



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2021 – 12:16 PM EDT

PDB ID : 7LJS  
Title : Porcine Dihydropyrimidine dehydrogenase (DPD) complexed with 5-Ethynyluracil (5EU) - Open Form  
Authors : Butrin, A.; Forouzesh, D.; Beaupre, B.; Wawrzak, Z.; Liu, D.; Moran, G.  
Deposited on : 2021-01-30  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

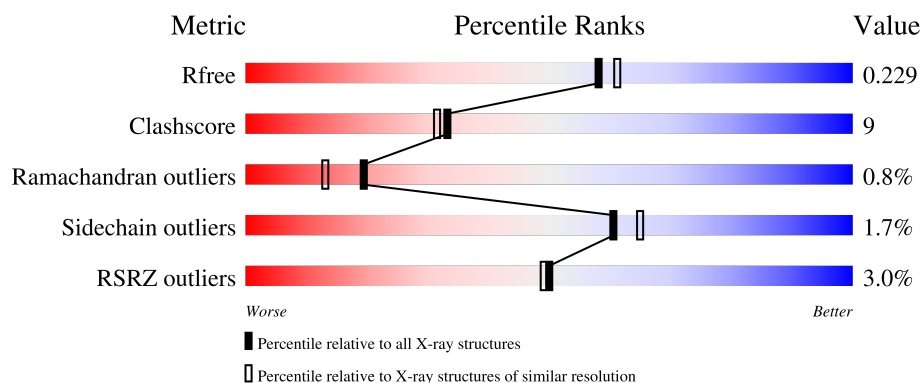
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1025	<div> <div>3%</div> <div>72%</div> <div>22%</div> <div>..</div> </div>
1	B	1025	<div> <div>3%</div> <div>71%</div> <div>23%</div> <div>..</div> </div>
1	C	1025	<div> <div>3%</div> <div>71%</div> <div>24%</div> <div>..</div> </div>
1	D	1025	<div> <div>3%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	1101	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33532 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.

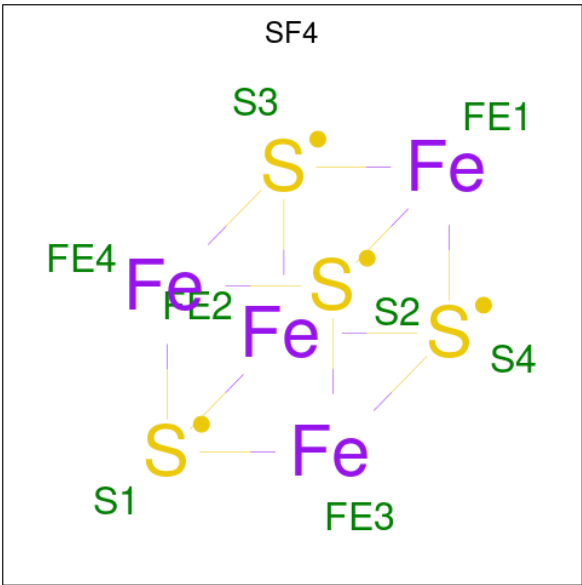
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1005	Total	C	N	O	S	0	4	0
			7678	4869	1298	1456	55			
1	B	1004	Total	C	N	O	S	0	5	0
			7688	4874	1303	1456	55			
1	C	1010	Total	C	N	O	S	0	11	0
			7741	4915	1308	1464	54			
1	D	1014	Total	C	N	O	S	0	7	0
			7750	4914	1312	1468	56			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



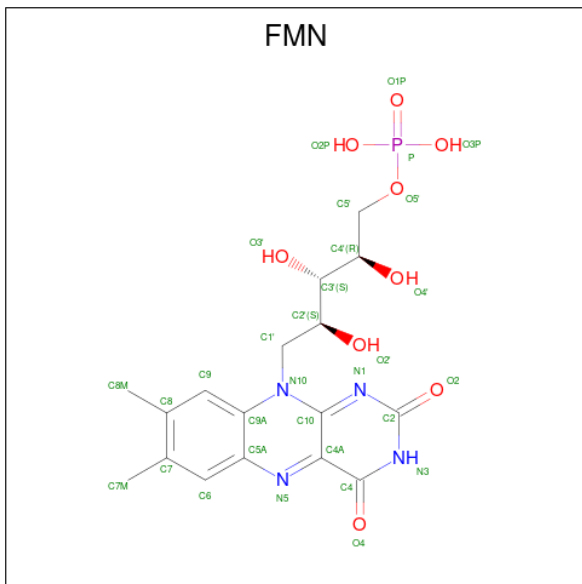
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

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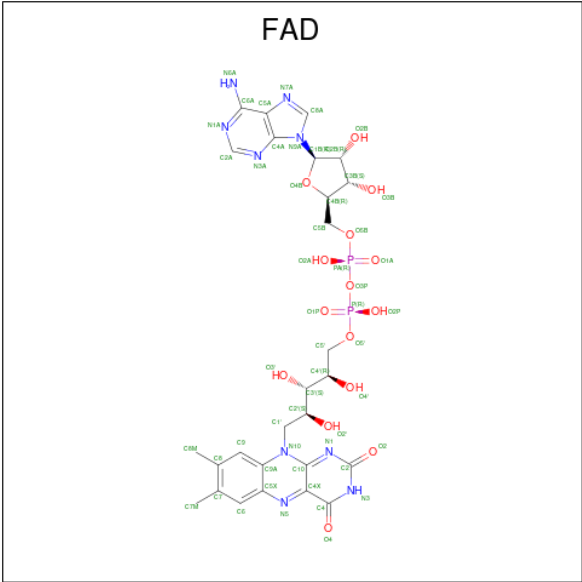
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



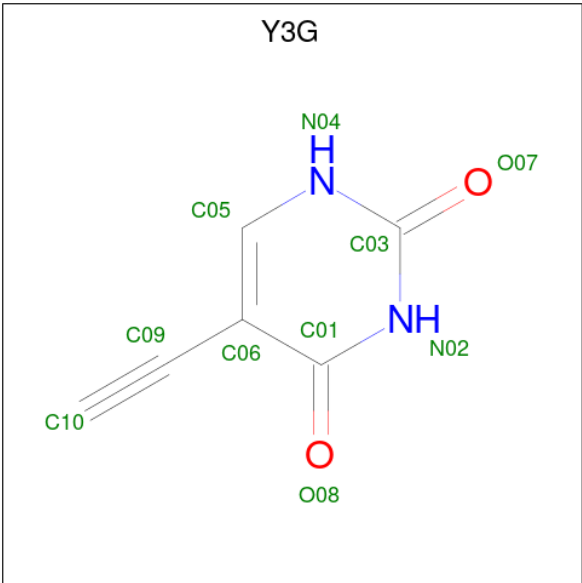
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	C	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	D	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is 5-ethynylpyrimidine-2,4(1H,3H)-dione (three-letter code: Y3G) (formula: C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	2	2		
5	B	1	Total	C	N	O	0	0
			10	6	2	2		
5	C	1	Total	C	N	O	0	0
			10	6	2	2		
5	D	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 6 is water.

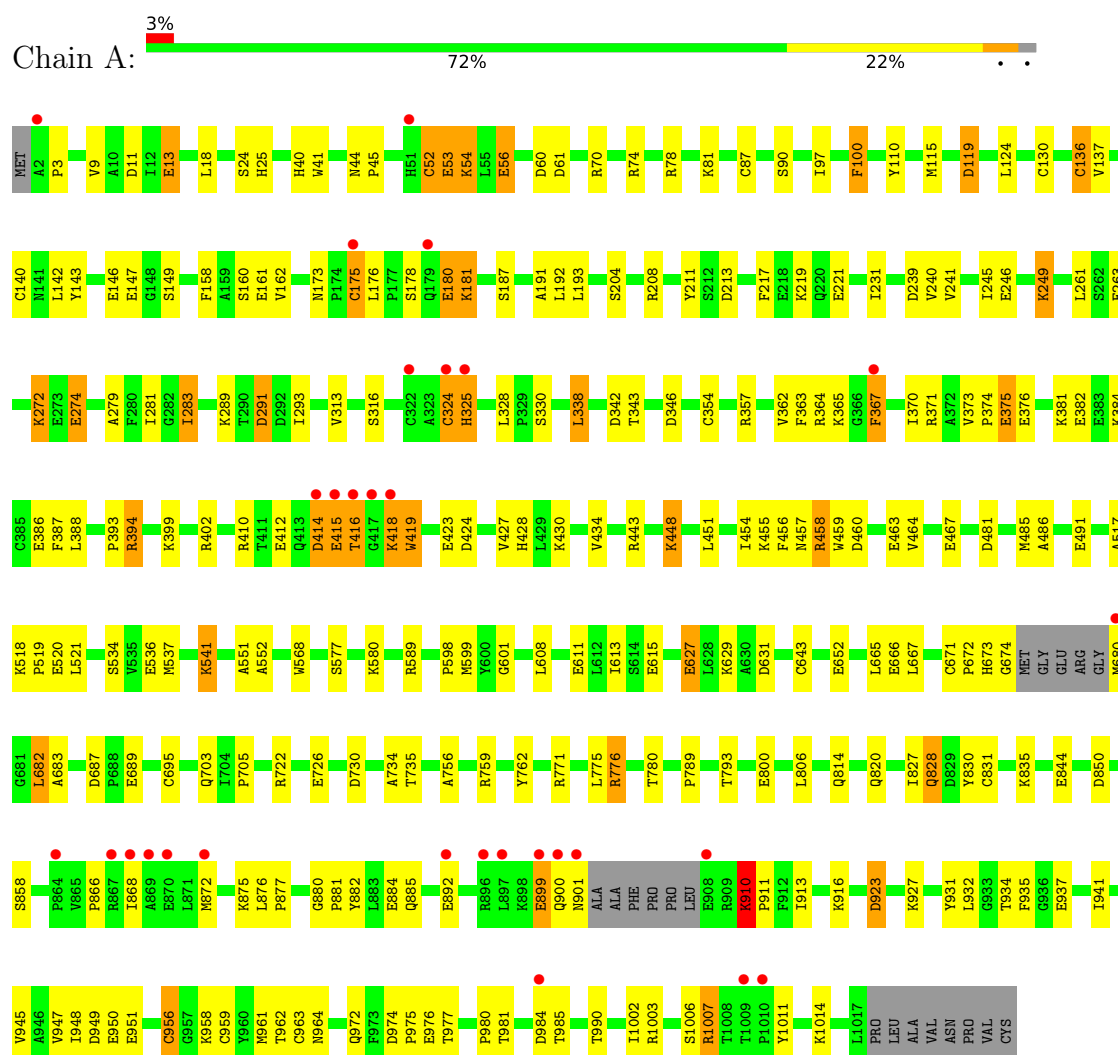
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	529	Total	O	0	0
			529	529		
6	B	490	Total	O	0	0
			490	490		
6	C	593	Total	O	0	0
			593	593		
6	D	559	Total	O	0	0
			559	559		



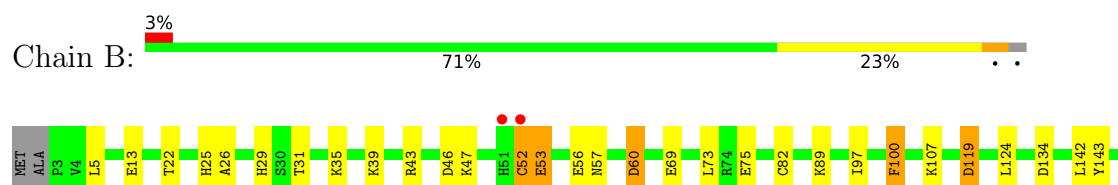
### 3 Residue-property plots

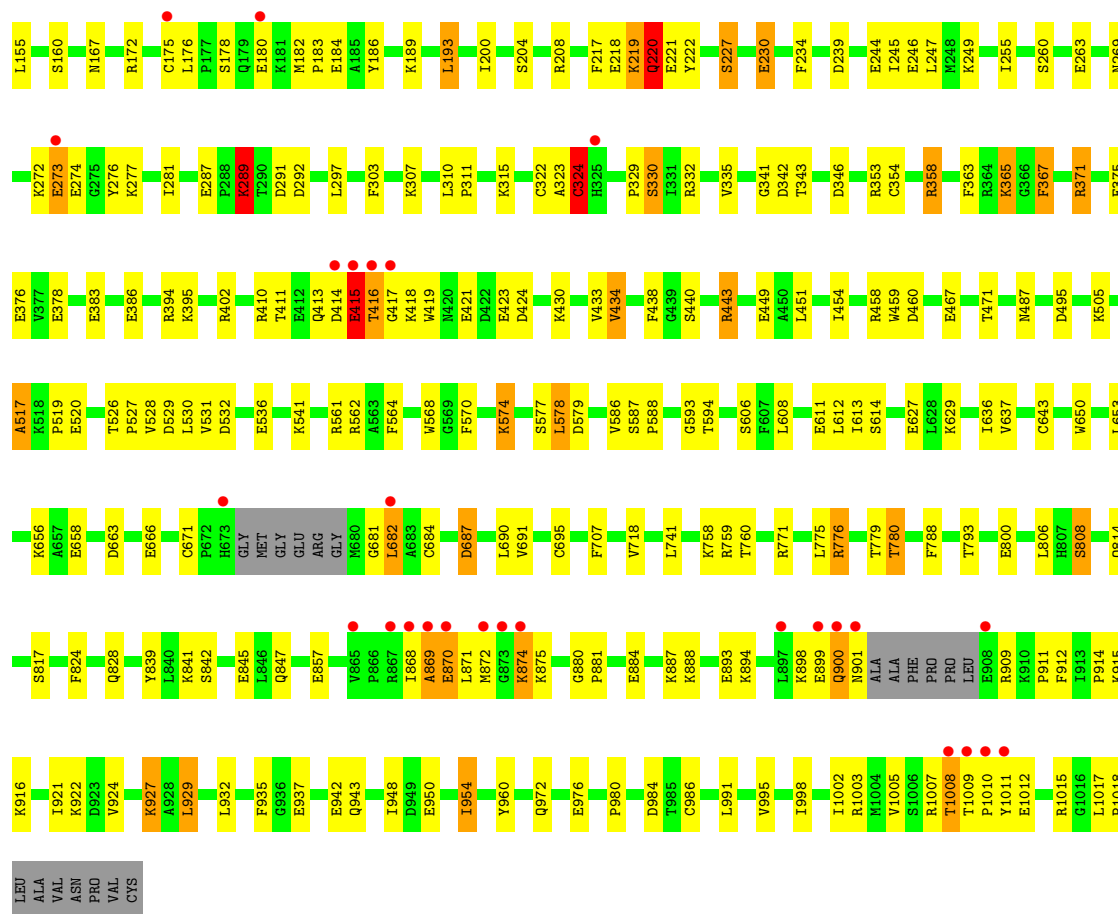
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

