARG:HG2	2:D:126:ARG:O	2.12	0.50
2:D:13:LYS:HA	2:D:65:PHE:CE1	2.47	0.50
1:G:687:ARG:NH1	1:G:687:ARG:HG3	2.27	0.50
2:F:66:PRO:HG3	2:H:69:LEU:CD1	2.41	0.50
1:G:542:LEU:HA	1:G:570:VAL:O	2.12	0.50
2:B:137:ASN:ND2	2:B:140:GLU:CB	2.75	0.50
2:F:88:ALA:O	2:F:91:VAL:HB	2.12	0.49
1:G:620:ARG:NH1	1:G:683:THR:HB	2.27	0.49
1:C:544:ALA:HB3	1:C:590:THR:OG1	2.12	0.49
1:G:575:TYR:CZ	1:G:579:CYS:HB2	2.47	0.49
2:F:69:LEU:CD1	2:H:66:PRO:HG3	2.43	0.49
2:H:105:LEU:HD13	2:H:124:MET:HE3	1.93	0.49
1:C:576:ARG:HB3	1:C:578:SER:OG	2.12	0.49
1:C:634:PHE:HA	3:C:999:FMN:O2	2.12	0.49
1:G:516:LYS:HA	1:G:519:VAL:CG1	2.42	0.49
2:B:125:ILE:C	2:B:127:GLU:N	2.66	0.49
1:E:523:LEU:HB2	2:F:145:MET:CE	2.40	0.49
1:C:695:PRO:HG2	1:C:698:TYR:CD1	2.47	0.49
1:E:596:GLY:CA	1:E:636:ALA:HB3	2.35	0.49
1:G:627:GLY:HA2	3:G:999:FMN:O2'	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:ASP:OD1	2:H:66:PRO:HD2	2.12	0.49
1:C:620:ARG:HG3	1:C:620:ARG:HH11	1.77	0.49
2:D:47:GLU:O	2:D:51:MET:HG3	2.12	0.49
1:G:644:LYS:NZ	1:G:648:LEU:HD21	2.27	0.49
1:C:518:LEU:O	1:C:522:VAL:HG12	2.13	0.48
1:G:546:GLU:HG3	1:G:593:PHE:CD1	2.48	0.48
1:G:612:LEU:CD1	1:G:613:LYS:H	2.24	0.48
1:C:539:VAL:O	1:C:567:PRO:HA	2.14	0.48
1:A:637:PHE:O	1:A:641:ILE:HG23	2.13	0.48
1:G:529:MET:O	1:G:533:MET:HB2	2.12	0.48
1:E:559:ALA:O	1:E:562:SER:HB2	2.13	0.48
2:F:4:LEU:CD2	2:F:9:ILE:HG13	2.43	0.48
1:G:692:ILE:HD12	2:H:44:THR:CG2	2.43	0.48
2:D:105:LEU:O	2:D:109:MET:HG2	2.13	0.48
1:E:577:LEU:HD21	1:E:608:SER:HB2	1.95	0.48
2:F:26:THR:HG22	2:F:63:ILE:O	2.14	0.48
1:G:545:THR:HB	1:G:550:SER:HB2	1.94	0.48
1:E:689:LYS:O	1:E:692:ILE:HG22	2.13	0.48
2:F:13:LYS:HG2	2:H:6:GLU:HG3	1.94	0.48
2:B:123:GLU:C	2:B:125:ILE:H	2.17	0.48
2:H:48:LEU:HD23	2:H:51:MET:HE2	1.95	0.48
2:F:55:VAL:HB	2:F:63:ILE:CD1	2.44	0.48
1:G:533:MET:O	1:G:536:ARG:HB2	2.13	0.48
1:G:538:ARG:HG3	1:G:538:ARG:NH1	2.28	0.48
1:G:575:TYR:OH	1:G:579:CYS:HB2	2.14	0.48
2:F:121:VAL:HA	2:F:124:MET:CE	2.44	0.48
1:G:523:LEU:O	1:G:527:MET:HG2	2.13	0.48
2:H:46:ALA:O	2:H:50:ASP:N	2.47	0.48
1:E:540:THR:HB	1:E:586:LEU:HD23	1.96	0.47
1:E:609:LEU:O	1:E:609:LEU:HD23	2.14	0.47
1:C:662:LEU:HD12	1:C:662:LEU:N	2.29	0.47
1:G:609:LEU:HD22	1:G:644:LYS:HE2	1.95	0.47
1:A:514:PRO:HG2	1:A:517:VAL:HB	1.96	0.47
2:F:55:VAL:HB	2:F:63:ILE:HD11	1.95	0.47
1:E:677:PHE:C	1:E:679:ALA:H	2.17	0.47
1:A:592:THR:HG22	1:A:593:PHE:N	2.29	0.47
1:A:622:ALA:HB1	1:A:654:THR:HG22	1.97	0.47
1:E:610:PHE:HB2	1:E:611:MET:CE	2.44	0.47
1:E:673:ALA:HA	1:E:676:THR:CG2	2.43	0.47
1:C:550:SER:OG	1:C:626:LEU:HD22	2.13	0.47
2:H:55:VAL:HG22	2:H:71:MET:CE	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ASP:OD1	1:A:662:LEU:HB2	2.15	0.47
2:B:5:THR:O	2:B:6:GLU:C	2.53	0.47
1:C:525:ALA:HB1	2:D:41:GLN:HE22	1.80	0.47
2:D:129:ASP:OD1	2:D:134:GLY:N	2.47	0.47
2:F:23:GLY:O	2:H:3:GLN:NE2	2.47	0.47
1:A:696:LYS:HG3	1:A:697:LEU:N	2.30	0.47
1:C:680:ALA:O	1:C:684:PHE:HB2	2.15	0.47
2:F:13:LYS:O	2:F:16:PHE:HB3	2.15	0.47
2:H:97:ASN:CG	2:H:98:GLY:H	2.18	0.47
1:A:529:MET:HG2	2:B:36:MET:HE2	1.97	0.47
2:D:13:LYS:O	2:D:16:PHE:HB3	2.14	0.47
2:H:83:GLU:O	2:H:86:ARG:HG3	2.14	0.47
1:E:603:GLU:O	1:E:605:LEU:N	2.48	0.47
2:F:65:PHE:HB3	2:F:66:PRO:HD3	1.97	0.46
1:A:543:PHE:CE2	1:A:551:GLU:HB2	2.50	0.46
1:A:515:LEU:CD1	2:B:144:MET:HE1	2.45	0.46
1:G:687:ARG:HG3	1:G:687:ARG:HH11	1.80	0.46
1:A:546:GLU:HG2	1:A:599:PRO:HB3	1.98	0.46
2:F:105:LEU:HD13	2:F:105:LEU:O	2.14	0.46
1:G:601:ASN:ND2	1:G:601:ASN:H	2.13	0.46
2:D:78:ASP:C	2:D:80:ASP:H	2.17	0.46
1:G:601:ASN:HD22	1:G:601:ASN:H	1.60	0.46
1:E:675:GLN:O	1:E:679:ALA:HB2	2.15	0.46
1:A:685:ASP:OD2	1:E:682:GLU:HG3	2.16	0.46
1:E:663:SER:O	1:E:665:GLN:N	2.49	0.46
1:G:545:THR:HG21	1:G:551:GLU:HB2	1.96	0.46
1:C:682:GLU:O	1:C:684:PHE:N	2.49	0.46
2:D:65:PHE:HB3	2:D:66:PRO:HD3	1.97	0.46
1:A:577:LEU:HD21	1:A:605:LEU:HD12	1.98	0.46
1:C:596:GLY:CA	1:C:636:ALA:HB3	2.46	0.46
2:D:86:ARG:HG2	5:D:169:HOH:O	2.16	0.46
1:E:623:VAL:CG1	1:E:641:ILE:HD11	2.45	0.46
2:F:116:LEU:HD22	2:F:116:LEU:C	2.36	0.46
2:B:105:LEU:O	2:B:105:LEU:HD23	2.16	0.46
2:B:78:ASP:OD2	2:B:80:ASP:HB2	2.16	0.46
2:B:123:GLU:C	2:B:125:ILE:N	2.69	0.46
2:D:105:LEU:HD13	2:D:105:LEU:O	2.16	0.46
2:D:82:GLU:O	2:D:86:ARG:HB2	2.15	0.46
1:G:642:ASP:CG	1:G:656:MET:HB2	2.37	0.46
1:G:622:ALA:HB1	1:G:672:TRP:CZ2	2.51	0.46
1:G:687:ARG:HG3	2:H:46:ALA:CB	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:591:SER:O	1:E:599:PRO:HD3	2.16	0.45
1:E:643:GLN:HA	1:E:643:GLN:OE1	2.16	0.45
1:A:633:ARG:HG3	1:A:633:ARG:HH11	1.80	0.45
1:A:527:MET:CE	2:B:75:LYS:HG2	2.46	0.45
1:C:545:THR:HG1	3:C:999:FMN:P	2.39	0.45
1:E:515:LEU:HD13	1:E:515:LEU:O	2.16	0.45
1:E:673:ALA:CA	1:E:676:THR:HG22	2.46	0.45
2:H:69:LEU:C	2:H:69:LEU:HD13	2.36	0.45
1:A:514:PRO:HG2	1:A:517:VAL:CG2	2.47	0.45
1:A:519:VAL:CG1	2:B:145:MET:HG2	2.46	0.45
1:C:530:ARG:HH22	2:D:83:GLU:HG2	1.82	0.45
1:E:571:CYS:SG	1:E:573:ASP:OD1	2.75	0.45
2:B:117:THR:HG22	2:B:118:ASP:N	2.31	0.45
1:E:527:MET:SD	2:F:75:LYS:HG2	2.56	0.45
2:F:137:ASN:HD21	2:F:140:GLU:CG	2.23	0.45
1:G:531:LYS:C	1:G:533:MET:N	2.70	0.45
1:G:516:LYS:HG3	2:H:144:MET:HE1	1.99	0.45
1:G:516:LYS:HG3	2:H:144:MET:HE2	1.98	0.45
1:C:606:LYS:O	1:C:609:LEU:HB2	2.17	0.45
2:H:26:THR:HA	2:H:63:ILE:O	2.17	0.45
1:C:576:ARG:C	1:C:578:SER:N	2.70	0.45
2:F:117:THR:HG22	2:F:119:GLU:HB3	1.99	0.45
1:G:619:PHE:C	1:G:619:PHE:CD1	2.90	0.45
2:H:13:LYS:O	2:H:16:PHE:HB3	2.17	0.45
2:B:36:MET:HG2	2:B:41:GLN:HE22	1.82	0.45
1:G:531:LYS:O	1:G:533:MET:N	2.50	0.45
1:G:675:GLN:HE21	1:G:675:GLN:HA	1.82	0.45
2:B:129:ASP:OD1	2:B:134:GLY:N	2.50	0.45
1:E:524:PHE:HD2	2:F:19:PHE:CZ	2.34	0.45
1:C:536:ARG:HG2	1:C:565:PHE:HA	1.99	0.44
2:D:105:LEU:CD1	2:D:124:MET:HE3	2.45	0.44
1:E:677:PHE:C	1:E:679:ALA:N	2.71	0.44
2:H:26:THR:HB	2:H:62:THR:HB	2.00	0.44
1:A:695:PRO:HB2	1:A:698:TYR:HD1	1.82	0.44
1:E:521:ALA:O	1:E:524:PHE:HB3	2.17	0.44
2:F:117:THR:CG2	2:F:119:GLU:HB3	2.47	0.44
2:H:138:TYR:HA	2:H:141:PHE:HB3	1.99	0.44
1:E:572:MET:C	1:E:574:LYS:H	2.21	0.44
2:F:116:LEU:CD1	2:F:116:LEU:H	2.30	0.44
1:E:522:VAL:CG2	2:F:88:ALA:HB1	2.47	0.44
1:G:576:ARG:NE	1:G:578:SER:OG	2.41	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:582:GLU:O	1:G:583:GLU:HB2	2.17	0.44
1:A:513:ILE:H	1:A:513:ILE:HD12	1.79	0.44
1:A:542:LEU:HA	1:A:570:VAL:O	2.16	0.44
2:B:115:LYS:HD2	2:B:115:LYS:H	1.82	0.44
2:B:126:ARG:HB2	2:B:126:ARG:HH11	1.82	0.44
1:C:536:ARG:HG2	1:C:564:ALA:O	2.17	0.44
2:H:48:LEU:HA	2:H:51:MET:HE2	1.99	0.44
2:H:97:ASN:CG	2:H:98:GLY:N	2.71	0.44
1:A:598:CYS:HG	1:A:603:GLU:HG2	1.78	0.44
1:C:641:ILE:HD11	1:C:645:LEU:HD11	1.98	0.44
1:G:537:VAL:HG13	1:G:565:PHE:CD2	2.53	0.44
2:H:125:ILE:HG23	2:H:136:VAL:HG23	1.99	0.44
1:A:537:VAL:HA	5:A:65:HOH:O	2.16	0.44
1:C:629:SER:HB3	1:C:660:ASP:OD2	2.17	0.44
1:G:639:HIS:O	1:G:643:GLN:HB2	2.17	0.44
2:B:85:ILE:O	2:B:88:ALA:HB3	2.17	0.44