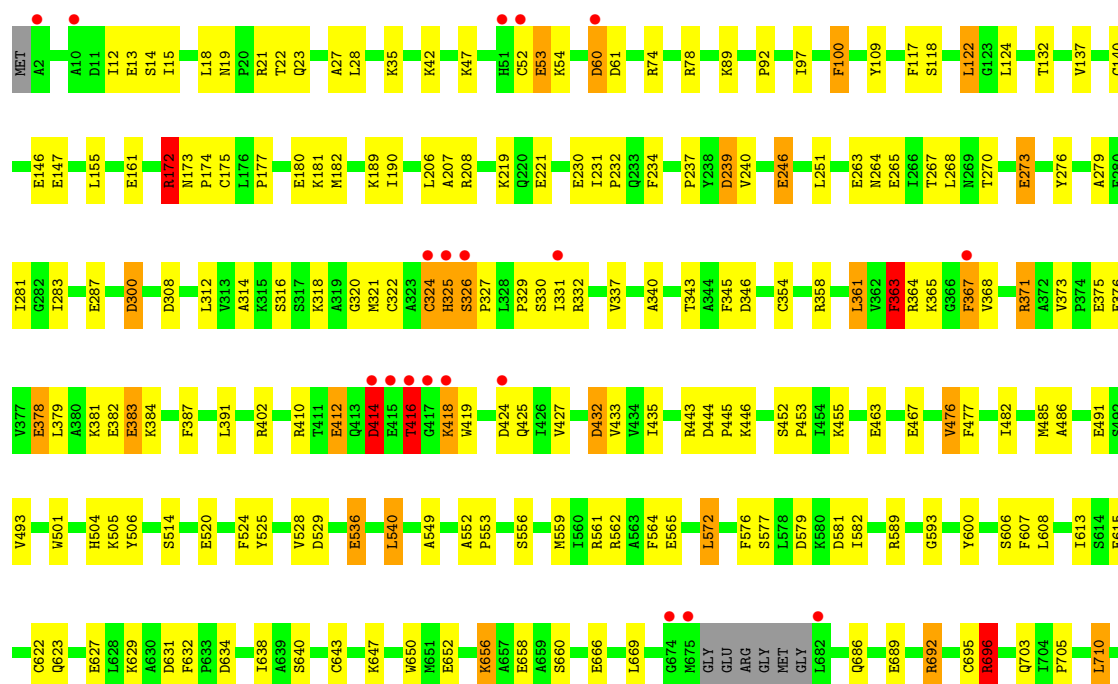


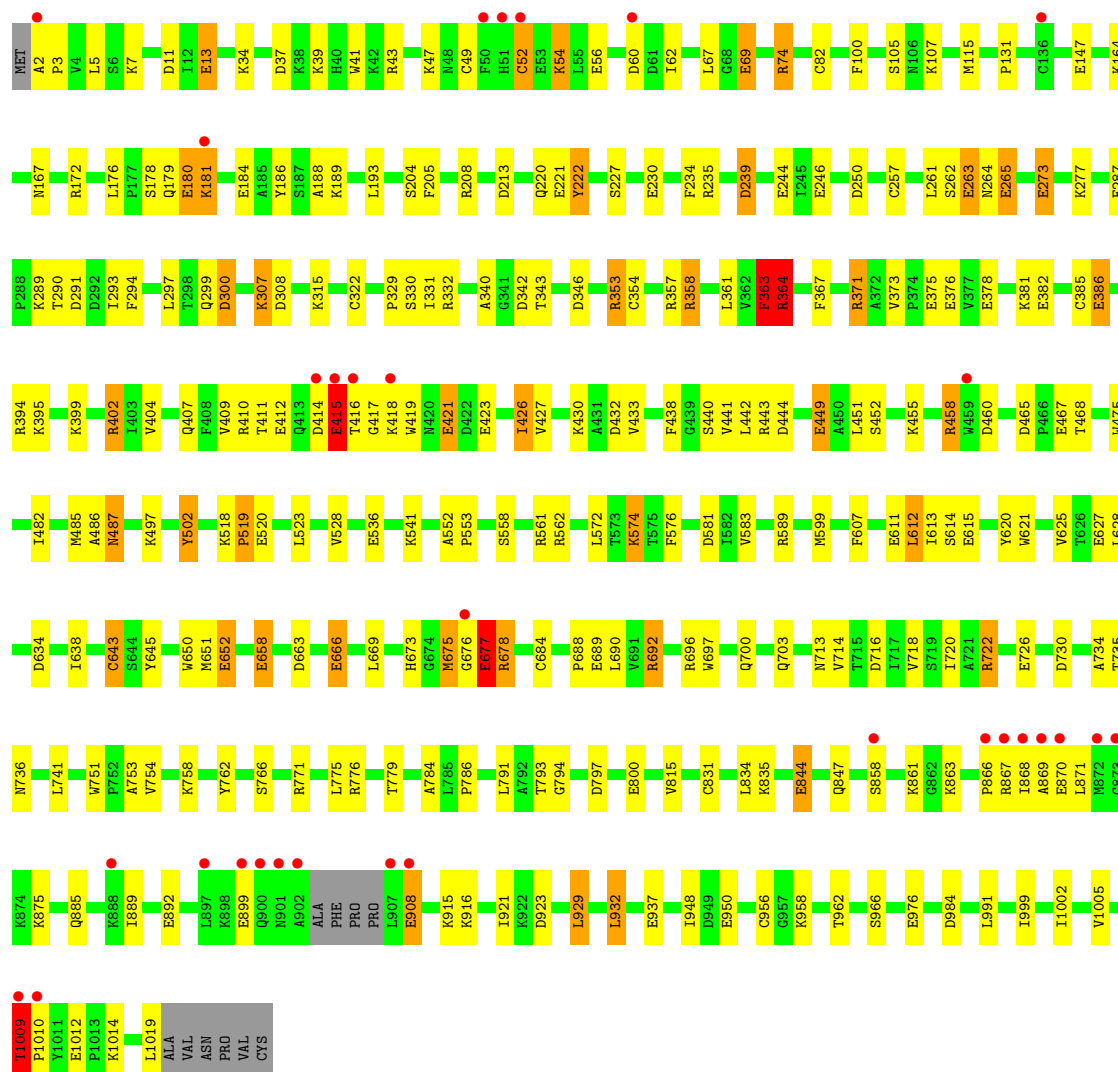
- Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]





• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.03Å 160.05Å 164.07Å 90.00° 95.95° 90.00°	Depositor
Resolution (Å)	45.62 – 2.00 45.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	77.1 (45.62-2.00) 77.1 (45.62-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.172 , 0.229 0.172 , 0.229	Depositor DCC
$R_{free}$ test set	10692 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: Y3G, SF4, FAD, FMN

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	1.43	96/7849 (1.2%)	1.20	47/10635 (0.4%)
1	B	1.43	98/7865 (1.2%)	1.23	62/10655 (0.6%)
1	C	1.50	129/7945 (1.6%)	1.25	70/10772 (0.6%)
1	D	1.55	129/7936 (1.6%)	1.28	66/10754 (0.6%)
All	All	1.48	452/31595 (1.4%)	1.24	245/42816 (0.6%)

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	3
1	B	0	3
1	C	0	3
1	D	0	5
All	All	0	14

All (452) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	519	PRO	N-CD	-20.33	1.19	1.47
1	D	265	GLU	CG-CD	18.56	1.79	1.51
1	A	956	CYS	CB-SG	14.74	2.07	1.82
1	D	265	GLU	CB-CG	12.59	1.76	1.52
1	C	60	ASP	CB-CG	11.67	1.76	1.51
1	C	956	CYS	CB-SG	11.40	2.01	1.82
1	D	800	GLU	CG-CD	11.25	1.68	1.51
1	A	324	CYS	CB-SG	10.86	2.00	1.82
1	D	184	GLU	CD-OE1	10.58	1.37	1.25
1	D	60	ASP	CB-CG	10.41	1.73	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	956	CYS	CB-SG	10.30	1.99	1.82
1	D	265	GLU	CD-OE2	10.11	1.36	1.25
1	C	536	GLU	CD-OE2	10.01	1.36	1.25
1	B	666	GLU	CD-OE2	9.76	1.36	1.25
1	C	324	CYS	CB-SG	9.66	1.98	1.82
1	D	984	ASP	CB-CG	9.65	1.72	1.51
1	C	375	GLU	CD-OE2	9.57	1.36	1.25
1	A	536	GLU	CD-OE1	9.40	1.35	1.25
1	C	175	CYS	CB-SG	9.37	1.98	1.82
1	B	60	ASP	CB-CG	9.29	1.71	1.51
1	C	800	GLU	CD-OE1	9.21	1.35	1.25
1	B	371	ARG	CG-CD	9.08	1.74	1.51
1	B	884	GLU	CG-CD	9.05	1.65	1.51
1	C	884	GLU	CD-OE2	8.97	1.35	1.25
1	A	52	CYS	CB-SG	8.82	1.97	1.82
1	A	136	CYS	CB-SG	8.80	1.97	1.82
1	A	87	CYS	CB-SG	8.78	1.97	1.82
1	C	884	GLU	CD-OE1	8.77	1.35	1.25
1	B	246	GLU	CD-OE2	8.73	1.35	1.25
1	B	884	GLU	CD-OE2	8.73	1.35	1.25
1	C	263	GLU	CG-CD	8.62	1.64	1.51
1	B	376	GLU	CD-OE2	8.55	1.35	1.25
1	A	541	LYS	CE-NZ	8.54	1.70	1.49
1	D	367	PHE	CE2-CZ	8.51	1.53	1.37
1	B	695	CYS	CB-SG	8.49	1.96	1.82
1	B	800	GLU	CB-CG	-8.49	1.36	1.52
1	C	908	GLU	CB-CG	8.44	1.68	1.52
1	B	246	GLU	CB-CG	8.41	1.68	1.52
1	D	684	CYS	CB-SG	8.39	1.96	1.82
1	B	273	GLU	CD-OE2	8.38	1.34	1.25
1	C	263	GLU	CD-OE1	8.32	1.34	1.25
1	D	378	GLU	CG-CD	8.28	1.64	1.51
1	C	13	GLU	CD-OE2	8.18	1.34	1.25
1	D	184	GLU	CG-CD	8.17	1.64	1.51
1	A	467	GLU	CG-CD	8.16	1.64	1.51
1	B	217	PHE	CE2-CZ	8.16	1.52	1.37
1	B	230	GLU	CG-CD	8.15	1.64	1.51
1	B	13	GLU	CD-OE1	8.13	1.34	1.25
1	D	487	ASN	CB-CG	8.10	1.69	1.51
1	B	1012	GLU	CG-CD	8.08	1.64	1.51
1	A	313	VAL	CB-CG2	8.07	1.69	1.52
1	C	800	GLU	CD-OE2	8.07	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	870	GLU	CG-CD	8.01	1.64	1.51
1	B	263	GLU	CG-CD	8.00	1.64	1.51
1	A	140	CYS	CB-SG	7.99	1.95	1.82
1	A	800	GLU	CD-OE1	7.95	1.34	1.25
1	A	884	GLU	CD-OE2	7.85	1.34	1.25
1	D	376	GLU	CD-OE2	7.84	1.34	1.25
1	D	815	VAL	CB-CG1	7.74	1.69	1.52
1	C	703	GLN	CG-CD	7.72	1.68	1.51
1	D	762	TYR	CE1-CZ	-7.70	1.28	1.38
1	C	528	VAL	CB-CG1	7.69	1.69	1.52
1	B	788	PHE	CE2-CZ	7.68	1.51	1.37
1	C	908	GLU	CG-CD	7.67	1.63	1.51
1	D	415	GLU	CG-CD	7.66	1.63	1.51
1	B	53	GLU	CD-OE2	7.64	1.34	1.25
1	D	800	GLU	CD-OE2	7.62	1.34	1.25
1	D	1012	GLU	CG-CD	7.56	1.63	1.51
1	D	375	GLU	CD-OE2	7.56	1.33	1.25
1	A	263	GLU	CD-OE2	7.54	1.33	1.25
1	B	937	GLU	CG-CD	7.52	1.63	1.51
1	B	375	GLU	CD-OE1	7.51	1.33	1.25
1	D	265	GLU	CD-OE1	7.45	1.33	1.25
1	C	13	GLU	CG-CD	7.45	1.63	1.51
1	C	615	GLU	CD-OE1	7.45	1.33	1.25
1	A	615	GLU	CG-CD	7.39	1.63	1.51
1	C	899	GLU	CG-CD	7.37	1.62	1.51
1	D	364	ARG	CG-CD	7.35	1.70	1.51
1	B	950	GLU	CG-CD	7.30	1.62	1.51
1	D	541	LYS	CD-CE	7.28	1.69	1.51
1	C	1012	GLU	CD-OE1	7.27	1.33	1.25
1	D	620	TYR	CD1-CE1	7.24	1.50	1.39
1	C	265	GLU	CG-CD	7.24	1.62	1.51
1	D	382	GLU	CG-CD	7.24	1.62	1.51
1	A	221	GLU	CG-CD	7.22	1.62	1.51
1	A	984	ASP	CB-CG	7.16	1.66	1.51
1	C	378	GLU	CD-OE1	7.15	1.33	1.25
1	B	324	CYS	CB-SG	7.15	1.94	1.82
1	A	828	GLN	CG-CD	7.15	1.67	1.51
1	C	660	SER	CB-OG	7.14	1.51	1.42
1	C	273	GLU	CD-OE1	7.13	1.33	1.25
1	C	640	SER	CB-OG	7.12	1.51	1.42
1	C	875	LYS	CD-CE	7.11	1.69	1.51
1	A	652	GLU	CG-CD	7.10	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	927	LYS	CB-CG	7.09	1.71	1.52
1	D	666	GLU	CD-OE1	7.09	1.33	1.25
1	B	75	GLU	CD-OE1	7.08	1.33	1.25
1	B	884	GLU	CB-CG	7.07	1.65	1.52
1	B	143	TYR	CD2-CE2	7.06	1.50	1.39
1	C	828	GLN	CG-CD	7.06	1.67	1.51
1	B	467	GLU	CD-OE1	6.99	1.33	1.25
1	C	375	GLU	CG-CD	6.96	1.62	1.51
1	C	446	LYS	CE-NZ	6.96	1.66	1.49
1	D	899	GLU	CG-CD	6.96	1.62	1.51
1	D	449	GLU	CG-CD	6.95	1.62	1.51
1	B	274	GLU	CD-OE2	6.94	1.33	1.25
1	A	580	LYS	CE-NZ	6.93	1.66	1.49
1	D	52	CYS	CB-SG	6.92	1.94	1.82
1	C	467	GLU	CD-OE2	6.91	1.33	1.25
1	B	937	GLU	CB-CG	6.90	1.65	1.52
1	C	230	GLU	CB-CG	6.89	1.65	1.52
1	B	277	LYS	CE-NZ	6.88	1.66	1.49
1	C	161	GLU	CD-OE1	6.88	1.33	1.25
1	A	274	GLU	CD-OE2	6.88	1.33	1.25
1	B	817	SER	CB-OG	6.87	1.51	1.42
1	C	817	SER	CB-OG	6.85	1.51	1.42
1	B	143	TYR	CZ-OH	6.84	1.49	1.37
1	C	146	GLU	CG-CD	6.84	1.62	1.51
1	A	951	GLU	CB-CG	6.83	1.65	1.52
1	D	69	GLU	CG-CD	6.82	1.62	1.51
1	D	412	GLU	CB-CG	-6.82	1.39	1.52
1	B	808	SER	CB-OG	-6.80	1.33	1.42
1	A	931	TYR	CD2-CE2	-6.79	1.29	1.39
1	C	506	TYR	CD1-CE1	6.78	1.49	1.39
1	D	273	GLU	CG-CD	6.77	1.62	1.51
1	D	227	SER	CB-OG	-6.77	1.33	1.42
1	C	1012	GLU	CD-OE2	6.76	1.33	1.25
1	D	107	LYS	CE-NZ	6.75	1.66	1.49
1	C	263	GLU	CB-CG	6.75	1.65	1.52
1	A	375	GLU	CD-OE2	6.74	1.33	1.25
1	B	684	CYS	CB-SG	6.71	1.93	1.82
1	C	476	VAL	CB-CG1	6.71	1.67	1.52
1	D	528	VAL	CB-CG2	-6.67	1.38	1.52
1	D	950	GLU	CD-OE2	6.67	1.32	1.25
1	A	274	GLU	CG-CD	6.64	1.61	1.51
1	C	221	GLU	CD-OE1	6.62	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	GLU	CG-CD	6.62	1.61	1.51
1	D	536	GLU	CD-OE1	6.60	1.32	1.25
1	C	666	GLU	CG-CD	6.60	1.61	1.51
1	C	376	GLU	CD-OE2	6.59	1.32	1.25
1	C	622	CYS	CB-SG	6.55	1.93	1.82
1	C	844	GLU	CG-CD	6.55	1.61	1.51
1	B	758	LYS	CE-NZ	6.54	1.65	1.49
1	D	315	LYS	CE-NZ	6.54	1.65	1.49
1	C	950	GLU	CG-CD	6.54	1.61	1.51
1	D	54	LYS	CD-CE	6.50	1.67	1.51
1	B	175	CYS	CB-SG	6.49	1.93	1.82
1	A	221	GLU	CD-OE2	6.49	1.32	1.25
1	A	434	VAL	CB-CG1	-6.48	1.39	1.52
1	B	568	TRP	CE3-CZ3	6.46	1.49	1.38
1	B	421	GLU	CD-OE2	6.46	1.32	1.25
1	D	378	GLU	CB-CG	6.45	1.64	1.52
1	C	117	PHE	CG-CD1	-6.45	1.29	1.38
1	A	375	GLU	CG-CD	6.44	1.61	1.51
1	D	180	GLU	CG-CD	6.44	1.61	1.51
1	B	505	LYS	CD-CE	6.43	1.67	1.51
1	C	467	GLU	CB-CG	6.42	1.64	1.52
1	C	627	GLU	CD-OE2	6.42	1.32	1.25
1	A	460	ASP	CB-CG	6.42	1.65	1.51
1	A	263	GLU	CD-OE1	6.41	1.32	1.25
1	D	976	GLU	CD-OE1	6.41	1.32	1.25
1	A	263	GLU	CG-CD	6.40	1.61	1.51
1	A	800	GLU	CG-CD	6.39	1.61	1.51
1	C	884	GLU	CG-CD	6.39	1.61	1.51
1	C	689	GLU	CD-OE2	6.38	1.32	1.25
1	D	449	GLU	CB-CG	-6.38	1.40	1.52
1	B	536	GLU	CD-OE1	6.38	1.32	1.25
1	C	615	GLU	CD-OE2	6.38	1.32	1.25
1	C	615	GLU	CG-CD	6.38	1.61	1.51
1	A	60	ASP	CB-CG	6.37	1.65	1.51
1	D	689	GLU	CD-OE2	6.37	1.32	1.25
1	A	110	TYR	CZ-OH	6.36	1.48	1.37
1	C	367	PHE	CE1-CZ	6.34	1.49	1.37
1	B	82	CYS	CB-SG	6.31	1.93	1.82
1	D	607	PHE	CE1-CZ	6.28	1.49	1.37
1	D	652	GLU	CG-CD	6.27	1.61	1.51
1	A	884	GLU	CD-OE1	6.27	1.32	1.25
1	B	119	ASP	CB-CG	6.27	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	892	GLU	CD-OE2	6.26	1.32	1.25
1	A	844	GLU	CD-OE2	6.25	1.32	1.25
1	C	950	GLU	CD-OE2	6.24	1.32	1.25
1	C	109	TYR	CE1-CZ	6.24	1.46	1.38
1	D	692	ARG	CZ-NH2	6.24	1.41	1.33
1	D	7	LYS	CD-CE	6.20	1.66	1.51
1	D	754	VAL	CB-CG1	6.20	1.65	1.52
1	D	82	CYS	CB-SG	6.18	1.92	1.82
1	C	273	GLU	CD-OE2	6.17	1.32	1.25
1	B	378	GLU	CD-OE2	6.17	1.32	1.25
1	D	666	GLU	CD-OE2	6.17	1.32	1.25
1	A	671	CYS	CB-SG	6.17	1.92	1.82
1	C	463	GLU	CD-OE1	6.16	1.32	1.25
1	D	950	GLU	CD-OE1	6.16	1.32	1.25
1	A	666	GLU	CG-CD	6.15	1.61	1.51
1	D	467	GLU	CG-CD	6.15	1.61	1.51
1	B	671	CYS	CB-SG	6.14	1.92	1.82
1	D	689	GLU	CD-OE1	6.14	1.32	1.25
1	D	766	SER	CB-OG	6.13	1.50	1.42
1	A	666	GLU	CD-OE2	6.12	1.32	1.25
1	D	386	GLU	CG-CD	6.09	1.61	1.51
1	B	230	GLU	CD-OE1	6.08	1.32	1.25
1	D	1012	GLU	CD-OE1	6.08	1.32	1.25
1	D	892	GLU	CG-CD	6.07	1.61	1.51
1	A	950	GLU	CD-OE2	6.07	1.32	1.25
1	C	367	PHE	CD2-CE2	6.07	1.51	1.39
1	A	354	CYS	CB-SG	6.07	1.92	1.82
1	C	181	LYS	CD-CE	6.06	1.66	1.51
1	D	421	GLU	CD-OE2	6.06	1.32	1.25
1	C	976	GLU	CD-OE2	6.05	1.32	1.25
1	B	330	SER	CB-OG	6.05	1.50	1.42
1	C	695	CYS	CB-SG	6.05	1.92	1.82
1	C	909	ARG	CG-CD	6.05	1.67	1.51
1	D	449	GLU	CD-OE1	6.04	1.32	1.25
1	D	2	ALA	CA-CB	6.02	1.65	1.52
1	D	180	GLU	CD-OE2	6.02	1.32	1.25
1	D	1005	VAL	CB-CG2	-6.01	1.40	1.52
1	B	658	GLU	CG-CD	6.01	1.60	1.51
1	B	363	PHE	CB-CG	-6.00	1.41	1.51
1	C	180	GLU	CD-OE1	6.00	1.32	1.25
1	B	386	GLU	CD-OE1	6.00	1.32	1.25
1	D	561	ARG	CZ-NH1	5.99	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	13	GLU	CD-OE2	5.97	1.32	1.25
1	B	487	ASN	CB-CG	5.97	1.64	1.51
1	C	424	ASP	CB-CG	5.96	1.64	1.51
1	D	751	TRP	CB-CG	5.96	1.60	1.50
1	C	627	GLU	CB-CG	5.95	1.63	1.52