1:E:539:VAL:O	1:E:567:PRO:HA	2.18	0.44
1:E:652:GLN:NE2	1:E:655:PRO:HA	2.33	0.44
1:G:541:ILE:HG12	1:G:587:LEU:HB2	1.99	0.44
1:A:694:ILE:HB	1:A:695:PRO:CD	2.48	0.44
1:C:536:ARG:NH2	1:C:562:SER:O	2.51	0.44
1:C:577:LEU:H	1:C:577:LEU:CD2	2.30	0.44
1:E:587:LEU:HD22	1:E:622:ALA:HB3	1.99	0.44
2:F:26:THR:HG22	2:F:63:ILE:C	2.37	0.44
2:H:55:VAL:HG22	2:H:71:MET:HE3	2.00	0.44
2:H:65:PHE:HB3	2:H:66:PRO:HD3	1.98	0.44
1:C:581:GLU:CD	1:C:617:ASN:HB2	2.38	0.43
2:D:123:GLU:HA	2:D:123:GLU:OE2	2.17	0.43
2:D:29:THR:CG2	2:D:52:ILE:HG13	2.45	0.43
1:G:640:ASP:O	1:G:644:LYS:HB3	2.17	0.43
2:H:3:GLN:HB3	2:H:3:GLN:HE21	1.55	0.43
1:A:623:VAL:HG12	1:A:624:PHE:N	2.32	0.43
1:C:549:LYS:HB2	3:C:999:FMN:O3P	2.19	0.43
2:D:141:PHE:O	2:D:144:MET:HB3	2.19	0.43
1:E:653:LEU:HD13	1:E:653:LEU:O	2.18	0.43
1:G:644:LYS:NZ	1:G:648:LEU:HD11	2.33	0.43
1:A:620:ARG:HH22	1:E:687:ARG:HA	1.82	0.43
1:C:546:GLU:C	1:C:548:GLY:H	2.21	0.43
1:C:690:GLN:H	1:C:690:GLN:CD	2.20	0.43
2:D:79:THR:O	2:D:79:THR:CG2	2.67	0.43
1:E:610:PHE:HB2	1:E:611:MET:HE1	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:621:TYR:CD2	1:E:645:LEU:HD13	2.53	0.43
2:H:117:THR:HB	2:H:120:GLU:HG2	2.01	0.43
2:H:55:VAL:O	2:H:57:ALA:N	2.46	0.43
1:A:546:GLU:OE1	1:C:633:ARG:NH2	2.51	0.43
1:E:533:MET:C	1:E:535:SER:N	2.71	0.43
1:A:590:THR:O	1:A:625:GLY:HA2	2.18	0.43
2:B:137:ASN:ND2	2:B:137:ASN:C	2.71	0.43
2:B:5:THR:O	2:B:8:GLN:N	2.52	0.43
1:E:529:MET:HG2	2:F:36:MET:HE3	2.00	0.43
1:E:582:GLU:HG2	1:E:583:GLU:H	1.78	0.43
1:C:519:VAL:HG13	2:D:145:MET:SD	2.59	0.43
1:C:576:ARG:O	1:C:577:LEU:C	2.57	0.43
1:C:609:LEU:O	1:C:611:MET:N	2.52	0.43
2:D:4:LEU:O	2:D:5:THR:CB	2.65	0.43
1:E:592:THR:HG21	1:E:596:GLY:HA2	2.00	0.43
1:E:693:GLN:NE2	1:E:696:LYS:HZ3	2.15	0.43
1:G:519:VAL:O	1:G:522:VAL:HG12	2.19	0.43
1:A:659:GLY:C	1:A:665:GLN:HG3	2.38	0.43
1:C:624:PHE:CE1	1:C:669:PHE:HA	2.54	0.43
1:C:670:ARG:HG3	1:C:670:ARG:HH11	1.84	0.43
1:E:553:LEU:HD12	1:E:626:LEU:HD11	2.01	0.43
1:G:592:THR:OG1	1:G:635:CYS:HA	2.18	0.43
2:B:126:ARG:CB	2:B:126:ARG:HH11	2.32	0.43
1:E:583:GLU:HA	1:E:583:GLU:OE1	2.18	0.43
1:E:581:GLU:OE2	1:E:617:ASN:CB	2.67	0.43
1:E:680:ALA:O	1:E:684:PHE:HB2	2.19	0.43
2:B:48:LEU:HD23	2:B:51:MET:CE	2.49	0.43
1:G:568:LYS:HG3	1:G:570:VAL:HG23	2.00	0.43
1:A:694:ILE:HB	1:A:695:PRO:HD2	2.01	0.42
2:B:29:THR:HG21	2:B:49:GLN:CD	2.39	0.42
1:C:592:THR:HG21	1:C:596:GLY:HA2	2.02	0.42
1:E:619:PHE:C	1:E:619:PHE:CD1	2.92	0.42
1:E:675:GLN:O	1:E:679:ALA:CB	2.67	0.42
1:G:513:ILE:H	1:G:513:ILE:CD1	2.24	0.42
1:A:515:LEU:HD23	2:B:124:MET:HG2	2.00	0.42
1:A:577:LEU:O	1:A:578:SER:C	2.56	0.42
1:E:530:ARG:HG2	1:E:530:ARG:HH11	1.85	0.42
1:A:689:LYS:NZ	1:A:689:LYS:CB	2.82	0.42
1:E:513:ILE:CD1	1:E:513:ILE:N	2.81	0.42
1:G:615:LEU:HG	1:G:617:ASN:O	2.20	0.42
2:H:65:PHE:N	2:H:66:PRO:CD	2.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:GLU:O	1:A:667:ASP:C	2.58	0.42
2:B:3:GLN:CD	2:B:3:GLN:N	2.73	0.42
1:C:670:ARG:O	1:C:674:VAL:HG23	2.19	0.42
1:E:663:SER:O	1:E:664:GLY:C	2.58	0.42
1:G:522:VAL:CG2	2:H:91:VAL:HG21	2.42	0.42
2:H:41:GLN:HB2	2:H:41:GLN:HE21	1.60	0.42
2:H:57:ALA:O	2:H:59:GLY:N	2.53	0.42
1:A:587:LEU:HD22	1:A:622:ALA:HB3	2.02	0.42
1:E:610:PHE:CZ	1:E:640:ASP:HB3	2.55	0.42
1:E:681:CYS:HA	1:E:686:VAL:HG23	2.02	0.42
2:B:126:ARG:HB2	2:B:126:ARG:NH1	2.35	0.42
2:B:130:ILE:CG1	2:B:140:GLU:HG2	2.50	0.42
1:C:519:VAL:O	1:C:522:VAL:HG13	2.20	0.42
1:C:628:SER:H	3:C:999:FMN:H1'1	1.83	0.42
1:G:652:GLN:HE21	1:G:655:PRO:HA	1.82	0.42
1:A:672:TRP:HA	1:A:675:GLN:CG	2.50	0.42
2:D:56:ASP:OD2	2:D:59:GLY:HA2	2.20	0.42
2:F:17:SER:HA	2:F:20:ASP:HB3	2.02	0.42
2:F:56:ASP:OD1	2:F:62:THR:O	2.38	0.42
1:G:563:CYS:O	1:G:564:ALA:HB2	2.20	0.42
2:B:3:GLN:NE2	2:B:3:GLN:N	2.68	0.41
1:C:631:TYR:HA	1:C:632:PRO:HD3	1.91	0.41
1:C:691:HIS:O	1:C:692:ILE:C	2.58	0.41
1:E:610:PHE:HZ	1:E:640:ASP:HB3	1.85	0.41
2:F:128:ALA:HB2	2:F:144:MET:SD	2.60	0.41
1:A:545:THR:HG1	3:A:999:FMN:P	2.42	0.41
1:E:598:CYS:O	1:E:599:PRO:O	2.38	0.41
1:A:583:GLU:HG3	5:A:15:HOH:O	2.20	0.41
2:B:138:TYR:CZ	2:B:142:VAL:HG21	2.55	0.41
1:C:598:CYS:SG	1:C:606:LYS:HB2	2.61	0.41
1:G:519:VAL:HA	1:G:522:VAL:CG1	2.51	0.41
2:D:143:GLN:O	2:D:147:ALA:HB2	2.20	0.41
2:F:26:THR:HG21	2:F:62:THR:OG1	2.21	0.41
2:H:5:THR:HG23	2:H:8:GLN:NE2	2.35	0.41
1:C:697:LEU:HD23	1:C:697:LEU:C	2.41	0.41
1:G:686:VAL:O	1:G:687:ARG:C	2.57	0.41
2:F:127:GLU:O	2:F:144:MET:HE1	2.20	0.41
1:A:689:LYS:NZ	1:A:689:LYS:HB2	2.35	0.41
1:C:607:LYS:O	1:C:611:MET:HG2	2.21	0.41
1:C:638:ALA:O	1:C:641:ILE:HG23	2.20	0.41
1:C:649:GLY:O	1:C:650:ALA:C	2.59	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:675:GLN:HE21	1:G:675:GLN:CA	2.33	0.41
1:G:530:ARG:NH1	2:H:84:GLU:CD	2.73	0.41
1:A:592:THR:CG2	1:A:593:PHE:N	2.84	0.41
1:A:672:TRP:O	1:A:676:THR:HG22	2.20	0.41
1:C:692:ILE:HD12	2:D:44:THR:HG22	2.03	0.41
2:D:37:ARG:HG2	2:D:42:ASN:HD22	1.84	0.41
1:G:590:THR:O	1:G:625:GLY:HA2	2.21	0.41
1:G:653:LEU:HD11	1:G:679:ALA:HB3	2.03	0.41
2:H:42:ASN:C	2:H:42:ASN:HD22	2.24	0.41
1:G:527:MET:H	1:G:527:MET:HG2	1.68	0.41
2:H:29:THR:CG2	2:H:52:ILE:HG13	2.41	0.41
1:C:621:TYR:CE1	1:C:652:GLN:N	2.88	0.41
1:C:680:ALA:O	1:C:684:PHE:HD1	2.04	0.41
1:E:546:GLU:HB2	1:E:593:PHE:CZ	2.56	0.41
1:G:573:ASP:OD1	1:G:574:LYS:HG2	2.19	0.41
2:B:101:SER:OG	2:B:104:GLU:HG3	2.21	0.41
1:E:589:VAL:HA	1:E:624:PHE:O	2.21	0.41
1:G:524:PHE:HD2	2:H:19:PHE:CZ	2.39	0.41
1:G:579:CYS:HA	1:G:582:GLU:HG3	2.02	0.41
1:G:553:LEU:HD22	1:G:669:PHE:CG	2.56	0.41
1:A:581:GLU:OE2	1:A:617:ASN:N	2.44	0.40
1:A:528:LEU:HB3	2:B:51:MET:SD	2.61	0.40
1:C:621:TYR:CD1	1:C:621:TYR:N	2.89	0.40
1:C:670:ARG:HG3	1:C:670:ARG:NH1	2.36	0.40
1:E:537:VAL:HG21	1:E:684:PHE:CD2	2.56	0.40
1:E:561:PHE:CE1	1:E:677:PHE:HB2	2.55	0.40
1:G:644:LYS:HZ2	1:G:648:LEU:HD21	1.85	0.40
1:A:546:GLU:HG3	1:A:593:PHE:CE1	2.56	0.40
2:D:27:ILE:HB	2:D:63:ILE:HB	2.04	0.40
1:C:662:LEU:CD1	1:C:662:LEU:N	2.84	0.40
1:E:528:LEU:HD21	2:F:71:MET:CE	2.51	0.40
1:E:598:CYS:C	1:E:599:PRO:O	2.60	0.40
1:G:527:MET:CE	2:H:75:LYS:HG2	2.52	0.40
2:D:109:MET:HE3	2:D:109:MET:HA	2.03	0.40
1:G:654:THR:HG21	1:G:676:THR:HB	2.03	0.40
2:B:137:ASN:ND2	2:B:140:GLU:N	2.48	0.40
2:B:77:LYS:HA	2:B:77:LYS:HD3	1.91	0.40
1:C:696:LYS:HB2	1:C:696:LYS:HE2	1.93	0.40
2:D:137:ASN:ND2	2:D:137:ASN:C	2.75	0.40
2:H:57:ALA:C	2:H:59:GLY:H	2.24	0.40
2:H:74:ARG:O	2:H:77:LYS:HB3	2.21	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	187/219 (85%)	165 (88%)	17 (9%)	5 (3%)	5	7
1	C	186/219 (85%)	142 (76%)	34 (18%)	10 (5%)	2	2
1	E	187/219 (85%)	156 (83%)	19 (10%)	12 (6%)	1	1
1	G	185/219 (84%)	156 (84%)	22 (12%)	7 (4%)	3	4
2	B	143/149 (96%)	125 (87%)	16 (11%)	2 (1%)	11	20
2	D	143/149 (96%)	129 (90%)	10 (7%)	4 (3%)	5	7
2	F	143/149 (96%)	128 (90%)	11 (8%)	4 (3%)	5	7
2	H	143/149 (96%)	113 (79%)	22 (15%)	8 (6%)	2	1
All	All	1317/1472 (90%)	1114 (85%)	151 (12%)	52 (4%)	3	4