1	C	950	GLU	CB-CG	5.95	1.63	1.52
1	C	576	PHE	CG-CD1	5.95	1.47	1.38
1	A	363	PHE	CE1-CZ	5.95	1.48	1.37
1	A	382	GLU	CG-CD	5.93	1.60	1.51
1	C	839	TYR	CE1-CZ	-5.93	1.30	1.38
1	C	564	PHE	CE1-CZ	5.92	1.48	1.37
1	A	627	GLU	CD-OE2	5.92	1.32	1.25
1	D	376	GLU	CG-CD	5.92	1.60	1.51
1	A	589	ARG	CZ-NH2	5.91	1.40	1.33
1	C	19	ASN	CB-CG	5.91	1.64	1.51
1	A	491	GLU	CD-OE1	5.89	1.32	1.25
1	D	658	GLU	CD-OE2	5.89	1.32	1.25
1	B	234	PHE	CE2-CZ	5.86	1.48	1.37
1	A	137	VAL	CB-CG1	-5.85	1.40	1.52
1	C	696	ARG	CZ-NH1	5.85	1.40	1.33
1	B	353	ARG	CZ-NH1	5.84	1.40	1.33
1	D	246	GLU	CG-CD	5.84	1.60	1.51
1	A	695	CYS	CB-SG	5.84	1.92	1.82
1	D	589	ARG	CZ-NH2	5.82	1.40	1.33
1	A	643	CYS	CB-SG	-5.82	1.72	1.81
1	A	386	GLU	CD-OE1	5.81	1.32	1.25
1	C	893	GLU	CG-CD	5.81	1.60	1.51
1	C	378	GLU	CD-OE2	5.80	1.32	1.25
1	C	467	GLU	CD-OE1	5.80	1.32	1.25
1	C	565	GLU	CD-OE2	5.79	1.32	1.25
1	B	847	GLN	CG-CD	5.78	1.64	1.51
1	D	263	GLU	CD-OE2	5.78	1.32	1.25
1	D	371	ARG	CZ-NH2	5.78	1.40	1.33
1	A	386	GLU	CG-CD	5.77	1.60	1.51
1	B	180	GLU	CD-OE2	5.76	1.31	1.25
1	D	375	GLU	CG-CD	5.76	1.60	1.51
1	C	180	GLU	CD-OE2	5.76	1.31	1.25
1	C	647	LYS	CE-NZ	5.76	1.63	1.49
1	D	300	ASP	CB-CG	5.75	1.63	1.51
1	A	611	GLU	CD-OE1	5.74	1.31	1.25
1	C	696	ARG	CG-CD	5.74	1.66	1.51
1	C	652	GLU	CG-CD	5.73	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	LYS	CG-CD	5.73	1.72	1.52
1	A	882	TYR	CB-CG	-5.72	1.43	1.51
1	B	707	PHE	CE1-CZ	5.72	1.48	1.37
1	C	703	GLN	CB-CG	5.72	1.68	1.52
1	D	467	GLU	CD-OE1	5.71	1.31	1.25
1	B	13	GLU	CD-OE2	5.71	1.31	1.25
1	D	367	PHE	CE1-CZ	5.71	1.48	1.37
1	B	874	LYS	CB-CG	5.71	1.68	1.52
1	B	666	GLU	CD-OE1	5.71	1.31	1.25
1	D	541	LYS	CE-NZ	5.70	1.63	1.49
1	D	861	LYS	CE-NZ	5.68	1.63	1.49
1	C	984	ASP	CB-CG	5.68	1.63	1.51
1	B	69	GLU	CD-OE2	5.67	1.31	1.25
1	D	908	GLU	CG-CD	5.67	1.60	1.51
1	A	56	GLU	CG-CD	5.65	1.60	1.51
1	B	656	LYS	CD-CE	5.65	1.65	1.51
1	B	276	TYR	CB-CG	-5.65	1.43	1.51
1	D	800	GLU	CD-OE1	5.65	1.31	1.25
1	D	558	SER	CB-OG	5.64	1.49	1.42
1	B	986	CYS	CB-SG	5.63	1.91	1.82
1	A	951	GLU	CG-CD	5.63	1.60	1.51
1	D	475	TRP	CZ3-CH2	5.62	1.49	1.40
1	D	455	LYS	CG-CD	5.62	1.71	1.52
1	D	244	GLU	CG-CD	5.62	1.60	1.51
1	D	726	GLU	CD-OE1	5.62	1.31	1.25
1	C	658	GLU	CG-CD	5.62	1.60	1.51
1	A	689	GLU	CD-OE1	5.61	1.31	1.25
1	D	74	ARG	CZ-NH1	5.61	1.40	1.33
1	B	244	GLU	CD-OE2	5.61	1.31	1.25
1	A	119	ASP	CB-CG	5.61	1.63	1.51
1	B	287	GLU	CD-OE1	5.61	1.31	1.25
1	C	383	GLU	CD-OE2	5.61	1.31	1.25
1	D	714	VAL	CB-CG1	-5.60	1.41	1.52
1	A	289	LYS	CE-NZ	5.60	1.63	1.49
1	D	222	TYR	CZ-OH	5.60	1.47	1.37
1	B	184	GLU	CD-OE1	5.59	1.31	1.25
1	A	272	LYS	CE-NZ	5.59	1.63	1.49
1	B	371	ARG	CB-CG	5.59	1.67	1.52
1	D	520	GLU	CB-CG	-5.59	1.41	1.52
1	B	574	LYS	CE-NZ	5.58	1.62	1.49
1	B	637	VAL	CB-CG1	5.58	1.64	1.52
1	D	844	GLU	CD-OE2	5.57	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	337	VAL	CB-CG1	5.57	1.64	1.52
1	B	884	GLU	CD-OE1	5.57	1.31	1.25
1	D	342	ASP	CG-OD2	5.56	1.38	1.25
1	C	845	GLU	CD-OE1	5.56	1.31	1.25
1	D	186	TYR	CE2-CZ	5.56	1.45	1.38
1	B	800	GLU	CD-OE1	5.56	1.31	1.25
1	D	611	GLU	CD-OE2	5.55	1.31	1.25
1	C	937	GLU	CG-CD	5.55	1.60	1.51
1	A	81	LYS	CE-NZ	5.54	1.62	1.49
1	C	857	GLU	CD-OE2	5.53	1.31	1.25
1	B	371	ARG	CD-NE	5.53	1.55	1.46
1	A	875	LYS	CE-NZ	5.53	1.62	1.49
1	B	909	ARG	CZ-NH1	5.53	1.40	1.33
1	C	367	PHE	CD1-CE1	5.53	1.50	1.39
1	B	893	GLU	CG-CD	5.51	1.60	1.51
1	C	666	GLU	CD-OE2	5.50	1.31	1.25
1	C	287	GLU	CD-OE2	5.50	1.31	1.25
1	C	382	GLU	CD-OE1	5.50	1.31	1.25
1	D	643	CYS	CB-SG	-5.50	1.72	1.81
1	C	828	GLN	CD-NE2	5.49	1.46	1.32
1	D	863	LYS	CE-NZ	5.49	1.62	1.49
1	B	367	PHE	CD2-CE2	5.48	1.50	1.39
1	B	935	PHE	CE2-CZ	5.46	1.47	1.37
1	D	230	GLU	CD-OE2	5.46	1.31	1.25
1	A	467	GLU	CB-CG	5.46	1.62	1.52
1	C	958	LYS	CD-CE	5.46	1.64	1.51
1	B	1005	VAL	CB-CG2	-5.45	1.41	1.52
1	C	276	TYR	CG-CD1	-5.44	1.32	1.39
1	B	564	PHE	CG-CD1	5.43	1.46	1.38
1	C	745	LYS	CE-NZ	5.43	1.62	1.49
1	A	211	TYR	CD2-CE2	-5.41	1.31	1.39
1	D	627	GLU	CG-CD	5.41	1.60	1.51
1	D	385	CYS	CB-SG	5.41	1.91	1.82
1	C	800	GLU	CG-CD	5.41	1.60	1.51
1	A	162	VAL	CB-CG2	5.41	1.64	1.52
1	C	887	LYS	CE-NZ	5.40	1.62	1.49
1	B	586	VAL	CB-CG1	5.40	1.64	1.52
1	D	703	GLN	CD-NE2	5.39	1.46	1.32
1	A	53	GLU	CD-OE1	5.39	1.31	1.25
1	A	130	CYS	CB-SG	5.39	1.91	1.82
1	C	556	SER	CB-OG	5.39	1.49	1.42
1	C	514	SER	CB-OG	5.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	402	ARG	CZ-NH1	5.38	1.40	1.33
1	C	520	GLU	CD-OE2	5.38	1.31	1.25
1	A	161	GLU	CB-CG	5.37	1.62	1.52
1	A	927	LYS	CD-CE	5.37	1.64	1.51
1	C	589	ARG	CZ-NH2	5.37	1.40	1.33
1	B	611	GLU	CD-OE1	5.36	1.31	1.25
1	D	844	GLU	CD-OE1	5.36	1.31	1.25
1	D	184	GLU	CB-CG	5.36	1.62	1.52
1	A	464	VAL	CB-CG2	-5.35	1.41	1.52
1	B	227	SER	CB-OG	-5.35	1.35	1.42
1	D	576	PHE	CB-CG	5.34	1.60	1.51
1	A	680	MET	CG-SD	5.33	1.95	1.81
1	C	326	SER	CB-OG	5.33	1.49	1.42
1	D	677	GLU	CD-OE2	5.33	1.31	1.25
1	A	884	GLU	CG-CD	5.33	1.59	1.51
1	A	892	GLU	CG-CD	5.32	1.59	1.51
1	C	246	GLU	CG-CD	5.32	1.59	1.51
1	C	565	GLU	CD-OE1	5.32	1.31	1.25
1	D	221	GLU	CD-OE1	5.32	1.31	1.25
1	A	146	GLU	CB-CG	5.31	1.62	1.52
1	B	800	GLU	CD-OE2	5.31	1.31	1.25
1	D	69	GLU	CD-OE2	5.31	1.31	1.25
1	C	525	TYR	CE2-CZ	5.31	1.45	1.38
1	A	158	PHE	CE1-CZ	5.31	1.47	1.37
1	C	300	ASP	CG-OD1	5.31	1.37	1.25
1	C	21	ARG	CZ-NH1	5.30	1.40	1.33
1	D	2	ALA	CA-C	5.30	1.66	1.52
1	B	505	LYS	CE-NZ	5.29	1.62	1.49
1	B	927	LYS	CD-CE	5.29	1.64	1.51
1	A	689	GLU	CD-OE2	5.29	1.31	1.25
1	B	376	GLU	CG-CD	5.29	1.59	1.51
1	B	857	GLU	CB-CG	5.28	1.62	1.52
1	C	561	ARG	CG-CD	5.28	1.65	1.51
1	B	402	ARG	CZ-NH2	5.28	1.40	1.33
1	A	762	TYR	CD2-CE2	-5.28	1.31	1.39
1	C	844	GLU	CD-OE1	5.28	1.31	1.25
1	D	875	LYS	CD-CE	5.28	1.64	1.51
1	A	376	GLU	CD-OE2	5.27	1.31	1.25
1	C	965	ASP	CB-CG	5.27	1.62	1.51
1	C	147	GLU	CG-CD	5.27	1.59	1.51
1	B	824	PHE	CE1-CZ	5.26	1.47	1.37
1	D	958	LYS	CG-CD	5.26	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	899	GLU	CG-CD	5.26	1.59	1.51
1	B	434	VAL	CB-CG1	-5.26	1.41	1.52
1	B	273	GLU	CG-CD	5.26	1.59	1.51
1	D	375	GLU	CB-CG	5.26	1.62	1.52
1	C	1007	ARG	CB-CG	-5.25	1.38	1.52
1	B	375	GLU	CG-CD	5.25	1.59	1.51
1	B	180	GLU	CG-CD	5.25	1.59	1.51
1	C	376	GLU	CG-CD	5.25	1.59	1.51
1	D	74	ARG	CB-CG	-5.25	1.38	1.52
1	D	574	LYS	CB-CG	-5.24	1.38	1.52
1	B	322	CYS	CB-SG	-5.24	1.73	1.81
1	D	870	GLU	CG-CD	5.22	1.59	1.51
1	A	246	GLU	CG-CD	5.22	1.59	1.51
1	C	656	LYS	CD-CE	5.22	1.64	1.51
1	C	140	CYS	CB-SG	5.22	1.91	1.82
1	C	632	PHE	CE1-CZ	5.22	1.47	1.37
1	A	147	GLU	CG-CD	5.21	1.59	1.51
1	A	835	LYS	CB-CG	5.21	1.66	1.52
1	A	419	TRP	CB-CG	-5.19	1.41	1.50
1	A	910	LYS	CD-CE	5.19	1.64	1.51
1	C	221	GLU	CD-OE2	5.18	1.31	1.25
1	B	888	LYS	CE-NZ	5.18	1.61	1.49
1	A	726	GLU	CD-OE1	5.17	1.31	1.25
1	A	703	GLN	CB-CG	-5.17	1.38	1.52
1	C	276	TYR	CE1-CZ	-5.16	1.31	1.38
1	B	56	GLU	CB-CG	-5.16	1.42	1.52
1	C	35	LYS	CE-NZ	5.16	1.61	1.49
1	B	611	GLU	CD-OE2	5.15	1.31	1.25
1	D	74	ARG	CZ-NH2	5.15	1.39	1.33
1	D	502	TYR	CG-CD1	5.14	1.45	1.39
1	A	240	VAL	CB-CG2	-5.13	1.42	1.52
1	D	697	TRP	CB-CG	-5.13	1.41	1.50
1	D	246	GLU	CD-OE1	5.12	1.31	1.25
1	B	960	TYR	CD2-CE2	5.12	1.47	1.39
1	C	607	PHE	CE2-CZ	5.10	1.47	1.37
1	A	885	GLN	CG-CD	5.09	1.62	1.51
1	A	382	GLU	CD-OE1	5.09	1.31	1.25
1	D	181	LYS	CE-NZ	5.09	1.61	1.49
1	B	367	PHE	CE1-CZ	5.09	1.47	1.37
1	C	13	GLU	CD-OE1	5.09	1.31	1.25
1	A	963	CYS	CB-SG	5.09	1.90	1.82
1	A	414	ASP	CB-CG	5.08	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	257	CYS	CB-SG	-5.08	1.73	1.81
1	D	358	ARG	CZ-NH2	5.07	1.39	1.33
1	C	53	GLU	CD-OE2	5.07	1.31	1.25
1	D	718	VAL	CB-CG2	-5.07	1.42	1.52
1	B	627	GLU	CG-CD	5.05	1.59	1.51
1	C	805	PHE	CB-CG	-5.05	1.42	1.51
1	D	415	GLU	CB-CG	5.05	1.61	1.52
1	C	42	LYS	CD-CE	5.05	1.63	1.51
1	C	117	PHE	CE1-CZ	-5.04	1.27	1.37
1	C	234	PHE	CB-CG	5.04	1.59	1.51
1	C	564	PHE	CD2-CE2	5.04	1.49	1.39
1	D	870	GLU	CD-OE1	5.04	1.31	1.25
1	A	830	TYR	CE1-CZ	-5.04	1.32	1.38
1	D	611	GLU	CB-CG	5.04	1.61	1.52
1	A	443	ARG	CZ-NH1	5.03	1.39	1.33
1	C	383	GLU	CG-CD	5.03	1.59	1.51
1	B	1011	TYR	CE1-CZ	-5.03	1.32	1.38
1	D	167	ASN	CB-CG	-5.02	1.39	1.51
1	D	875	LYS	CB-CG	5.02	1.66	1.52
1	A	13	GLU	CD-OE1	5.01	1.31	1.25
1	A	217	PHE	CE2-CZ	5.00	1.46	1.37
1	D	581	ASP	CB-CG	5.00	1.62	1.51

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ASP	CB-CG-OD2	-13.09	106.52	118.30
1	A	175	CYS	CA-CB-SG	-12.75	91.05	114.00
1	B	52	CYS	CA-CB-SG	-11.29	93.67	114.00
1	D	60	ASP	CB-CG-OD1	11.24	128.42	118.30
1	C	1015	ARG	NE-CZ-NH2	-10.93	114.84	120.30
1	D	561	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	D	561	ARG	NE-CZ-NH2	-10.67	114.96	120.30
1	C	562	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	C	208	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	C	965	ASP	CB-CG-OD2	10.54	127.79	118.30
1	C	219	LYS	CD-CE-NZ	-10.53	87.47	111.70
1	D	402	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	D	562	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	D	115	MET	CG-SD-CE	9.97	116.15	100.20
1	A	460	ASP	CB-CG-OD1	9.94	127.25	118.30
1	B	909	ARG	NE-CZ-NH2	-9.83	115.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	432	ASP	CB-CG-OD1	9.54	126.89	118.30
1	C	562	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	B	239	ASP	CB-CG-OD2	9.40	126.76	118.30
1	D	346	ASP	CB-CG-OD1	9.37	126.73	118.30
1	A	981	THR	CA-CB-CG2	-9.21	99.50	112.40
1	D	776	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	C	1015	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	D	797	ASP	CB-CG-OD1	8.78	126.20	118.30
1	D	432	ASP	CB-CG-OD2	-8.77	110.40	118.30
1	D	11	ASP	CB-CG-OD1	8.72	126.15	118.30
1	C	208	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	C	634	ASP	CB-CG-OD1	8.54	125.98	118.30
1	C	346	ASP	CB-CG-OD1	8.50	125.95	118.30
1	A	78	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	A	324	CYS	CA-CB-SG	8.32	128.98	114.00
1	D	932	LEU	CB-CG-CD2	-8.24	97.00	111.00
1	B	239	ASP	CB-CG-OD1	-8.14	110.97	118.30
1	C	446	LYS	CD-CE-NZ	8.13	130.39	111.70
1	D	771	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	909	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	D	923	ASP	CB-CG-OD1	-7.92	111.18	118.30
1	D	663	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	D	797	ASP	CB-CG-OD2	-7.72	111.36	118.30
1	A	722	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	D	353	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	599	MET	CA-CB-CG	-7.62	100.35	113.30
1	B	741	LEU	CB-CG-CD1	-7.43	98.37	111.00
1	C	361	LEU	CB-CG-CD2	-7.40	98.43	111.00
1	A	70	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	A	246	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	D	364	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	C	747	ASP	CB-CG-OD2	7.36	124.92	118.30
1	C	384	LYS	CD-CE-NZ	-7.35	94.80	111.70
1	A	342	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	B	371	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	A	776	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	B	780	THR	OG1-CB-CG2	-7.19	93.46	110.00
1	A	771	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	687	ASP	CB-CG-OD1	7.14	124.72	118.30
1	D	213	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	692	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	B	529	ASP	CB-CG-OD2	7.04	124.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	D	663	ASP	CB-CG-OD1	7.00	124.60	118.30
1	C	710	LEU	CB-CG-CD1	-6.96	99.17	111.00
1	A	291	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	B	458	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	D	265	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	B	346	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	338	LEU	CB-CG-CD1	-6.91	99.25	111.00
1	B	395	LYS	CD-CE-NZ	6.84	127.44	111.70
1	C	741	LEU	CB-CG-CD1	-6.84	99.37	111.00
1	C	432	ASP	CB-CG-OD1	6.83	124.45	118.30
1	B	1017	LEU	CA-CB-CG	6.79	130.91	115.30
1	A	674	GLY	N-CA-C	6.78	130.05	113.10
1	C	505	LYS	CD-CE-NZ	-6.76	96.14	111.70
1	A	342	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	371	ARG	CA-CB-CG	6.71	128.15	113.40
1	C	172	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	D	451	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	C	485	MET	CG-SD-CE	-6.68	89.50	100.20
1	D	634	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	239	ASP	CB-CG-OD2	6.62	124.26	118.30
1	D	60	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	C	827	ILE	CG1-CB-CG2	-6.59	96.91	111.40
1	B	297	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	B	365	LYS	CD-CE-NZ	-6.58	96.57	111.70
1	A	249	LYS	CD-CE-NZ	-6.54	96.67	111.70
1	C	669	LEU	CA-CB-CG	-6.52	100.30	115.30
1	D	250	ASP	CB-CG-OD1	-6.50	112.44	118.30
1	C	122	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	C	1007	ARG	CG-CD-NE	-6.48	98.19	111.80
1	D	37	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	C	28	LEU	CB-CG-CD1	-6.46	100.02	111.00
1	A	831	CYS	CA-CB-SG	-6.45	102.39	114.00
1	D	741	LEU	CB-CG-CD2	-6.40	100.11	111.00
1	D	426	ILE	CG1-CB-CG2	-6.40	97.32	111.40
1	A	78	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	B	578	LEU	CA-CB-CG	-6.39	100.59	115.30
1	C	74	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	932	LEU	CB-CG-CD1	-6.33	100.23	111.00
1	D	628	LEU	CB-CG-CD1	-6.31	100.28	111.00
1	C	239	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	46	ASP	CB-CG-OD1	6.28	123.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	C	909	ARG	C-N-CA	-6.25	106.09	121.70
1	A	682	LEU	CB-CG-CD1	6.24	121.61	111.00
1	A	239	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	835	LYS	CD-CE-NZ	-6.20	97.44	111.70
1	B	771	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	172	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	61	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	932[A]	LEU	CB-CG-CD1	-6.10	100.62	111.00
1	C	932[B]	LEU	CB-CG-CD1	-6.10	100.62	111.00
1	C	835	LYS	CD-CE-NZ	-6.08	97.71	111.70
1	D	363	PHE	CB-CG-CD1	-6.06	116.56	120.80
1	B	839	TYR	CZ-CE2-CD2	-6.05	114.36	119.80
1	C	1003	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	771	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	300	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	579	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	B	371	ARG	CG-CD-NE	5.99	124.37	111.80
1	A	443	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	371	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	D	54	LYS	CB-CG-CD	5.97	127.13	111.60
1	B	922	LYS	CD-CE-NZ	-5.97	97.98	111.70
1	C	759	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	1008	THR	C-N-CA	5.96	136.59	121.70
1	B	189	LYS	CD-CE-NZ	-5.94	98.04	111.70
1	B	937	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	C	371	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	C	1003	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	B	5	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	D	730	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	342	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	B	332	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	481	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	C	540	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	D	669	LEU	CA-CB-CG	-5.78	102.01	115.30
1	A	910	LYS	CD-CE-NZ	5.76	124.94	111.70
1	B	43	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	C	965	ASP	OD1-CG-OD2	-5.69	112.48	123.30
1	D	612	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	A	455	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	C	435	ILE	CG1-CB-CG2	5.66	123.84	111.40
1	D	300	ASP	CB-CG-OD2	5.65	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	682	LEU	CB-CG-CD1	5.63	120.57	111.00
1	D	690	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	A	671	CYS	CA-CB-SG	-5.59	103.93	114.00
1	B	687	ASP	CB-CG-OD1	5.58	123.33	118.30
1	D	599	MET	CG-SD-CE	-5.58	91.28	100.20
1	B	929	LEU	CA-CB-CG	-5.57	102.49	115.30
1	B	353	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	872	MET	CG-SD-CE	5.56	109.10	100.20
1	D	465	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	B	289	LYS	CD-CE-NZ	5.54	124.43	111.70
1	B	532	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	812	VAL	CG1-CB-CG2	-5.53	102.05	110.90
1	D	722	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	213	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	412	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	B	776	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	759	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	1003	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	283	ILE	C-N-CA	-5.50	110.75	122.30
1	B	155	LEU	CB-CG-CD2	5.49	120.34	111.00
1	C	581	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	D	519	PRO	CA-N-CD	5.49	119.39	111.70
1	B	495	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	665	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	B	424	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	402	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	984	ASP	CB-CG-OD1	5.46	123.22	118.30
1	C	414	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	923	ASP	CB-CG-OD2	5.45	123.21	118.30
1	D	43	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	B	691	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	A	631	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	977	THR	CA-CB-CG2	5.42	119.99	112.40
1	A	850	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	61	ASP	CB-CG-OD1	5.41	123.17	118.30
1	D	49	CYS	CA-CB-SG	-5.40	104.27	114.00
1	D	115	MET	CA-CB-CG	-5.40	104.12	113.30
1	C	984	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	1015	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	C	776	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	C	155	LEU	CB-CG-CD1	-5.39	101.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	529	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	189	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	C	937	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	D	172	ARG	CB-CG-CD	-5.37	97.64	111.60
1	A	680	MET	CG-SD-CE	5.36	108.77	100.20
1	C	363	PHE	CB-CA-C	-5.35	99.70	110.40
1	B	277	LYS	CD-CE-NZ	5.33	123.97	111.70
1	B	517	ALA	C-N-CA	-5.33	108.38	121.70
1	D	357	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	161	GLU	OE1-CD-OE2	5.32	129.68	123.30
1	C	455	LYS	CD-CE-NZ	-5.31	99.48	111.70
1	C	337	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	A	1007	ARG	CG-CD-NE	-5.28	100.71	111.80
1	C	898	LYS	CD-CE-NZ	-5.28	99.56	111.70
1	B	771	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	410	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	D	794	GLY	N-CA-C	-5.27	99.92	113.10
1	D	523	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	B	924	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	B	927	LYS	CD-CE-NZ	5.24	123.75	111.70
1	D	984	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	308	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	193	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	394	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	929	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	A	213	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	189	LYS	CD-CE-NZ	-5.21	99.73	111.70
1	A	371	ARG	CG-CD-NE	5.19	122.70	111.80
1	C	230	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	D	37	ASP	CB-CG-OD1	5.18	122.97	118.30
1	C	974	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	762	TYR	CG-CD2-CE2	-5.16	117.17	121.30
1	C	78	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	C	371	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	459	TRP	CA-CB-CG	-5.15	103.91	113.70
1	B	134	ASP	CB-CG-OD1	5.14	122.92	118.30
1	C	572	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	530	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	B	887	LYS	CB-CG-CD	-5.13	98.26	111.60
1	A	667	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	C	579	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	B	653	LEU	CB-CG-CD1	-5.11	102.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	887	LYS	CD-CE-NZ	-5.11	99.94	111.70
1	D	361	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	D	932	LEU	CA-CB-CG	-5.10	103.57	115.30
1	A	806	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	C	172	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	984	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	1000	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	760	THR	CA-CB-CG2	-5.07	105.31	112.40
1	D	458	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	62	ILE	CG1-CB-CG2	5.05	122.52	111.40
1	B	759	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	279	ALA	N-CA-CB	5.02	117.13	110.10
1	B	220	GLN	N-CA-CB	-5.02	101.57	110.60
1	C	308	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	B	874	LYS	CB-CG-CD	5.01	124.63	111.60
1	D	984	ASP	OD1-CG-OD2	-5.01	113.78	123.30
1	A	974	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	D	67	LEU	CA-CB-CG	-5.01	103.78	115.30
1	B	561	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	ASP	Peptide
1	A	418	LYS	Peptide
1	A	672	PRO	Peptide
1	B	324	CYS	Peptide
1	B	415	GLU	Peptide
1	B	954	ILE	Peptide
1	C	264	ASN	Peptide
1	C	325	HIS	Peptide
1	C	416	THR	Peptide
1	D	1009	THR	Peptide
1	D	415	GLU	Peptide
1	D	486	ALA	Peptide
1	D	676	GLY	Peptide
1	D	677	GLU	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	7678	0	7707	128	0
1	B	7688	0	7715	147	1
1	C	7741	0	7767	156	0
1	D	7750	0	7781	143	1
2	A	32	0	0	2	0
2	B	32	0	0	1	0
2	C	32	0	0	1	0
2	D	32	0	0	0	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	C	31	0	19	2	0
3	D	31	0	19	4	0
4	A	53	0	31	2	0
4	B	53	0	31	2	0
4	C	53	0	31	1	0
4	D	53	0	31	1	0
5	A	10	0	0	1	0
5	B	10	0	0	2	0
5	C	10	0	0	2	0
5	D	10	0	0	1	0
6	A	529	0	0	26	0
6	B	490	0	0	28	1
6	C	593	0	0	25	2
6	D	559	0	0	30	1
All	All	33532	0	31170	538	3