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	609	LEU
1	C	689	LYS
2	D	5	THR
2	D	78	ASP
2	D	79	THR
1	E	695	PRO
1	G	603	GLU
1	G	632	PRO
1	G	695	PRO
1	A	619	PHE
2	B	132	GLY
1	C	610	PHE
1	C	648	LEU
1	C	683	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	690	GLN
1	E	564	ALA
1	E	582	GLU
1	E	583	GLU
1	E	604	LYS
1	E	664	GLY
2	F	24	ASP
2	F	115	LYS
2	F	129	ASP
1	G	564	ALA
2	H	56	ASP
2	H	58	ASP
1	A	609	LEU
1	E	603	GLU
2	F	78	ASP
1	G	514	PRO
1	G	532	THR
1	A	601	ASN
1	A	695	PRO
1	E	573	ASP
1	E	685	ASP
2	H	71	MET
2	B	4	LEU
1	C	612	LEU
1	C	649	GLY
1	G	531	LYS
2	H	57	ALA
2	H	127	GLU
1	A	629	SER
1	C	607	LYS
2	D	56	ASP
1	E	599	PRO
1	E	594	GLY
1	E	632	PRO
2	H	96	GLY
2	H	130	ILE
2	H	98	GLY
1	C	548	GLY

### 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	157/190 (83%)	138 (88%)	19 (12%)	5	9
1	C	154/190 (81%)	137 (89%)	17 (11%)	6	12
1	E	155/190 (82%)	139 (90%)	16 (10%)	7	14
1	G	154/190 (81%)	134 (87%)	20 (13%)	4	7
2	B	124/127 (98%)	115 (93%)	9 (7%)	14	27
2	D	122/127 (96%)	114 (93%)	8 (7%)	16	32
2	F	124/127 (98%)	114 (92%)	10 (8%)	11	23
2	H	119/127 (94%)	114 (96%)	5 (4%)	30	54
All	All	1109/1268 (88%)	1005 (91%)	104 (9%)	8	17