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 9.

All (538) 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:371:ARG:CG	1:B:371:ARG:CD	1.74	1.65
1:D:265:GLU:CG	1:D:265:GLU:CB	1.76	1.56
1:C:60:ASP:CG	1:C:60:ASP:CB	1.76	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LYS:NZ	1:A:541:LYS:CE	1.70	1.52
1:D:265:GLU:CG	1:D:265:GLU:CD	1.79	1.50
1:C:956:CYS:CB	1:C:956:CYS:SG	2.01	1.46
1:A:956:CYS:CB	1:A:956:CYS:SG	2.07	1.42
1:B:449:GLU:OE1	6:B:1201:HOH:O	1.53	1.22
1:A:399:LYS:NZ	6:A:1201:HOH:O	1.77	1.15
1:A:1007:ARG:NH1	6:A:1202:HOH:O	1.89	1.04
1:C:410[B]:ARG:HD2	1:D:427:VAL:HG22	1.43	1.01
1:C:391:LEU:HD23	1:C:410[B]:ARG:HH12	1.23	1.00
1:C:54:LYS:NZ	6:C:1204:HOH:O	1.97	0.98
1:D:675:MET:O	1:D:678:ARG:NH2	1.97	0.97
1:A:54:LYS:HE2	1:A:54:LYS:HA	1.46	0.97
1:B:414:ASP:HB3	1:B:415:GLU:OE1	1.66	0.95
1:B:520:GLU:OE2	6:B:1202:HOH:O	1.86	0.92
1:C:172:ARG:NH2	6:C:1208:HOH:O	2.02	0.91
1:A:430:LYS:NZ	6:A:1205:HOH:O	2.02	0.89
1:C:861:LYS:NZ	6:C:1213:HOH:O	2.05	0.88
1:D:299:GLN:OE1	6:D:1202:HOH:O	1.91	0.88
1:D:52:CYS:SG	6:D:1345:HOH:O	2.33	0.87
1:A:901:ASN:ND2	6:A:1209:HOH:O	2.08	0.86
1:C:331:ILE:HD12	1:C:433:VAL:HG21	1.58	0.85
1:D:273:GLU:OE1	6:D:1203:HOH:O	1.94	0.84
1:C:722:ARG:NH1	6:C:1201:HOH:O	1.72	0.84
1:C:324:CYS:O	6:C:1203:HOH:O	1.97	0.83
1:B:119:ASP:OD2	6:B:1203:HOH:O	1.97	0.83
1:D:443:ARG:NE	6:D:1209:HOH:O	2.10	0.82
1:B:39:LYS:NZ	6:B:1207:HOH:O	2.13	0.82
1:C:365:LYS:HE2	1:C:419:TRP:NE1	1.94	0.82
1:D:1009:THR:HB	1:D:1010:PRO:HD3	1.61	0.81
1:A:872:MET:O	6:A:1203:HOH:O	1.99	0.81
1:B:416:THR:HG23	1:B:418:LYS:HB2	1.61	0.81
1:C:783:ARG:HD3	6:C:1202:HOH:O	1.82	0.80
1:A:249:LYS:NZ	6:A:1213:HOH:O	2.16	0.79
1:A:324:CYS:SG	6:A:1700:HOH:O	2.41	0.79
1:A:1006:SER:O	6:A:1204:HOH:O	2.00	0.78
1:A:923:ASP:OD1	1:D:937:GLU:HG2	1.83	0.78
1:B:415:GLU:HB2	1:B:416:THR:HG22	1.66	0.77
1:B:1018:PRO:O	6:B:1204:HOH:O	2.01	0.77
1:C:631:ASP:OD2	6:C:1207:HOH:O	2.01	0.77
1:A:964:ASN:OD1	6:A:1206:HOH:O	2.03	0.77
1:D:866:PRO:HB2	1:D:868:ILE:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLU:O	1:A:416:THR:OG1	2.02	0.76
1:B:875:LYS:NZ	6:B:1209:HOH:O	2.18	0.76
1:C:402:ARG:NH2	6:C:1216:HOH:O	2.19	0.76
1:D:394:ARG:NH1	1:D:421:GLU:OE1	2.18	0.76
1:C:391:LEU:CD2	1:C:410[B]:ARG:HH12	1.98	0.75
1:C:443:ARG:NH2	6:C:1214:HOH:O	2.10	0.75
1:C:173:ASN:OD1	6:C:1211:HOH:O	2.04	0.75
1:C:391:LEU:HD23	1:C:410[B]:ARG:NH1	2.00	0.74
1:B:828:GLN:NE2	6:B:1211:HOH:O	2.20	0.74
1:C:410[B]:ARG:HD2	1:D:427:VAL:CG2	2.17	0.74
1:D:666:GLU:OE1	6:D:1205:HOH:O	2.06	0.74
1:C:872:MET:O	6:C:1210:HOH:O	2.04	0.74
1:A:173:ASN:OD1	6:A:1207:HOH:O	2.05	0.74
1:A:577:SER:O	6:A:1208:HOH:O	2.05	0.74
1:B:167[B]:ASN:OD1	1:B:911:PRO:HA	1.88	0.73
1:D:716:ASP:OD2	6:D:1204:HOH:O	2.05	0.73
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.69	0.73
1:D:131:PRO:HB2	1:D:373:VAL:HG11	1.69	0.73
1:D:722:ARG:NH2	6:D:1206:HOH:O	2.08	0.72
1:A:457:ASN:HB3	1:A:463:GLU:HG3	1.72	0.72
1:B:1018:PRO:O	6:B:1205:HOH:O	2.05	0.72
1:D:371:ARG:NH1	6:D:1211:HOH:O	2.20	0.72
1:B:901:ASN:ND2	6:B:1212:HOH:O	2.21	0.72
1:D:658:GLU:OE1	6:D:1207:HOH:O	2.09	0.71
1:A:673:HIS:O	6:A:1210:HOH:O	2.09	0.70
1:C:322:CYS:SG	1:C:324:CYS:HB2	2.32	0.70
1:B:976:GLU:OE2	6:B:1206:HOH:O	2.09	0.69
1:A:427:VAL:HG22	1:B:410[B]:ARG:HD2	1.73	0.69
1:A:520:GLU:HG2	1:B:25:HIS:CE1	2.27	0.69
1:D:645:TYR:O	6:D:1208:HOH:O	2.09	0.69
1:A:175:CYS:SG	6:A:1207:HOH:O	2.38	0.68
1:C:368[A]:VAL:HG13	1:D:386:GLU:OE2	1.94	0.68
1:D:652:GLU:OE2	6:D:1210:HOH:O	2.12	0.67
1:B:272:LYS:NZ	6:B:1216:HOH:O	2.26	0.67
1:C:881:PRO:HA	1:C:884:GLU:HG3	1.77	0.67
1:D:844:GLU:O	1:D:847:GLN:HG3	1.95	0.67
1:A:793:THR:HB	1:A:814:GLN:HB2	1.77	0.66
2:A:1101:SF4:FE2	2:A:1101:SF4:S1	1.86	0.66
1:D:179:GLN:NE2	6:D:1219:HOH:O	2.28	0.66
1:C:381:LYS:NZ	1:D:381:LYS:NZ	2.44	0.66
1:D:13:GLU:CD	6:D:1215:HOH:O	2.34	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLU:C	1:B:417:GLY:H	2.00	0.65
1:D:399:LYS:HD2	1:D:404:VAL:HG21	1.78	0.65
1:B:841:LYS:NZ	6:B:1218:HOH:O	2.28	0.65
1:B:943:GLN:HB2	1:B:1007:ARG:HD3	1.77	0.65
1:B:841:LYS:NZ	6:B:1215:HOH:O	2.26	0.65
1:D:1010:PRO:HA	6:D:1432:HOH:O	1.97	0.65
1:D:443:ARG:CZ	6:D:1209:HOH:O	2.42	0.65
1:D:678:ARG:NH1	6:D:1223:HOH:O	2.30	0.64
1:A:274:GLU:OE2	6:A:1212:HOH:O	2.15	0.64
1:C:793:THR:HG22	1:C:814:GLN:HB2	1.79	0.64
1:C:365:LYS:HE2	1:C:419:TRP:CD1	2.33	0.64
1:B:230:GLU:OE1	6:B:1208:HOH:O	2.15	0.64
1:D:487:ASN:ND2	6:D:1222:HOH:O	2.29	0.64
1:D:343:THR:HA	4:D:1106:FAD:HM73	1.80	0.64
1:D:395:LYS:HE2	1:D:407:GLN:OE1	1.97	0.64
1:B:60:ASP:OD1	1:B:894:LYS:NZ	2.21	0.63
1:D:263:GLU:HG3	1:D:449:GLU:HB3	1.80	0.63
2:C:1101:SF4:FE2	2:C:1101:SF4:S1	1.90	0.63
1:A:178:SER:OG	1:A:180:GLU:OE2	2.15	0.63
1:A:54:LYS:HD3	1:A:56:GLU:H	1.64	0.62
1:A:458:ARG:NH1	1:A:459:TRP:CZ2	2.68	0.62
1:B:842:SER:OG	1:B:914:PRO:HB3	2.00	0.62
2:A:1101:SF4:FE4	2:A:1101:SF4:S3	1.92	0.62
2:B:1101:SF4:FE1	2:B:1101:SF4:S3	1.91	0.62
1:C:321:MET:HG2	1:C:322:CYS:HB2	1.81	0.62
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.82	0.61
1:C:762:TYR:OH	1:D:779[B]:THR:HG22	2.00	0.61
1:D:299:GLN:HB3	6:D:1202:HOH:O	2.00	0.61
1:D:180:GLU:OE2	1:D:180:GLU:N	2.22	0.61
1:A:261:LEU:HD21	1:A:451:LEU:HD21	1.82	0.61
1:D:779[B]:THR:HG21	1:D:932:LEU:HD13	1.83	0.61
1:D:332:ARG:HG2	1:D:332:ARG:HH11	1.65	0.61
1:B:358:ARG:HG3	1:B:358:ARG:HH11	1.66	0.61
1:A:373:VAL:HG23	1:A:375:GLU:HG2	1.83	0.60
1:A:866:PRO:HB2	1:A:868:ILE:HD12	1.82	0.60
1:C:381:LYS:NZ	1:D:381:LYS:HZ1	1.99	0.60
1:C:373:VAL:HG12	1:D:47:LYS:HD3	1.84	0.60
1:C:741:LEU:HD23	1:D:775[B]:LEU:HG	1.83	0.60
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.37	0.60
1:C:536:GLU:H	1:C:922:LYS:HE3	1.66	0.60
1:D:1009:THR:CB	1:D:1010:PRO:HD3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410[B]:ARG:NH2	1:C:427:VAL:HG23	2.16	0.60
1:C:364:ARG:HG3	1:C:364:ARG:HH11	1.67	0.60
1:D:330:SER:O	1:D:330:SER:OG	2.17	0.60
1:B:775:LEU:O	1:B:779:THR:HG23	2.02	0.59
1:D:164:LYS:NZ	1:D:239:ASP:OD2	2.26	0.59
1:C:177:PRO:HG2	1:C:182:MET:SD	2.42	0.59
1:C:834:LEU:HD21	1:C:921:ILE:HD11	1.83	0.59
1:A:457:ASN:HB3	1:A:463:GLU:CG	2.33	0.59
1:C:12:ILE:HA	1:C:15:ILE:HG22	1.83	0.59
1:B:200:ILE:HD13	1:B:245:ILE:HD11	1.83	0.59
1:B:200:ILE:CD1	1:B:245:ILE:HD11	2.33	0.58
1:A:343:THR:HA	4:A:1106:FAD:HM73	1.84	0.58
1:B:416:THR:CG2	1:B:418:LYS:HB2	2.33	0.58
1:B:872:MET:O	1:B:874:LYS:HG3	2.03	0.58
1:B:954:ILE:HD13	1:B:998:ILE:HD11	1.86	0.58
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.39	0.58
1:D:188:ALA:HB1	1:D:277:LYS:HG3	1.84	0.58
1:B:1007:ARG:HD2	6:B:1530:HOH:O	2.03	0.58
1:D:178:SER:HB3	1:D:181:LYS:HE2	1.86	0.57
1:D:307:LYS:NZ	1:D:440:SER:OG	2.25	0.57
1:A:241:VAL:O	1:A:245[A]:ILE:HG13	2.05	0.57
1:A:365:LYS:HG2	1:A:419:TRP:CZ2	2.40	0.57
1:C:340:ALA:HB2	1:C:363:PHE:CD2	2.39	0.57
1:D:643:CYS:HB2	1:D:650:TRP:CE2	2.39	0.57
6:C:1337:HOH:O	1:D:430:LYS:HG2	2.05	0.57
1:A:52:CYS:HB3	1:A:384:LYS:HG2	1.87	0.56
1:C:320:GLY:O	1:C:322:CYS:N	2.38	0.56
1:B:613:ILE:HG22	5:B:1107:Y3G:C10	2.36	0.56
1:B:307:LYS:HE2	1:B:440:SER:OG	2.05	0.56
1:B:875:LYS:HE2	6:B:1209:HOH:O	2.06	0.56
1:C:412:GLU:OE2	1:D:430:LYS:NZ	2.39	0.56
1:B:875:LYS:CE	6:B:1209:HOH:O	2.54	0.56
1:B:394:ARG:NH2	1:B:423:GLU:OE1	2.39	0.55
1:B:718:VAL:HG21	1:B:780:THR:HG22	1.86	0.55
1:C:432:ASP:OD2	6:C:1215:HOH:O	2.18	0.55
1:B:249:LYS:HE3	1:B:255:ILE:HD12	1.87	0.55
1:C:391:LEU:CD2	1:C:410[B]:ARG:NH1	2.62	0.55
1:A:985:THR:HG22	1:A:1014:LYS:NZ	2.22	0.55
1:A:74:ARG:NH2	6:A:1229:HOH:O	2.30	0.55
1:A:948:ILE:HD13	1:A:980:PRO:HG2	1.89	0.55
1:B:415:GLU:O	1:B:417:GLY:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLU:O	1:C:273:GLU:HG2	2.07	0.55
1:B:219:LYS:HG3	1:B:260:SER:OG	2.06	0.55
1:B:413:GLN:HG3	1:B:419:TRP:CE2	2.42	0.55
1:B:413:GLN:HG2	1:B:417:GLY:O	2.07	0.55
1:C:577[A]:SER:HB3	6:C:1380:HOH:O	2.05	0.55
1:A:394:ARG:NH2	1:A:423:GLU:OE2	2.37	0.55
1:B:57:ASN:ND2	1:B:898:LYS:HB2	2.21	0.55
1:A:367:PHE:CE2	1:A:370:ILE:HD12	2.42	0.55
1:C:52:CYS:HB2	1:C:383:GLU:O	2.07	0.55
1:C:316:SER:OG	1:C:326:SER:O	2.19	0.55
1:C:779[A]:THR:HG22	1:C:808:SER:HB3	1.89	0.55
1:A:175:CYS:SG	1:A:176:LEU:N	2.80	0.54
1:D:205:PHE:CE1	1:D:497:LYS:HG3	2.42	0.54
1:C:124:LEU:HG	1:C:240:VAL:HG13	1.90	0.54
1:C:358:ARG:HD2	6:C:1460:HOH:O	2.06	0.54
1:D:263:GLU:O	1:D:264:ASN:HB2	2.08	0.54
1:C:613:ILE:HG22	5:C:1107:Y3G:C10	2.37	0.54
1:D:394:ARG:NH2	1:D:421:GLU:OE1	2.40	0.54
1:B:1010:PRO:HD2	1:B:1010:PRO:O	2.08	0.54
1:C:89:LYS:HD2	1:D:41:TRP:CE2	2.43	0.54
1:C:381:LYS:HZ2	1:D:381:LYS:HZ1	1.55	0.54
1:D:793:THR:HG22	3:D:1105:FMN:O5'	2.07	0.54
1:B:219:LYS:O	1:B:220:GLN:O	2.26	0.54
1:A:428:HIS:O	1:B:410[A]:ARG:NH1	2.40	0.53
1:B:663:ASP:OD2	6:B:1210:HOH:O	2.19	0.53
1:D:1009:THR:HB	1:D:1010:PRO:CD	2.37	0.53
1:A:828:GLN:HG2	1:B:22:THR:HG21	1.91	0.53
1:C:387:PHE:N	1:C:387:PHE:CD1	2.76	0.53
1:A:828:GLN:CG	1:B:22:THR:HG21	2.38	0.53
1:B:343:THR:HA	4:B:1106:FAD:HM73	1.89	0.53
1:C:137:VAL:HG12	6:C:1286:HOH:O	2.08	0.53
1:B:415:GLU:C	1:B:417:GLY:N	2.63	0.52
1:D:371:ARG:NH1	6:D:1212:HOH:O	2.20	0.52
1:D:415:GLU:C	1:D:417:GLY:N	2.62	0.52
1:C:783:ARG:NH1	6:C:1202:HOH:O	1.95	0.52
1:D:291:ASP:OD2	1:D:293:ILE:HG23	2.08	0.52
1:B:413:GLN:HG3	1:B:419:TRP:CZ2	2.44	0.52
1:B:1008:THR:OG1	1:B:1009:THR:N	2.40	0.52
1:A:316:SER:OG	1:A:328:LEU:HD23	2.09	0.52
1:A:945:VAL:HG13	1:A:1007:ARG:HG3	1.92	0.52
1:B:172:ARG:HG3	6:B:1545:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ARG:NH1	6:D:1211:HOH:O	2.42	0.52
1:A:534:SER:HB2	1:A:541:LYS:HE3	1.91	0.52
1:B:218:GLU:OE1	4:B:1106:FAD:H1B	2.10	0.52
1:A:13:GLU:HG2	6:A:1280:HOH:O	2.09	0.52
1:A:627:GLU:HB3	6:A:1222:HOH:O	2.10	0.52
1:B:193:LEU:N	1:B:193:LEU:HD22	2.25	0.52
1:C:340:ALA:HB2	1:C:363:PHE:HD2	1.73	0.52
1:C:834:LEU:HD21	1:C:921:ILE:CD1	2.40	0.52
1:B:269:ASN:O	1:B:273:GLU:CD	2.49	0.51
1:A:362:VAL:HG22	1:A:388:LEU:HB2	1.92	0.51
1:A:424:ASP:OD1	1:A:424:ASP:N	2.41	0.51
1:B:97:ILE:HA	1:B:100:PHE:CD2	2.46	0.51
1:D:438:PHE:HA	6:D:1212:HOH:O	2.10	0.51
1:D:468:THR:HA	1:D:502:TYR:CD1	2.45	0.51
1:B:218:GLU:O	1:B:219:LYS:O	2.29	0.51
1:C:47:LYS:HD3	1:D:373:VAL:HG12	1.93	0.51
1:C:190:ILE:HD13	1:C:206:LEU:HD13	1.92	0.51
1:C:381:LYS:HZ2	1:D:381:LYS:NZ	2.09	0.51
1:B:570:PHE:HB2	1:B:636:ILE:HB	1.93	0.51
1:A:910:LYS:HG2	1:A:911:PRO:HD2	1.93	0.50
1:B:948:ILE:HD13	1:B:980:PRO:HG2	1.93	0.50
1:C:552:ALA:HB2	3:C:1105:FMN:HM73	1.93	0.50
1:C:656:LYS:NZ	6:C:1241:HOH:O	2.43	0.50
1:D:287:GLU:OE2	1:D:444:ASP:HB2	2.12	0.50
1:A:412:GLU:OE1	1:B:430:LYS:NZ	2.35	0.50
1:C:710:LEU:HD22	1:C:720:ILE:HG22	1.91	0.50
1:B:329:PRO:O	1:B:354:CYS:HB3	2.11	0.50
1:A:416:THR:HB	1:A:418:LYS:HE2	1.94	0.50
1:D:574:LYS:HB3	1:D:614:SER:HB2	1.94	0.50
1:D:779[B]:THR:CG2	1:D:932:LEU:HD13	2.41	0.50
1:D:915:LYS:HG2	6:D:1241:HOH:O	2.09	0.50
1:B:410[B]:ARG:NH1	6:B:1214:HOH:O	2.23	0.50
1:A:394:ARG:HH22	1:A:423:GLU:CD	2.16	0.50
1:C:22:THR:HG22	1:C:23:GLN:N	2.27	0.50
1:D:180:GLU:H	1:D:180:GLU:CD	2.11	0.49
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.93	0.49
1:C:325:HIS:NE2	1:C:901:ASN:ND2	2.60	0.49
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.12	0.49
1:C:956:CYS:SG	1:C:956:CYS:CA	2.96	0.49
1:A:219:LYS:HE3	6:A:1691:HOH:O	2.11	0.49
1:A:272:LYS:NZ	6:A:1240:HOH:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:TYR:CE1	1:D:999:ILE:HD11	2.48	0.49
1:C:613:ILE:CG2	5:C:1107:Y3G:C10	2.90	0.49
1:C:97:ILE:HA	1:C:100:PHE:CD2	2.48	0.49
1:A:517:ALA:O	1:A:519:PRO:HD3	2.11	0.49
1:C:577[B]:SER:HB2	6:C:1380:HOH:O	2.13	0.49
1:C:846:LEU:HD22	1:C:849:TRP:CE2	2.48	0.49
1:D:340:ALA:HB2	1:D:363:PHE:CD1	2.48	0.49
1:D:613:ILE:HG22	5:D:1107:Y3G:C10	2.42	0.49
1:A:44:ASN:HB2	1:A:45:PRO:HD2	1.95	0.49
1:B:643:CYS:HB2	1:B:650:TRP:CD2	2.48	0.49
1:B:471:THR:HB	6:B:1410:HOH:O	2.11	0.49
1:B:793:THR:HB	1:B:814:GLN:HB2	1.95	0.49
1:C:1011:TYR:OH	6:C:1205:HOH:O	1.98	0.49
1:A:124:LEU:HD13	1:A:160:SER:HB2	1.95	0.48
1:A:972:GLN:O	1:A:980:PRO:HA	2.12	0.48
1:C:371:ARG:NH2	6:C:1248:HOH:O	2.46	0.48
1:C:593:GLY:HA3	1:C:606:SER:OG	2.13	0.48
1:D:834:LEU:HD21	1:D:921:ILE:HD11	1.94	0.48
1:A:367:PHE:CD1	1:B:367:PHE:CZ	3.01	0.48
1:C:381:LYS:HZ3	1:D:381:LYS:NZ	2.11	0.48
1:C:536:GLU:H	1:C:922:LYS:CE	2.25	0.48