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	LEU
1	A	519	VAL
1	A	523	LEU
1	A	532	THR
1	A	537	VAL
1	A	555	TRP
1	A	560	LEU
1	A	583	GLU
1	A	584	ARG
1	A	586	LEU
1	A	609	LEU
1	A	641	ILE
1	A	643	GLN
1	A	653	LEU
1	A	665	GLN
1	A	675	GLN
1	A	683	THR
1	A	696	LYS
1	A	697	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	3	GLN
2	B	6	GLU
2	B	18	LEU
2	B	42	ASN
2	B	70	THR
2	B	80	ASP
2	B	122	ASP
2	B	137	ASN
2	B	145	MET
1	C	512	GLU
1	C	519	VAL
1	C	522	VAL
1	C	523	LEU
1	C	532	THR
1	C	555	TRP
1	C	556	ASP
1	C	560	LEU
1	C	567	PRO
1	C	584	ARG
1	C	586	LEU
1	C	619	PHE
1	C	633	ARG
1	C	641	ILE
1	C	643	GLN
1	C	648	LEU
1	C	685	ASP
2	D	26	THR
2	D	45	GLU
2	D	69	LEU
2	D	76	MET
2	D	80	ASP
2	D	119	GLU
2	D	137	ASN
2	D	144	MET
1	E	523	LEU
1	E	555	TRP
1	E	560	LEU
1	E	583	GLU
1	E	586	LEU
1	E	588	VAL
1	E	609	LEU
1	E	640	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	653	LEU
1	E	671	SER
1	E	675	GLN
1	E	682	GLU
1	E	683	THR
1	E	685	ASP
1	E	690	GLN
1	E	695	PRO
2	F	4	LEU
2	F	18	LEU
2	F	26	THR
2	F	30	LYS
2	F	42	ASN
2	F	71	MET
2	F	86	ARG
2	F	116	LEU
2	F	137	ASN
2	F	144	MET
1	G	513	ILE
1	G	515	LEU
1	G	516	LYS
1	G	527	MET
1	G	537	VAL
1	G	555	TRP
1	G	556	ASP
1	G	560	LEU
1	G	582	GLU
1	G	585	LEU
1	G	586	LEU
1	G	601	ASN
1	G	607	LYS
1	G	611	MET
1	G	666	GLU
1	G	675	GLN
1	G	687	ARG
1	G	693	GLN
1	G	697	LEU
1	G	698	TYR
2	H	3	GLN
2	H	42	ASN
2	H	86	ARG
2	H	105	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	144	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	HIS
1	A	652	GLN
1	A	675	GLN
1	A	690	GLN
2	B	3	GLN
2	B	41	GLN
2	B	42	ASN
2	B	135	GLN
2	B	137	ASN
2	B	143	GLN
1	C	675	GLN
1	C	691	HIS
2	D	8	GLN
2	D	41	GLN
2	D	42	ASN
2	D	135	GLN
2	D	137	ASN
1	E	652	GLN
1	E	675	GLN
1	E	690	GLN
1	E	693	GLN
2	F	41	GLN
2	F	42	ASN
2	F	135	GLN
2	F	137	ASN
1	G	601	ASN
1	G	617	ASN
1	G	652	GLN
1	G	675	GLN
1	G	691	HIS
2	H	3	GLN
2	H	8	GLN
2	H	41	GLN
2	H	42	ASN
2	H	53	ASN
2	H	135	GLN

### 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 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	$\# Z  > 2$
3	FMN	A	999	-	31,33,33	6.14	20 (64%)	40,50,50	3.46	18 (45%)
3	FMN	G	999	-	31,33,33	5.95	20 (64%)	40,50,50	3.44	16 (40%)
3	FMN	E	999	-	31,33,33	6.17	20 (64%)	40,50,50	3.44	15 (37%)
3	FMN	C	999	-	31,33,33	6.07	20 (64%)	40,50,50	3.46	17 (42%)

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
3	FMN	A	999	-	-	2/18/18/18	0/3/3/3
3	FMN	G	999	-	-	2/18/18/18	0/3/3/3
3	FMN	E	999	-	-	1/18/18/18	0/3/3/3
3	FMN	C	999	-	-	2/18/18/18	0/3/3/3

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FMN	C4A-C10	23.14	1.61	1.38
3	E	999	FMN	C4A-C10	22.64	1.61	1.38
3	C	999	FMN	C4A-C10	22.60	1.61	1.38
3	G	999	FMN	C4A-C10	21.77	1.60	1.38
3	A	999	FMN	C4-N3	10.35	1.51	1.33
3	E	999	FMN	C4-N3	10.30	1.51	1.33
3	G	999	FMN	C4-N3	9.93	1.50	1.33
3	E	999	FMN	C9-C9A	9.93	1.60	1.40
3	C	999	FMN	C4-N3	9.81	1.50	1.33
3	C	999	FMN	C5A-N5	9.67	1.51	1.35
3	C	999	FMN	C9-C9A	9.59	1.59	1.40
3	G	999	FMN	C9-C9A	9.50	1.59	1.40
3	A	999	FMN	C9-C9A	9.34	1.59	1.40
3	E	999	FMN	C9A-N10	9.08	1.50	1.38
3	G	999	FMN	C5A-N5	9.07	1.50	1.35
3	C	999	FMN	C9A-N10	8.95	1.50	1.38
3	E	999	FMN	C5A-N5	8.82	1.49	1.35
3	A	999	FMN	C5A-N5	8.54	1.49	1.35
3	G	999	FMN	C9A-N10	8.22	1.49	1.38
3	A	999	FMN	C9A-N10	8.10	1.49	1.38
3	E	999	FMN	C9A-C5A	6.42	1.55	1.42
3	G	999	FMN	C9A-C5A	6.10	1.54	1.42
3	C	999	FMN	C9A-C5A	6.03	1.54	1.42
3	E	999	FMN	C2'-C3'	-5.99	1.42	1.53
3	A	999	FMN	C2-N3	5.82	1.49	1.38
3	A	999	FMN	C9A-C5A	5.70	1.54	1.42
3	E	999	FMN	C8-C7	5.63	1.54	1.40
3	A	999	FMN	C8-C7	5.59	1.54	1.40
3	G	999	FMN	C8-C7	5.55	1.54	1.40
3	C	999	FMN	C6-C7	5.52	1.51	1.37
3	C	999	FMN	C8-C7	5.46	1.54	1.40
3	A	999	FMN	C6-C7	5.46	1.51	1.37
3	A	999	FMN	C2'-C3'	-5.39	1.43	1.53
3	C	999	FMN	C2-N3	5.26	1.48	1.38
3	A	999	FMN	C5'-C4'	5.23	1.59	1.51
3	G	999	FMN	C6-C7	5.22	1.51	1.37
3	E	999	FMN	C6-C7	5.22	1.51	1.37
3	A	999	FMN	O3'-C3'	5.19	1.55	1.43
3	G	999	FMN	C2-N3	5.15	1.48	1.38
3	G	999	FMN	O3'-C3'	5.11	1.55	1.43
3	E	999	FMN	C2-N3	5.10	1.48	1.38
3	C	999	FMN	C2'-C3'	-4.88	1.44	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	999	FMN	O3'-C3'	4.73	1.54	1.43
3	G	999	FMN	C2'-C3'	-4.71	1.44	1.53
3	E	999	FMN	C10-N1	4.56	1.39	1.33
3	E	999	FMN	O3'-C3'	4.48	1.53	1.43
3	E	999	FMN	C5'-C4'	4.39	1.58	1.51
3	G	999	FMN	C10-N1	4.39	1.38	1.33
3	G	999	FMN	C5'-C4'	4.37	1.58	1.51
3	E	999	FMN	O2'-C2'	-4.08	1.34	1.43
3	C	999	FMN	C10-N1	3.95	1.38	1.33
3	C	999	FMN	C6-C5A	3.91	1.47	1.41
3	E	999	FMN	C4-C4A	-3.84	1.34	1.41
3	G	999	FMN	O2'-C2'	-3.81	1.35	1.43
3	G	999	FMN	C6-C5A	3.75	1.47	1.41
3	A	999	FMN	C4-C4A	-3.73	1.34	1.41
3	A	999	FMN	C10-N1	3.72	1.38	1.33
3	G	999	FMN	C4-C4A	-3.57	1.35	1.41
3	C	999	FMN	O2'-C2'	-3.55	1.35	1.43
3	E	999	FMN	C6-C5A	3.52	1.47	1.41
3	A	999	FMN	O2'-C2'	-3.49	1.36	1.43
3	C	999	FMN	C4-C4A	-3.46	1.35	1.41
3	A	999	FMN	C6-C5A	3.41	1.47	1.41
3	A	999	FMN	C1'-N10	-3.31	1.44	1.48
3	C	999	FMN	C5'-C4'	3.28	1.56	1.51
3	E	999	FMN	C1'-N10	-3.01	1.45	1.48
3	A	999	FMN	P-O1P	-2.93	1.41	1.50
3	G	999	FMN	C1'-N10	-2.92	1.45	1.48
3	E	999	FMN	P-O1P	-2.69	1.41	1.50
3	G	999	FMN	P-O1P	-2.66	1.42	1.50
3	C	999	FMN	P-O1P	-2.63	1.42	1.50
3	E	999	FMN	C7M-C7	-2.45	1.46	1.51
3	A	999	FMN	P-O3P	-2.39	1.45	1.54
3	A	999	FMN	C7M-C7	-2.37	1.46	1.51
3	G	999	FMN	P-O3P	-2.33	1.45	1.54
3	C	999	FMN	P-O3P	-2.23	1.46	1.54
3	C	999	FMN	C1'-N10	-2.22	1.45	1.48
3	C	999	FMN	C7M-C7	-2.20	1.46	1.51
3	E	999	FMN	P-O3P	-2.08	1.46	1.54
3	G	999	FMN	C7M-C7	-2.07	1.46	1.51

All (66) bond angle outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	999	FMN	C4-N3-C2	11.36	124.73	115.14
3	G	999	FMN	C4-N3-C2	11.35	124.72	115.14
3	C	999	FMN	C4-N3-C2	11.27	124.66	115.14
3	A	999	FMN	C4-N3-C2	11.17	124.57	115.14
3	G	999	FMN	C1'-N10-C9A	8.31	124.83	118.29
3	E	999	FMN	C1'-N10-C9A	8.01	124.59	118.29
3	C	999	FMN	C1'-N10-C9A	7.77	124.41	118.29
3	G	999	FMN	C4A-N5-C5A	7.57	124.33	116.77
3	C	999	FMN	C4A-N5-C5A	7.56	124.33	116.77
3	E	999	FMN	C4A-N5-C5A	7.53	124.29	116.77
3	A	999	FMN	C4A-N5-C5A	7.28	124.05	116.77
3	A	999	FMN	C5A-C9A-N10	7.27	122.98	117.72
3	C	999	FMN	C5A-C9A-N10	6.18	122.19	117.72
3	E	999	FMN	C5A-C9A-N10	5.92	122.01	117.72
3	G	999	FMN	C5A-C9A-N10	5.87	121.97	117.72
3	E	999	FMN	C7M-C7-C6	-5.52	107.14	120.34
3	G	999	FMN	C7M-C7-C6	-5.33	107.58	120.34
3	A	999	FMN	C7M-C7-C6	-5.29	107.68	120.34
3	C	999	FMN	C7M-C7-C6	-5.21	107.88	120.34
3	E	999	FMN	C7M-C7-C8	4.85	130.67	120.74
3	G	999	FMN	C7M-C7-C8	4.77	130.52	120.74
3	A	999	FMN	C4A-C4-N3	-4.74	116.95	123.43
3	A	999	FMN	C7M-C7-C8	4.66	130.29	120.74
3	C	999	FMN	C7M-C7-C8	4.60	130.17	120.74
3	G	999	FMN	C4A-C4-N3	-4.51	117.27	123.43
3	E	999	FMN	C4A-C4-N3	-4.48	117.31	123.43
3	C	999	FMN	C4A-C4-N3	-4.46	117.33	123.43
3	C	999	FMN	C6-C5A-N5	4.04	123.50	119.05
3	A	999	FMN	C6-C5A-N5	4.02	123.47	119.05
3	A	999	FMN	C9A-N10-C10	-3.95	116.74	121.91
3	A	999	FMN	C1'-N10-C10	3.90	121.91	118.41
3	A	999	FMN	C1'-N10-C9A	3.88	121.35	118.29
3	G	999	FMN	C9A-N10-C10	-3.86	116.85	121.91
3	C	999	FMN	C9A-N10-C10	-3.85	116.87	121.91
3	E	999	FMN	C9A-N10-C10	-3.84	116.87	121.91
3	A	999	FMN	C9A-C5A-N5	-3.67	116.62	122.36
3	C	999	FMN	C9A-C5A-N5	-3.62	116.70	122.36
3	G	999	FMN	C6-C5A-N5	3.59	123.01	119.05
3	G	999	FMN	C9A-C5A-N5	-3.54	116.82	122.36
3	E	999	FMN	C9A-C5A-N5	-3.51	116.87	122.36
3	C	999	FMN	O5'-C5'-C4'	-3.44	100.18	109.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FMN	C5'-C4'-C3'	3.43	118.83	112.20
3	E	999	FMN	C6-C5A-N5	3.33	122.72	119.05
3	E	999	FMN	O3P-P-O2P	3.30	120.25	107.64
3	A	999	FMN	O5'-C5'-C4'	-3.22	100.77	109.36
3	G	999	FMN	O3P-P-O2P	3.16	119.70	107.64
3	C	999	FMN	O3P-P-O2P	3.13	119.62	107.64
3	A	999	FMN	O3P-P-O2P	3.13	119.61	107.64
3	A	999	FMN	C4'-C3'-C2'	3.09	119.79	113.36
3	A	999	FMN	O3'-C3'-C4'	-2.89	101.84	108.81
3	A	999	FMN	O4'-C4'-C5'	-2.64	103.97	109.92
3	C	999	FMN	C5'-C4'-C3'	2.61	117.25	112.20
3	E	999	FMN	C5'-C4'-C3'	2.59	117.20	112.20
3	G	999	FMN	O5'-C5'-C4'	-2.57	102.49	109.36
3	C	999	FMN	C4-C4A-N5	2.56	121.52	118.60
3	E	999	FMN	C4'-C3'-C2'	2.52	118.61	113.36
3	E	999	FMN	O5'-C5'-C4'	-2.51	102.67	109.36
3	C	999	FMN	C4-C4A-C10	-2.47	118.32	119.95
3	E	999	FMN	O3'-C3'-C4'	-2.42	102.98	108.81
3	G	999	FMN	C5'-C4'-C3'	2.39	116.82	112.20
3	G	999	FMN	C4'-C3'-C2'	2.30	118.15	113.36
3	C	999	FMN	C4'-C3'-C2'	2.29	118.12	113.36
3	A	999	FMN	O2P-P-O5'	2.23	112.67	106.73
3	G	999	FMN	C4-C4A-N5	2.16	121.07	118.60
3	C	999	FMN	O3'-C3'-C4'	-2.16	103.59	108.81
3	G	999	FMN	O3'-C3'-C4'	-2.15	103.62	108.81

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	999	FMN	C3'-C4'-C5'-O5'
3	C	999	FMN	O4'-C4'-C5'-O5'
3	A	999	FMN	O4'-C4'-C5'-O5'
3	G	999	FMN	O4'-C4'-C5'-O5'
3	G	999	FMN	C3'-C4'-C5'-O5'
3	A	999	FMN	C3'-C4'-C5'-O5'
3	E	999	FMN	O4'-C4'-C5'-O5'