1:C:686:GLN:HG2	1:C:714:VAL:CG1	2.43	0.48
1:B:221:GLU:O	1:B:221:GLU:HG2	2.13	0.48
1:B:718:VAL:CG2	1:B:780:THR:HG22	2.44	0.48
1:B:341:GLY:HA2	1:B:371:ARG:HB3	1.95	0.48
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.96	0.48
1:C:816:CYS:HB3	3:C:1105:FMN:O1P	2.13	0.48
1:D:394:ARG:CZ	1:D:421:GLU:OE1	2.61	0.48
1:D:962[A]:THR:CG2	1:D:991:LEU:HB3	2.44	0.48
1:A:97:ILE:HA	1:A:100:PHE:CD2	2.49	0.48
1:A:364:ARG:NH2	6:A:1255:HOH:O	2.46	0.48
1:B:204:SER:O	1:B:208:ARG:HG3	2.14	0.48
1:D:552:ALA:HB3	1:D:553:PRO:HD3	1.95	0.47
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.71	0.47
1:A:291:ASP:OD1	1:A:293:ILE:HG23	2.14	0.47
1:A:959:CYS:O	1:A:962[B]:THR:HG22	2.14	0.47
1:A:1007:ARG:CD	1:A:1011:TYR:HB2	2.44	0.47
1:D:395:LYS:HE2	1:D:407:GLN:CD	2.35	0.47
1:D:673:HIS:HB2	1:D:675:MET:HG2	1.94	0.47
1:B:311:PRO:O	1:B:315:LYS:HG3	2.14	0.47
1:B:410[A]:ARG:HG2	1:B:411:THR:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:THR:HA	4:C:1106:FAD:HM73	1.96	0.47
1:D:331:ILE:HD12	1:D:433:VAL:HG11	1.96	0.47
1:D:753:ALA:HB1	1:D:758:LYS:HA	1.96	0.47
1:A:958:LYS:HA	1:A:961:MET:HE2	1.97	0.47
1:D:866:PRO:CB	1:D:868:ILE:HD12	2.42	0.47
1:A:119:ASP:OD1	1:B:26:ALA:HB1	2.14	0.47
1:A:191:ALA:O	1:A:279:ALA:HA	2.15	0.47
1:A:381:LYS:HG3	1:A:387:PHE:HE1	1.79	0.47
1:B:335:VAL:HG22	1:B:433:VAL:HB	1.96	0.47
1:B:915:LYS:HZ3	1:B:915:LYS:HG3	1.50	0.47
1:D:962[B]:THR:HB	6:D:1201:HOH:O	2.14	0.47
1:A:730:ASP:OD1	6:A:1215:HOH:O	2.20	0.47
1:C:416:THR:OG1	1:C:418:LYS:HB2	2.15	0.47
1:D:69:GLU:OE1	6:D:1213:HOH:O	2.20	0.47
1:A:900:GLN:NE2	6:A:1264:HOH:O	2.47	0.47
1:A:858:SER:HB3	1:A:949:ASP:OD2	2.15	0.46
1:B:29:HIS:HB2	6:B:1516:HOH:O	2.16	0.46
1:B:443:ARG:NH2	6:B:1246:HOH:O	2.47	0.46
1:B:868:ILE:O	1:B:872:MET:HG2	2.14	0.46
1:C:410[B]:ARG:CD	1:D:427:VAL:HG22	2.29	0.46
1:D:962[A]:THR:HG21	1:D:991:LEU:HB3	1.96	0.46
1:C:122:LEU:N	1:C:122:LEU:HD12	2.30	0.46
1:C:124:LEU:HG	1:C:240:VAL:CG1	2.45	0.46
1:D:793:THR:HG21	3:D:1105:FMN:H3'	1.97	0.46
1:A:613:ILE:HG23	5:A:1107:Y3G:C10	2.46	0.46
1:C:686:GLN:HG2	1:C:714:VAL:HG12	1.96	0.46
1:A:756:ALA:N	1:B:942:GLU:OE1	2.38	0.46
1:D:572:LEU:HD13	1:D:638:ILE:HB	1.97	0.46
1:A:601:GLY:HA2	1:B:995:VAL:O	2.16	0.46
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.82	0.46
1:B:578:LEU:HA	1:B:578:LEU:HD23	1.54	0.46
1:B:183:PRO:HD2	1:B:186:TYR:CD1	2.51	0.46
1:B:845:GLU:HG3	1:B:912:PHE:CE2	2.50	0.46
1:B:899:GLU:O	1:B:900:GLN:HG3	2.16	0.46
1:B:779:THR:HG22	1:B:808:SER:HB3	1.97	0.46
1:B:869:ALA:HB3	1:B:870:GLU:OE1	2.15	0.46
1:C:582:ILE:HG21	1:D:1019:LEU:HD11	1.97	0.46
1:D:289:LYS:HG3	1:D:441:VAL:HG13	1.97	0.45
1:A:281:ILE:HD12	1:A:281:ILE:HG23	1.79	0.45
1:B:517:ALA:O	1:B:519:PRO:HD3	2.16	0.45
1:D:261:LEU:O	1:D:262:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:HIS:HE1	1:A:976:GLU:O	2.00	0.45
1:A:367:PHE:HD1	1:B:367:PHE:CZ	2.33	0.45
1:C:452:SER:HA	1:C:453:PRO:HA	1.73	0.45
1:B:526:THR:HB	1:B:527:PRO:HD2	1.98	0.45
1:C:246:GLU:OE2	1:C:908:GLU:HG2	2.16	0.45
1:D:373:VAL:HG13	6:D:1586:HOH:O	2.17	0.45
1:D:381:LYS:NZ	6:D:1257:HOH:O	2.50	0.45
1:B:687:ASP:HB3	1:B:690:LEU:HD12	1.99	0.45
1:C:1007:ARG:CD	1:C:1011:TYR:HB2	2.47	0.45
1:D:643:CYS:HB2	1:D:650:TRP:CD2	2.52	0.45
1:B:365:LYS:HG2	1:B:419:TRP:CH2	2.52	0.45
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	1.98	0.45
1:C:425:GLN:HG2	1:D:426:ILE:HD12	1.98	0.45
1:B:451:LEU:O	1:B:454:ILE:HG12	2.17	0.45
1:C:416:THR:HB	1:C:418:LYS:HE2	1.97	0.45
1:C:990:THR:O	1:C:990:THR:HG22	2.17	0.45
1:A:485:MET:HE2	1:B:31:THR:HG22	1.99	0.45
1:B:991:LEU:HD23	1:B:991:LEU:HA	1.73	0.45
1:C:735:THR:O	1:C:793:THR:OG1	2.35	0.45
1:D:868:ILE:O	1:D:871:LEU:N	2.33	0.45
1:A:932:LEU:HD22	1:B:760:THR:HG22	1.99	0.44
1:B:929:LEU:HD23	1:B:929:LEU:HA	1.76	0.44
1:A:18:LEU:HD11	1:A:975:PRO:HA	1.98	0.44
1:B:220:GLN:HB3	1:B:222:TYR:CE2	2.52	0.44
1:A:192:LEU:C	1:A:193:LEU:HD22	2.38	0.44
1:C:132:THR:HB	1:C:137:VAL:HG23	2.00	0.44
1:A:916:LYS:HB2	1:A:916:LYS:HE2	1.57	0.44
1:B:414:ASP:CB	1:B:415:GLU:OE1	2.54	0.44
1:B:415:GLU:OE1	1:B:415:GLU:N	2.50	0.44
1:D:410:ARG:HG2	1:D:411:THR:N	2.31	0.44
1:A:734:ALA:HA	1:A:735:THR:HA	1.71	0.44
1:B:562:ARG:HH11	1:B:562:ARG:HD2	1.66	0.44
1:A:947[A]:VAL:HG12	1:A:1003:ARG:O	2.18	0.44
1:B:1010:PRO:O	1:B:1010:PRO:CD	2.65	0.44
1:D:423:GLU:OE1	1:D:423:GLU:HA	2.18	0.44
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.82	0.44
1:B:193:LEU:HD23	1:B:281:ILE:HD13	1.98	0.44
1:B:528:VAL:O	1:B:531:VAL:HG23	2.18	0.44
1:B:880:GLY:HA3	1:B:881:PRO:HD2	1.82	0.44
1:D:443:ARG:CD	6:D:1209:HOH:O	2.61	0.44
1:D:193:LEU:N	1:D:193:LEU:HD22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:VAL:HB	1:D:612:LEU:CD1	2.47	0.44
1:A:293:ILE:HD11	1:A:393:PRO:HB2	2.00	0.44
1:C:283:ILE:HG13	1:C:482:ILE:HD12	2.00	0.44
1:D:885:GLN:O	1:D:889:ILE:HD12	2.18	0.44
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.65	0.43
1:B:577[A]:SER:HB3	6:B:1312:HOH:O	2.19	0.43
1:C:501:TRP:O	1:C:504:HIS:HB3	2.19	0.43
1:C:629:LYS:HA	1:C:629:LYS:HD2	1.80	0.43
1:D:688:PRO:HD3	1:D:720:ILE:CD1	2.47	0.43
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.18	0.43
1:B:613:ILE:CG2	5:B:1107:Y3G:C10	2.96	0.43
1:C:410[B]:ARG:HH11	1:C:410[B]:ARG:HD3	1.43	0.43
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	2.00	0.43
1:B:629:LYS:HE2	1:B:629:LYS:HA	2.00	0.43
1:B:776:ARG:NH1	6:B:1264:HOH:O	2.51	0.43
1:C:320:GLY:O	1:C:321:MET:C	2.56	0.43
1:C:623:GLN:HB3	1:D:5:LEU:HD12	2.00	0.43
1:C:207:ALA:HB1	1:C:251:LEU:HB3	2.00	0.43
1:D:205:PHE:CZ	1:D:497:LYS:HG3	2.53	0.43
1:D:402:ARG:NH2	6:D:1263:HOH:O	2.51	0.43
1:A:24:SER:OG	1:A:25:HIS:CD2	2.72	0.43
1:B:220:GLN:H	1:B:220:GLN:HG2	1.30	0.43
1:D:734:ALA:HA	1:D:735:THR:HA	1.79	0.43
1:B:681:GLY:C	1:B:682:LEU:HD23	2.39	0.43
1:C:696:ARG:NH1	1:C:696:ARG:HB2	2.33	0.43
1:A:381:LYS:HG3	1:A:387:PHE:CE1	2.53	0.43
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.79	0.43
1:B:124:LEU:HD13	1:B:160:SER:HB2	1.99	0.43
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.84	0.43
1:C:486:ALA:HB1	1:C:491:GLU:OE1	2.18	0.43
1:B:52:CYS:SG	1:B:383:GLU:HA	2.58	0.43
1:C:731:GLY:HA2	1:C:788:PHE:CZ	2.54	0.43
1:D:418:LYS:HG2	1:D:419:TRP:N	2.34	0.43
1:A:90:SER:HB2	1:A:136:CYS:HA	2.00	0.43
1:A:941:ILE:HD13	1:A:941:ILE:HA	1.67	0.43
1:B:289:LYS:HD2	1:B:438:PHE:O	2.19	0.43
1:B:869:ALA:C	1:B:871:LEU:H	2.21	0.43
1:B:972:GLN:O	1:B:980:PRO:HA	2.17	0.43
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.81	0.43
1:D:583:VAL:HB	1:D:612:LEU:HD13	2.01	0.43
1:A:9:VAL:HG12	1:A:11:ASP:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:CE2	1:B:89:LYS:HD2	2.54	0.42
1:A:283:ILE:HG21	1:A:283:ILE:HD13	1.77	0.42
1:A:598:PRO:HB2	1:B:73:LEU:HD13	2.01	0.42
1:B:182:MET:HE3	1:B:186:TYR:CD1	2.54	0.42
1:C:267:THR:OG1	1:C:270:THR:HG23	2.18	0.42
1:C:410[B]:ARG:HH21	1:C:427:VAL:HG23	1.82	0.42
1:C:572:LEU:HD13	1:C:638:ILE:HB	2.00	0.42
1:A:537:MET:HG3	1:A:789:PRO:HB3	2.00	0.42
1:A:776:ARG:O	1:A:780:THR:HG22	2.18	0.42
1:C:122:LEU:HD13	1:C:493:VAL:HG22	2.01	0.42
1:C:540:LEU:HA	1:C:540:LEU:HD23	1.75	0.42
1:C:941:ILE:HG21	1:C:941:ILE:HD13	1.81	0.42
1:D:290:THR:HA	6:D:1464:HOH:O	2.20	0.42
1:A:193:LEU:HD22	1:A:193:LEU:N	2.34	0.42
1:C:231:ILE:HA	1:C:232:PRO:HD3	1.81	0.42
1:C:549:ALA:HB2	1:C:814:GLN:HB3	2.01	0.42
1:D:458:ARG:C	1:D:460:ASP:H	2.22	0.42
1:A:231:ILE:HG21	1:A:231:ILE:HD13	1.71	0.42
1:A:521:LEU:HD23	1:A:521:LEU:HA	1.78	0.42
1:A:880:GLY:HA3	1:A:881:PRO:HD2	1.81	0.42
1:B:574:LYS:HB3	1:B:614:SER:HB2	2.01	0.42
1:C:410[B]:ARG:HB2	1:C:425:GLN:HB2	2.01	0.42
1:A:913:ILE:HG23	1:A:913:ILE:HD12	1.75	0.42
1:C:172:ARG:NH1	1:C:177:PRO:O	2.53	0.42
3:D:1105:FMN:H1'2	3:D:1105:FMN:H9	1.80	0.42
1:A:204:SER:O	1:A:208:ARG:HG3	2.20	0.42
1:C:416:THR:OG1	1:C:418:LYS:N	2.36	0.42
1:C:444:ASP:HA	1:C:445:PRO:HD3	1.93	0.42
1:A:552:ALA:HB3	1:A:820:GLN:OE1	2.19	0.42
1:C:410[B]:ARG:HG2	1:C:425:GLN:HB3	2.00	0.42
1:D:204:SER:O	1:D:208:ARG:HG3	2.20	0.42
1:B:587:SER:HA	1:B:588:PRO:C	2.40	0.42
1:C:865:VAL:CG1	1:C:866:PRO:HD2	2.50	0.42
1:D:54:LYS:HE2	1:D:56:GLU:HB2	2.01	0.42
1:C:118:SER:HA	1:C:524:PHE:HB2	2.02	0.42
1:D:234:PHE:CE2	1:D:353:ARG:HD3	2.55	0.42
1:D:364:ARG:HH12	1:D:371:ARG:HH11	1.68	0.42
1:D:518:LYS:HA	1:D:519:PRO:HD2	1.67	0.42
1:D:831:CYS:O	1:D:835:LYS:HG3	2.20	0.42
1:D:868:ILE:O	1:D:868:ILE:HG22	2.20	0.42
1:D:885:GLN:NE2	6:D:1273:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:929:LEU:HA	1:D:929:LEU:HD23	1.81	0.42
1:B:365:LYS:HB3	1:B:419:TRP:CH2	2.55	0.41
1:C:1009:THR:HA	1:C:1010:PRO:HD3	1.72	0.41
1:D:784:ALA:O	1:D:786:PRO:HD3	2.20	0.41
1:B:1007:ARG:HD2	1:B:1007:ARG:HH11	1.68	0.41
1:C:381:LYS:NZ	1:D:381:LYS:HZ3	2.16	0.41
1:C:553:PRO:O	1:C:559:MET:HE2	2.21	0.41
1:A:485:MET:O	1:B:35:LYS:HE3	2.21	0.41
1:A:568:TRP:CE2	1:A:827:ILE:HB	2.56	0.41
1:B:570:PHE:CB	1:B:636:ILE:HB	2.51	0.41
1:C:314:ALA:HB1	1:C:318:LYS:HD2	2.02	0.41
1:D:220:GLN:HG3	1:D:222:TYR:CZ	2.55	0.41
1:A:373:VAL:HB	1:A:374:PRO:HD2	2.01	0.41
1:A:910:LYS:HD3	1:A:911:PRO:N	2.35	0.41
1:C:22:THR:OG1	6:C:1212:HOH:O	2.05	0.41
1:C:692:ARG:HH11	1:C:692:ARG:HD2	1.67	0.41
1:C:1007:ARG:NE	1:C:1011:TYR:HB2	2.35	0.41
1:D:621:TRP:O	1:D:625:VAL:HG23	2.21	0.41
1:B:806:LEU:HD13	1:B:921:ILE:HG23	2.03	0.41
1:C:1015:ARG:HD3	1:D:615:GLU:O	2.20	0.41
1:C:1017:LEU:CA	6:C:1217:HOH:O	2.68	0.41
1:C:92:PRO:HA	1:D:34:LYS:HG3	2.02	0.41
1:C:948:ILE:HD13	1:C:980:PRO:HG2	2.02	0.41
1:D:793:THR:HG21	3:D:1105:FMN:C3'	2.51	0.41
1:B:107:LYS:HB3	6:B:1348:HOH:O	2.20	0.41
1:C:281[B]:ILE:HD11	1:C:476:VAL:CG1	2.50	0.41
1:C:378:GLU:HG2	6:C:1693:HOH:O	2.20	0.41
1:A:181:LYS:HA	1:A:181:LYS:HD2	1.78	0.41
1:A:485:MET:HB2	6:A:1471:HOH:O	2.20	0.41
1:B:594:THR:HB	6:B:1368:HOH:O	2.19	0.41
1:B:927:LYS:NZ	6:B:1257:HOH:O	2.49	0.41
1:C:329:PRO:O	1:C:354:CYS:HB3	2.21	0.41
1:D:692:ARG:O	1:D:696:ARG:HG3	2.20	0.41
1:D:791:LEU:N	1:D:791:LEU:HD12	2.36	0.41
1:A:143:TYR:HB2	1:A:149:SER:OG	2.21	0.41
1:A:448:LYS:HG3	1:A:456:PHE:CZ	2.56	0.41
1:B:219:LYS:O	1:B:220:GLN:C	2.59	0.41
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.84	0.41
1:C:331:ILE:O	1:C:332:ARG:HG2	2.21	0.41
1:C:379:LEU:HD23	1:C:379:LEU:HA	1.85	0.41
1:C:865:VAL:HG12	1:C:866:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:LEU:HD23	1:C:929:LEU:HA	1.79	0.41
1:C:948:ILE:HD13	1:C:948:ILE:HG21	1.81	0.41
1:D:1019:LEU:HD23	1:D:1019:LEU:HA	1.72	0.41
1:A:115:MET:HE3	6:A:1495:HOH:O	2.21	0.41
1:A:346:ASP:OD2	4:A:1106:FAD:H6	2.20	0.41
1:A:486:ALA:HB3	6:A:1298:HOH:O	2.21	0.41
1:A:629:LYS:HD2	1:A:629:LYS:HA	1.91	0.41
1:C:18:LEU:HD21	1:C:975:PRO:HA	2.03	0.41
1:C:414:ASP:OD1	1:C:416:THR:HG23	2.21	0.41
1:C:477:PHE:CD1	1:C:477:PHE:N	2.89	0.41
1:C:840:LEU:HD23	1:C:840:LEU:HA	1.93	0.41
1:C:897:LEU:HD23	1:C:897:LEU:HA	1.90	0.41
1:A:187[B]:SER:OG	6:A:1214:HOH:O	2.20	0.40
1:B:842:SER:HA	1:B:916:LYS:HG2	2.02	0.40
1:C:27:ALA:O	1:D:497:LYS:HE2	2.21	0.40
1:D:329:PRO:O	1:D:354:CYS:HB3	2.21	0.40
1:A:876:LEU:HA	1:A:877:PRO:HD2	1.90	0.40
1:A:934:THR:OG1	1:A:937:GLU:OE2	2.30	0.40
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.86	0.40
1:B:613:ILE:HG21	1:B:613:ILE:HD13	1.68	0.40
1:C:22:THR:CG2	1:C:23:GLN:N	2.83	0.40
1:D:235:ARG:HH11	1:D:235:ARG:HD2	1.76	0.40
1:D:651:MET:HE3	1:D:700:GLN:HG3	2.03	0.40
1:D:868:ILE:HB	1:D:871:LEU:HD12	2.03	0.40
1:A:454:ILE:O	1:A:454:ILE:HG13	2.20	0.40
1:B:200:ILE:HD13	1:B:245:ILE:CD1	2.51	0.40
1:C:345:PHE:HE2	1:C:387:PHE:HE2	1.70	0.40
1:C:643:CYS:HB2	1:C:650:TRP:CD1	2.56	0.40
1:C:734:ALA:HA	1:C:735:THR:HA	1.88	0.40
1:C:837:LEU:HD23	1:C:837:LEU:HA	1.93	0.40
1:C:1017:LEU:N	6:C:1217:HOH:O	2.44	0.40
1:D:176:LEU:HD23	1:D:176:LEU:HA	1.91	0.40
1:A:325:HIS:ND1	1:A:325:HIS:N	2.70	0.40
1:B:255:ILE:HD13	1:B:255:ILE:HG21	1.83	0.40
1:B:869:ALA:O	1:B:871:LEU:N	2.52	0.40
1:A:682:LEU:HD12	1:A:683:ALA:N	2.36	0.40
1:B:303:PHE:HD1	1:B:434:VAL:HG13	1.86	0.40
1:B:593:GLY:HA3	1:B:606:SER:OG	2.21	0.40
1:C:237:PRO:HB2	1:C:239:ASP:OD2	2.21	0.40
1:C:320:GLY:C	1:C:322:CYS:N	2.72	0.40
1:D:294:PHE:HA	1:D:297:LEU:HD12	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:O	1:D:677:GLU:OE1[2_746]	2.00	0.20
6:B:1634:HOH:O	6:C:1560:HOH:O[2_746]	2.15	0.05
6:C:1758:HOH:O	6:D:1728:HOH:O[1_655]	2.15	0.05