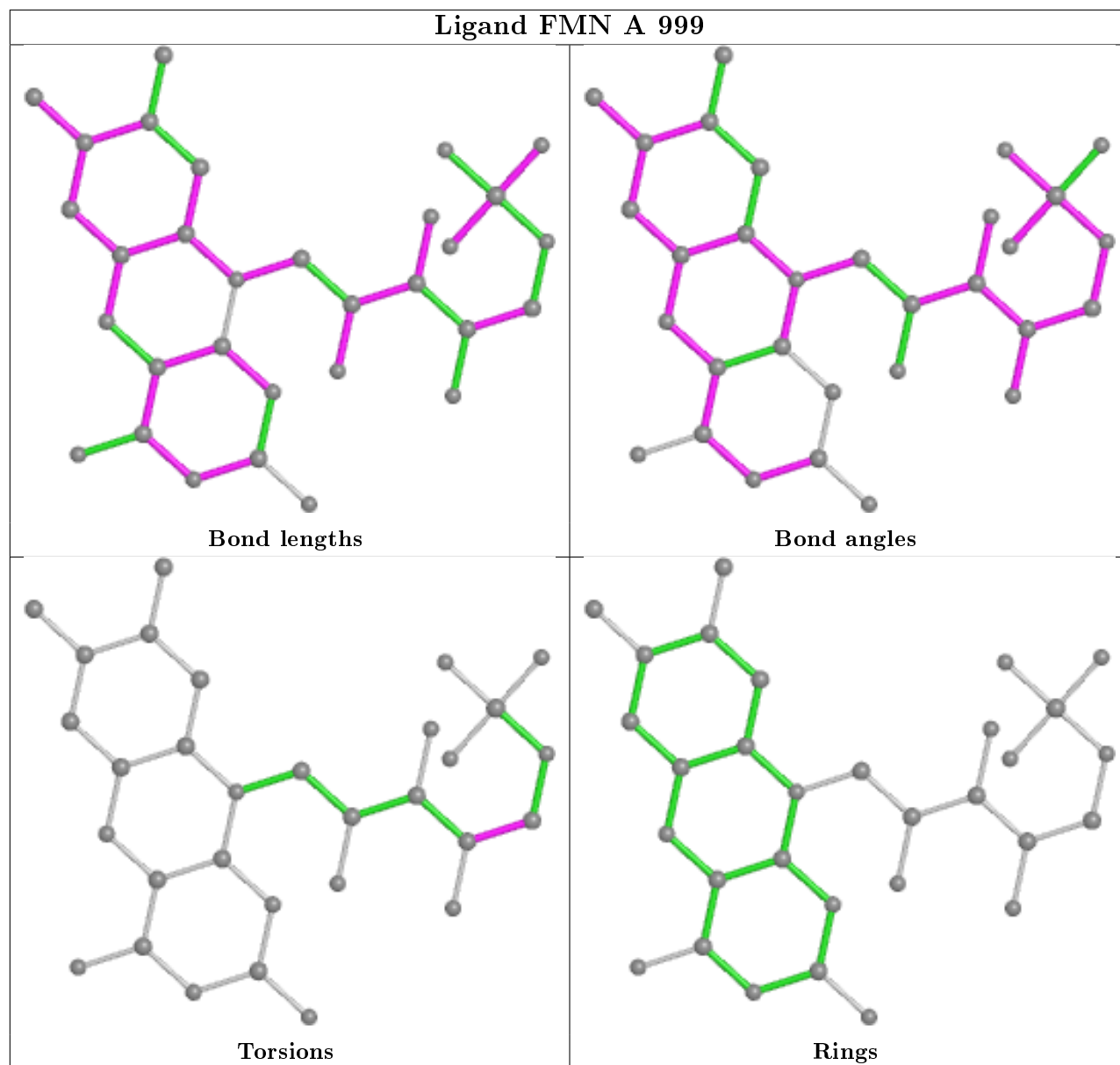
There are no ring outliers.

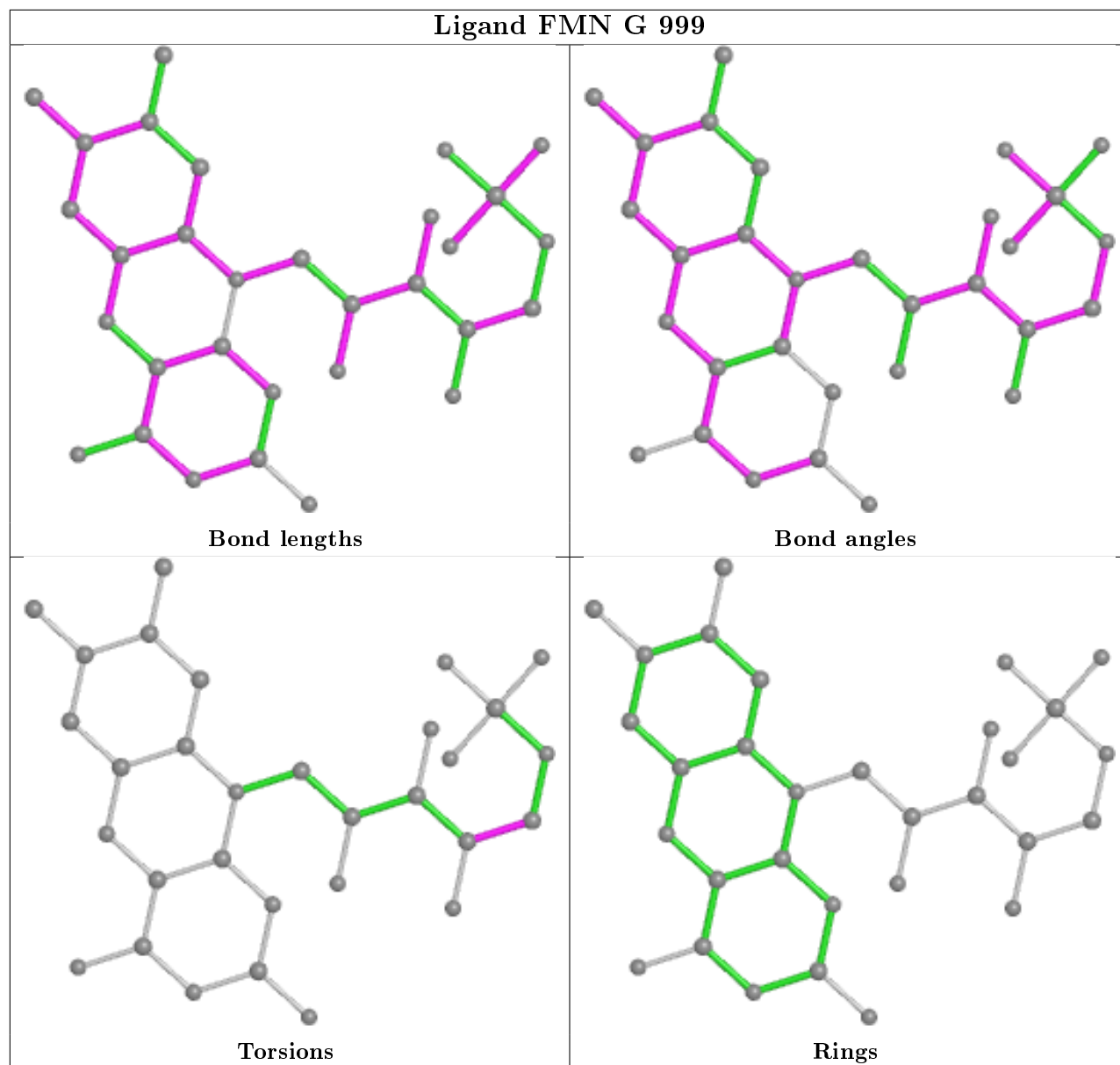
4 monomers are involved in 8 short contacts:

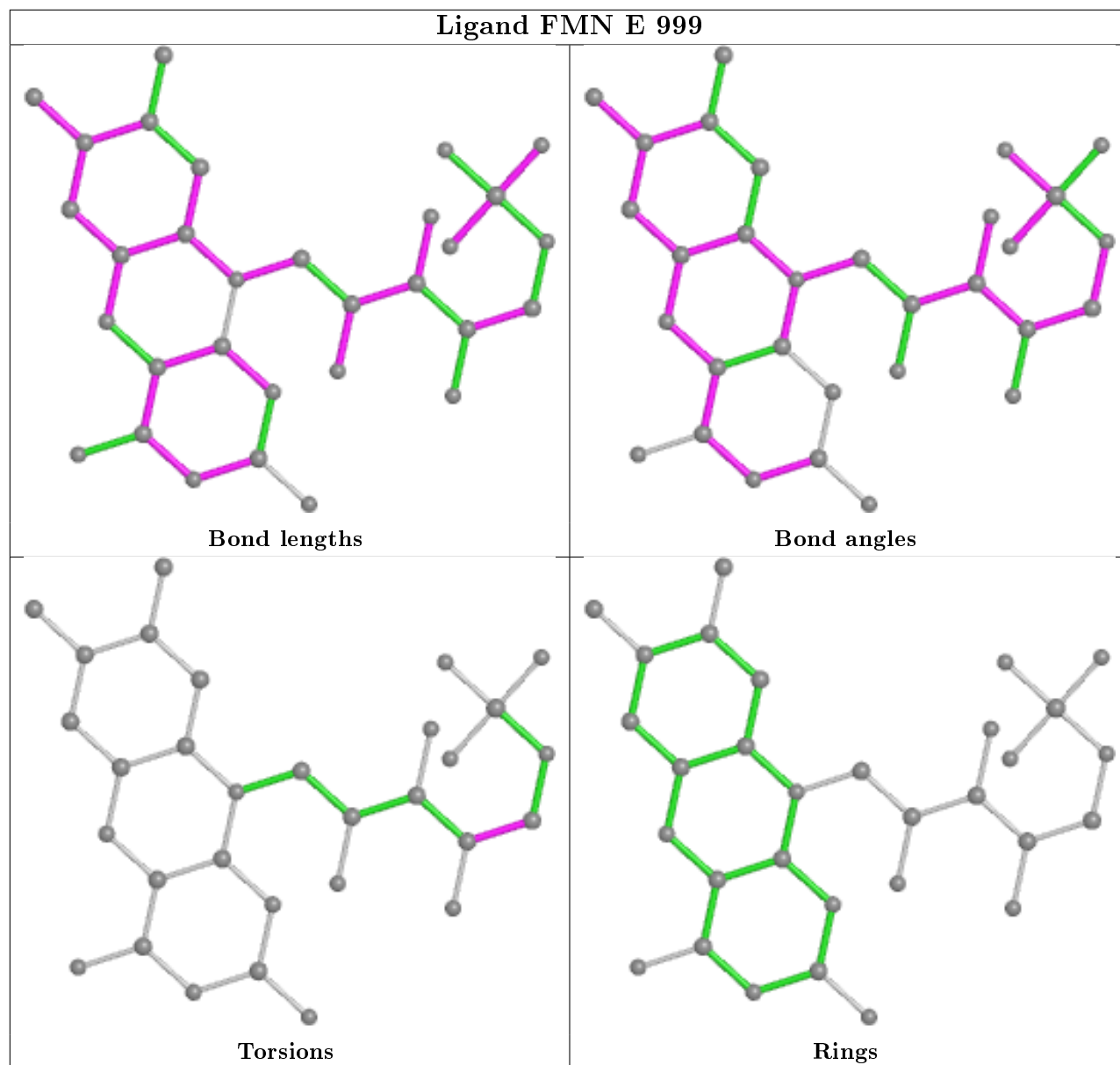
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	FMN	1	0
3	G	999	FMN	1	0
3	E	999	FMN	1	0
3	C	999	FMN	5	0

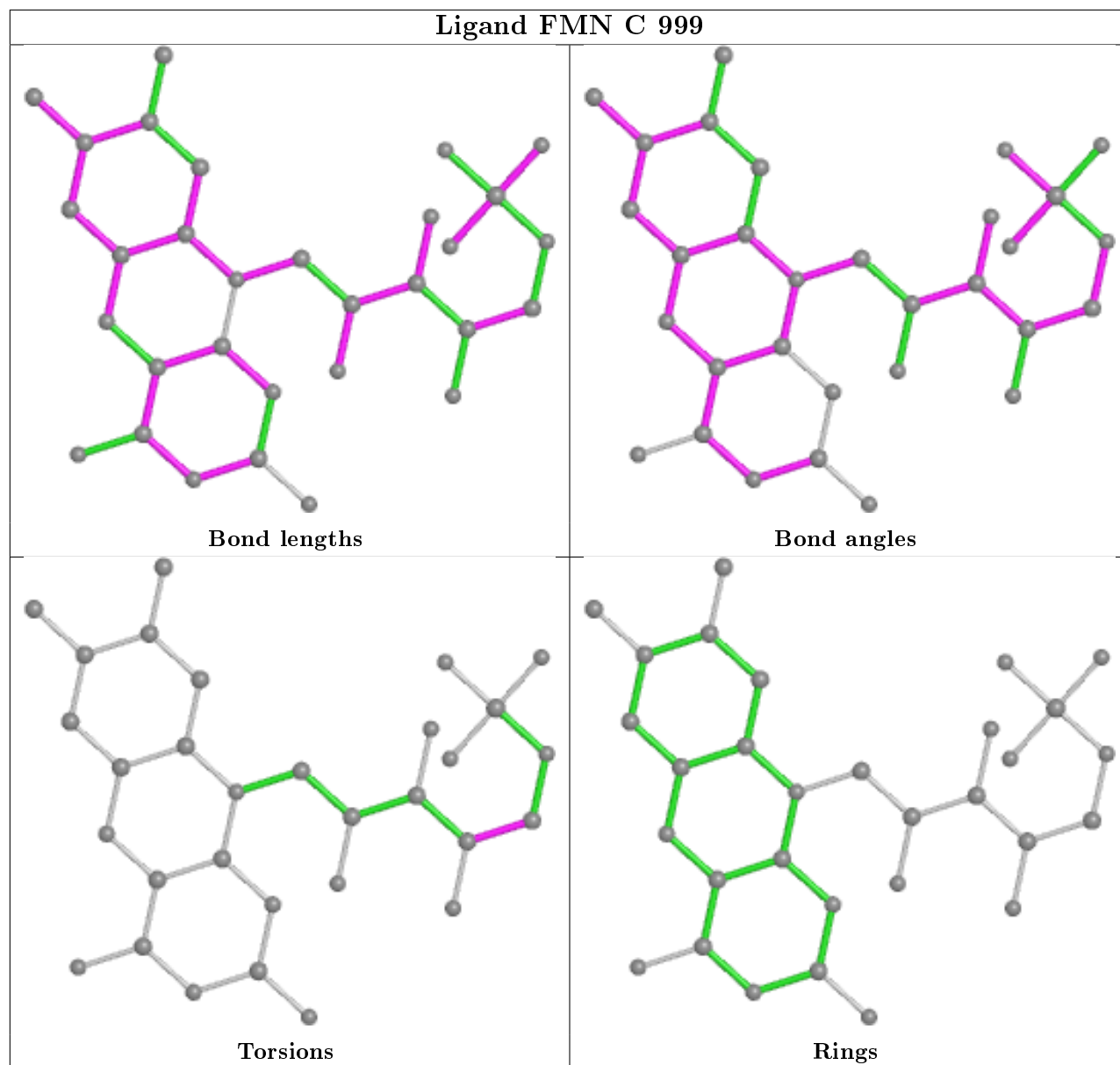
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	189/219 (86%)	-0.16	0 100 100	31, 51, 72, 86	0
1	C	188/219 (85%)	0.27	7 (3%) 41 45	32, 68, 94, 102	0
1	E	189/219 (86%)	0.11	3 (1%) 72 74	41, 69, 85, 92	0
1	G	187/219 (85%)	0.65	16 (8%) 10 10	48, 81, 98, 104	0
2	B	145/149 (97%)	-0.18	2 (1%) 75 77	34, 58, 86, 97	0
2	D	145/149 (97%)	-0.11	2 (1%) 75 77	27, 43, 72, 86	0
2	F	145/149 (97%)	-0.13	0 100 100	27, 55, 77, 87	0
2	H	145/149 (97%)	0.46	10 (6%) 16 17	52, 83, 102, 105	0
All	All	1333/1472 (90%)	0.13	40 (3%) 50 53	27, 64, 94, 105	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	686	VAL	5.1
1	G	593	PHE	4.2
1	C	593	PHE	3.7
1	G	681	CYS	3.7
2	H	92	PHE	3.4
1	G	628	SER	3.2
1	G	662	LEU	3.1
2	H	48	LEU	3.0
2	H	116	LEU	3.0
1	G	698	TYR	3.0
2	B	128	ALA	3.0
1	G	537	VAL	2.8
2	D	3	GLN	2.8
1	G	577	LEU	2.7
2	H	99	TYR	2.7
1	C	662	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	75	LYS	2.6
1	G	685	ASP	2.6
2	H	44	THR	2.5
1	C	594	GLY	2.5
1	E	641	ILE	2.4
1	G	647	HIS	2.4
1	C	615	LEU	2.4
1	G	564	ALA	2.4
1	G	633	ARG	2.4
1	C	580	LEU	2.4
1	G	653	LEU	2.4
2	H	138	TYR	2.3
1	G	649	GLY	2.3
1	G	677	PHE	2.3
2	H	49	GLN	2.3
2	H	127	GLU	2.3
2	H	136	VAL	2.2
2	H	100	ILE	2.2
1	E	645	LEU	2.2
1	E	577	LEU	2.2
1	C	582	GLU	2.2
2	B	130	ILE	2.1
1	C	691	HIS	2.1
1	G	630	MET	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](#)

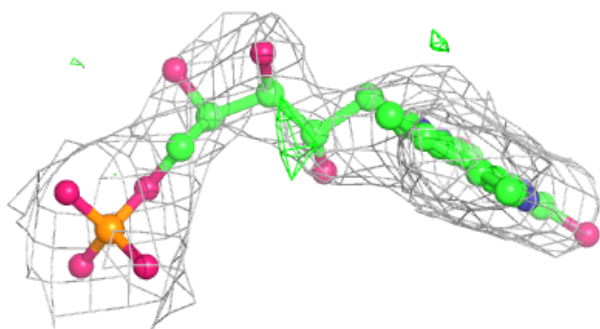
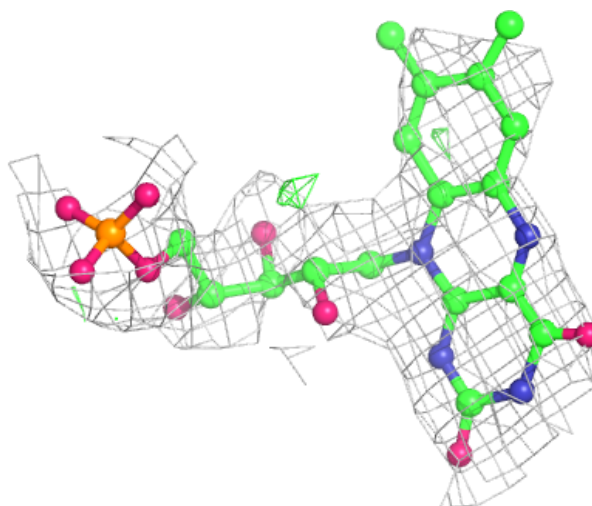
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	CA	B	204	1/1	0.80	0.06	77,77,77,77	0
3	FMN	G	999	31/31	0.88	0.26	93,97,99,99	0
3	FMN	C	999	31/31	0.89	0.25	91,93,94,95	0
4	CA	H	203	1/1	0.89	0.04	95,95,95,95	0
4	CA	H	201	1/1	0.94	0.13	88,88,88,88	0
4	CA	F	202	1/1	0.94	0.10	73,73,73,73	0
3	FMN	A	999	31/31	0.95	0.17	49,55,58,59	0
4	CA	F	201	1/1	0.96	0.14	63,63,63,63	0
4	CA	H	204	1/1	0.96	0.10	113,113,113,113	0
3	FMN	E	999	31/31	0.96	0.16	57,61,64,65	0
4	CA	D	203	1/1	0.97	0.16	37,37,37,37	0
4	CA	F	203	1/1	0.98	0.12	39,39,39,39	0
4	CA	D	204	1/1	0.98	0.14	36,36,36,36	0
4	CA	B	202	1/1	0.98	0.14	41,41,41,41	0
4	CA	B	203	1/1	0.98	0.05	61,61,61,61	0
4	CA	H	202	1/1	0.99	0.09	67,67,67,67	0
4	CA	B	201	1/1	0.99	0.12	44,44,44,44	0
4	CA	F	204	1/1	0.99	0.15	39,39,39,39	0
4	CA	D	201	1/1	0.99	0.12	43,43,43,43	0
4	CA	D	202	1/1	0.99	0.12	43,43,43,43	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 G 999:**

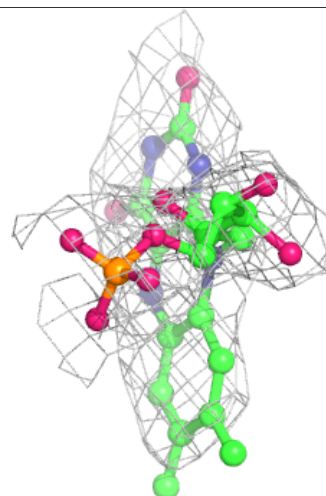
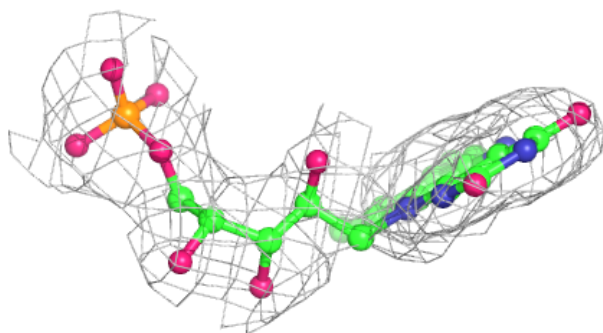
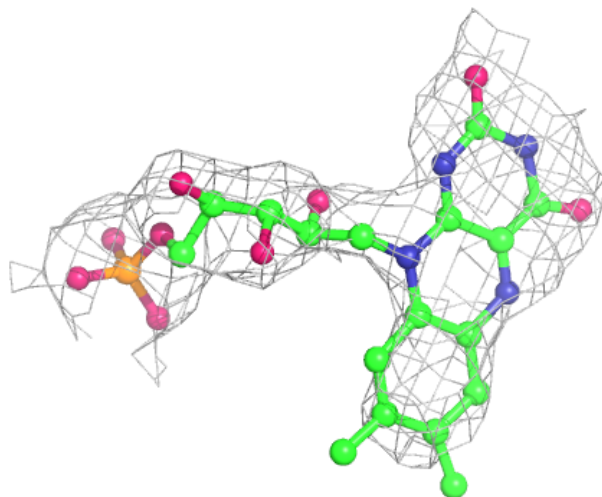
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





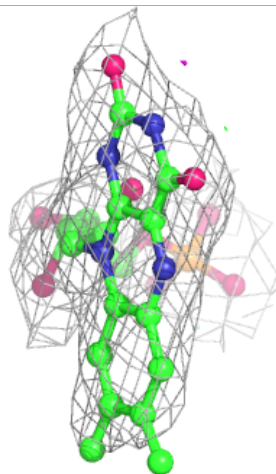
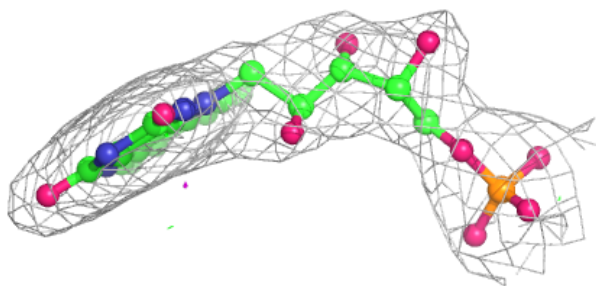
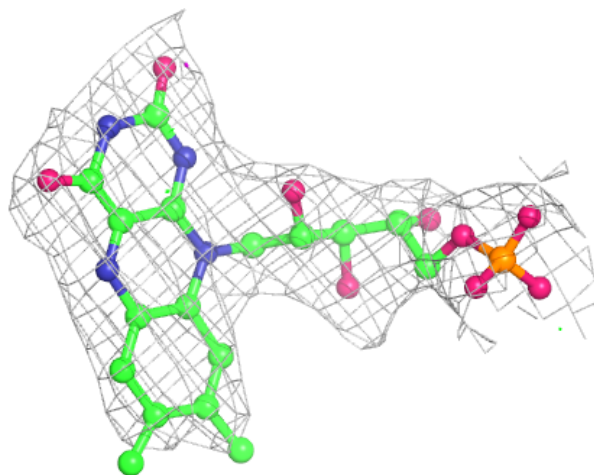
**Electron density around FMN C 999:**

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



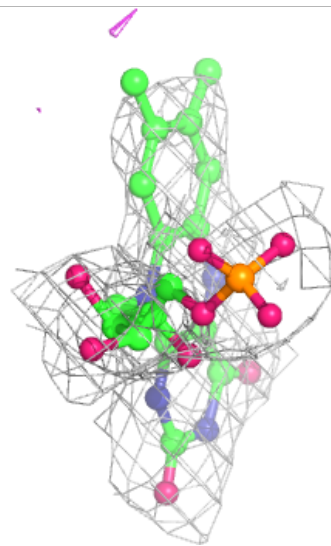
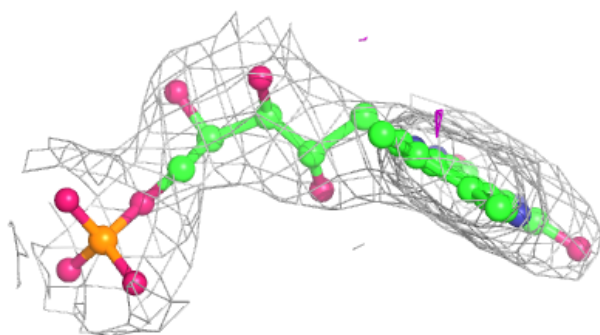
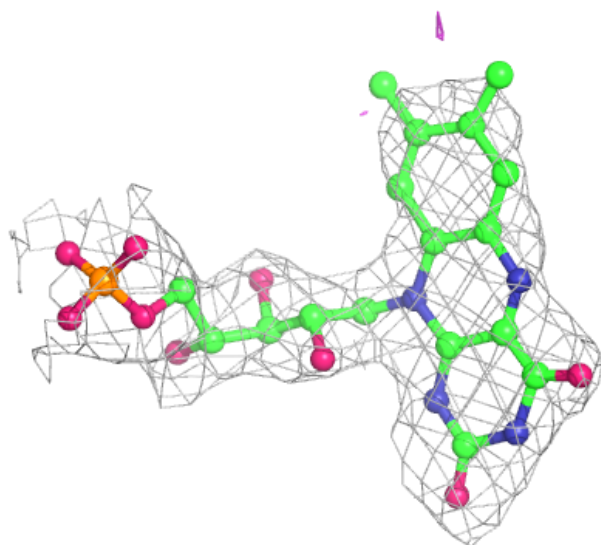
**Electron density around FMN A 999:**

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



**Electron density around FMN E 999:**

$2mF_o-DF_c$  (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.