## 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	1003/1025 (98%)	955 (95%)	41 (4%)	7 (1%)	22	16
1	B	1003/1025 (98%)	942 (94%)	49 (5%)	12 (1%)	13	7
1	C	1017/1025 (99%)	972 (96%)	43 (4%)	2 (0%)	47	44
1	D	1017/1025 (99%)	964 (95%)	41 (4%)	12 (1%)	13	7
All	All	4040/4100 (98%)	3833 (95%)	174 (4%)	33 (1%)	19	13

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
1	A	416	THR
1	B	219	LYS
1	B	220	GLN
1	B	324	CYS
1	B	330	SER
1	B	415	GLU
1	B	416	THR
1	B	870	GLU
1	B	900	GLN
1	C	416	THR
1	D	416	THR
1	D	677	GLU

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Mol	Chain	Res	Type
1	D	916	LYS
1	A	53	GLU
1	B	53	GLU
1	B	323	ALA
1	B	869	ALA
1	D	678	ARG
1	A	458	ARG
1	D	869	ALA
1	D	1009	THR
1	A	990	THR
1	B	227	SER
1	C	53	GLU
1	D	3	PRO
1	D	414	ASP
1	D	736	ASN
1	D	908	GLU
1	A	551	ALA
1	D	713	ASN
1	D	675	MET
1	A	3	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	842/854 (99%)	828 (98%)	14 (2%)	60	65
1	B	845/854 (99%)	833 (99%)	12 (1%)	67	72
1	C	852/854 (100%)	833 (98%)	19 (2%)	52	55
1	D	851/854 (100%)	835 (98%)	16 (2%)	57	61
All	All	3390/3416 (99%)	3329 (98%)	61 (2%)	60	63

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS

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Mol	Chain	Res	Type
1	A	100	PHE
1	A	180	GLU
1	A	181	LYS
1	A	325	HIS
1	A	330	SER
1	A	338	LEU
1	A	357	ARG
1	A	367	PHE
1	A	402	ARG
1	A	518	LYS
1	A	608	LEU
1	A	899	GLU
1	A	910	LYS
1	B	47	LYS
1	B	100	PHE
1	B	178	SER
1	B	289	LYS
1	B	324	CYS
1	B	358	ARG
1	B	443	ARG
1	B	460	ASP
1	B	541	LYS
1	B	608	LEU
1	B	932[A]	LEU
1	B	932[B]	LEU
1	C	14	SER
1	C	100	PHE
1	C	172	ARG
1	C	174	PRO
1	C	300	ASP
1	C	327	PRO
1	C	330	SER
1	C	361	LEU
1	C	363	PHE
1	C	367	PHE
1	C	414	ASP
1	C	418	LYS
1	C	608	LEU
1	C	696	ARG
1	C	745	LYS
1	C	915	LYS
1	C	922	LYS

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Mol	Chain	Res	Type
1	C	932[A]	LEU
1	C	932[B]	LEU
1	D	39	LYS
1	D	74	ARG
1	D	100	PHE
1	D	105	SER
1	D	300	ASP
1	D	307	LYS
1	D	322	CYS
1	D	358	ARG
1	D	363	PHE
1	D	364	ARG
1	D	452	SER
1	D	485	MET
1	D	858[A]	SER
1	D	858[B]	SER
1	D	867	ARG
1	D	1014	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	179	GLN
1	A	648	ASN
1	A	859	HIS
1	B	23	GLN
1	B	648	ASN
1	B	885	GLN
1	C	420	ASN
1	C	901	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

28 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$
3	FMN	A	1105	-	31,33,33	2.10	10 (32%)	40,50,50	2.49	11 (27%)
2	SF4	D	1103	1	0,12,12	0.00	-	-	-	-
4	FAD	B	1106	-	51,58,58	1.41	5 (9%)	60,89,89	2.27	11 (18%)
2	SF4	D	1104	1	0,12,12	0.00	-	-	-	-
2	SF4	A	1101	1	0,12,12	0.00	-	-	-	-
2	SF4	D	1102	1	0,12,12	0.00	-	-	-	-
2	SF4	B	1102	1	0,12,12	0.00	-	-	-	-
4	FAD	A	1106	-	51,58,58	1.61	8 (15%)	60,89,89	2.39	11 (18%)
2	SF4	B	1104	1	0,12,12	0.00	-	-	-	-
5	Y3G	B	1107	-	9,10,10	2.38	3 (33%)	6,13,13	7.16	5 (83%)
2	SF4	A	1104	1	0,12,12	0.00	-	-	-	-
2	SF4	D	1101	1	0,12,12	0.00	-	-	-	-
5	Y3G	A	1107	-	9,10,10	2.82	3 (33%)	6,13,13	7.12	4 (66%)
2	SF4	C	1102	1	0,12,12	0.00	-	-	-	-
2	SF4	B	1103	1	0,12,12	0.00	-	-	-	-
5	Y3G	C	1107	-	9,10,10	2.49	1 (11%)	6,13,13	5.03	4 (66%)
4	FAD	D	1106	-	51,58,58	1.31	6 (11%)	60,89,89	2.26	9 (15%)
2	SF4	C	1101	1	0,12,12	0.00	-	-	-	-
5	Y3G	D	1107	-	9,10,10	3.27	3 (33%)	6,13,13	5.57	3 (50%)
3	FMN	B	1105	-	31,33,33	2.83	7 (22%)	40,50,50	2.52	12 (30%)
3	FMN	D	1105	-	31,33,33	1.98	7 (22%)	40,50,50	2.72	13 (32%)
2	SF4	C	1104	1	0,12,12	0.00	-	-	-	-
2	SF4	A	1103	1	0,12,12	0.00	-	-	-	-
2	SF4	A	1102	1	0,12,12	0.00	-	-	-	-
2	SF4	C	1103	1	0,12,12	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SF4	B	1101	1	0,12,12	0.00	-	-		
4	FAD	C	1106	-	51,58,58	1.44	6 (11%)	60,89,89	2.30	9 (15%)
3	FMN	C	1105	-	31,33,33	2.19	11 (35%)	40,50,50	1.87	10 (25%)

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	1105	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1103	1	-	-	0/6/5/5
4	FAD	B	1106	-	-	4/30/50/50	0/6/6/6
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	A	1101	1	-	-	0/6/5/5
4	FAD	A	1106	-	-	3/30/50/50	0/6/6/6
2	SF4	B	1102	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
2	SF4	B	1104	1	-	-	0/6/5/5
5	Y3G	B	1107	-	-	0/0/2/2	0/1/1/1
2	SF4	A	1104	1	-	-	0/6/5/5
2	SF4	D	1101	1	-	-	0/6/5/5
5	Y3G	A	1107	-	-	0/0/2/2	0/1/1/1
2	SF4	C	1102	1	-	-	0/6/5/5
5	Y3G	C	1107	-	-	0/0/2/2	0/1/1/1
2	SF4	B	1103	1	-	-	0/6/5/5
4	FAD	D	1106	-	-	2/30/50/50	0/6/6/6
2	SF4	C	1101	1	-	-	0/6/5/5
5	Y3G	D	1107	-	-	0/0/2/2	0/1/1/1
3	FMN	B	1105	-	-	4/18/18/18	0/3/3/3
3	FMN	D	1105	-	-	2/18/18/18	0/3/3/3
2	SF4	C	1104	1	-	-	0/6/5/5
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
2	SF4	B	1101	1	-	-	0/6/5/5
4	FAD	C	1106	-	-	1/30/50/50	0/6/6/6
3	FMN	C	1105	-	-	2/18/18/18	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1107	Y3G	O08-C01	8.34	1.45	1.24
3	B	1105	FMN	C1'-N10	8.30	1.56	1.48
3	B	1105	FMN	C4A-C10	8.00	1.46	1.38
5	A	1107	Y3G	O08-C01	7.03	1.42	1.24
5	C	1107	Y3G	O08-C01	6.67	1.41	1.24
3	D	1105	FMN	C10-N1	6.62	1.41	1.33
3	B	1105	FMN	C4A-N5	6.55	1.42	1.33
3	C	1105	FMN	C4A-N5	5.90	1.41	1.33
3	A	1105	FMN	C4A-N5	5.89	1.41	1.33
5	B	1107	Y3G	O08-C01	5.72	1.38	1.24
3	B	1105	FMN	C10-N1	5.69	1.40	1.33
4	A	1106	FAD	C4X-C10	5.27	1.44	1.38
4	B	1106	FAD	C4X-C10	5.07	1.43	1.38
4	C	1106	FAD	C4-N3	4.54	1.40	1.33
4	B	1106	FAD	C5X-N5	4.50	1.42	1.35
4	D	1106	FAD	C4-N3	4.47	1.40	1.33
4	A	1106	FAD	C5X-N5	4.42	1.42	1.35
3	C	1105	FMN	C1'-N10	4.39	1.52	1.48
4	C	1106	FAD	C4X-C10	4.27	1.43	1.38
4	B	1106	FAD	C4-N3	4.17	1.40	1.33
4	A	1106	FAD	C4-N3	4.10	1.40	1.33
3	C	1105	FMN	C4A-C10	4.05	1.42	1.38
4	C	1106	FAD	C4X-N5	4.00	1.39	1.33
4	A	1106	FAD	C4-C4X	3.94	1.48	1.41
3	A	1105	FMN	C4A-C10	3.74	1.42	1.38
5	D	1107	Y3G	C06-C09	3.63	1.50	1.43
4	D	1106	FAD	C4X-C10	3.54	1.42	1.38
3	D	1105	FMN	C9-C8	3.43	1.46	1.37
4	C	1106	FAD	C5X-N5	3.37	1.40	1.35
3	A	1105	FMN	C10-N1	3.36	1.37	1.33
4	A	1106	FAD	P-O2P	-3.28	1.39	1.55
3	D	1105	FMN	C4A-N5	3.24	1.38	1.33
3	C	1105	FMN	C10-N1	3.22	1.37	1.33
4	D	1106	FAD	P-O2P	-3.17	1.40	1.55
3	A	1105	FMN	C4-C4A	-3.16	1.35	1.41
3	C	1105	FMN	C5A-N5	3.15	1.40	1.35
4	C	1106	FAD	C1'-N10	3.12	1.51	1.48
3	C	1105	FMN	C4-N3	3.09	1.38	1.33
4	A	1106	FAD	C10-N1	3.05	1.37	1.33
5	B	1107	Y3G	C03-N02	-3.01	1.32	1.38
3	A	1105	FMN	C1'-N10	3.01	1.51	1.48
5	A	1107	Y3G	C06-C09	3.00	1.49	1.43
4	D	1106	FAD	C1'-N10	-2.83	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1105	FMN	C5A-N5	2.77	1.39	1.35
3	B	1105	FMN	C4-N3	2.75	1.37	1.33
3	A	1105	FMN	C9A-C5A	-2.69	1.37	1.42
3	D	1105	FMN	C6-C7	2.55	1.44	1.37
4	C	1106	FAD	C9A-N10	2.54	1.41	1.38
4	A	1106	FAD	C1'-N10	2.53	1.50	1.48
3	C	1105	FMN	C8M-C8	2.49	1.56	1.51
5	D	1107	Y3G	C03-N02	-2.49	1.33	1.38
5	A	1107	Y3G	C03-N04	-2.49	1.33	1.38
5	B	1107	Y3G	C03-N04	-2.44	1.33	1.38
4	D	1106	FAD	O4B-C1B	-2.41	1.37	1.41
3	C	1105	FMN	C7M-C7	-2.37	1.46	1.51
3	B	1105	FMN	C2-N3	2.33	1.42	1.38
3	D	1105	FMN	C2-N1	-2.28	1.33	1.38
3	B	1105	FMN	C6-C5A	-2.27	1.38	1.41
3	A	1105	FMN	C9-C8	2.27	1.43	1.37
4	B	1106	FAD	C9A-N10	2.26	1.41	1.38
4	A	1106	FAD	C9A-N10	2.19	1.41	1.38
3	C	1105	FMN	C2-N1	2.17	1.42	1.38
3	C	1105	FMN	C9A-C5A	-2.17	1.38	1.42
3	A	1105	FMN	O4-C4	2.12	1.29	1.24
3	A	1105	FMN	C4'-C3'	2.06	1.57	1.53
4	B	1106	FAD	C4-C4X	2.02	1.44	1.41
4	D	1106	FAD	C4-C4X	2.02	1.44	1.41
3	C	1105	FMN	P-O2P	-2.01	1.47	1.54
3	D	1105	FMN	C7M-C7	2.01	1.55	1.51
3	A	1105	FMN	C8M-C8	2.00	1.55	1.51

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1107	Y3G	C06-C01-N02	-15.41	113.66	124.40
5	B	1107	Y3G	C06-C01-N02	-15.11	113.87	124.40
4	A	1106	FAD	C4-N3-C2	13.07	126.17	115.14
4	C	1106	FAD	C4-N3-C2	12.75	125.91	115.14
4	B	1106	FAD	C4-N3-C2	11.99	125.26	115.14
5	D	1107	Y3G	C06-C01-N02	-11.72	116.23	124.40
4	D	1106	FAD	C4-N3-C2	11.71	125.03	115.14
5	C	1107	Y3G	C06-C01-N02	-10.51	117.07	124.40
3	B	1105	FMN	C4-N3-C2	9.55	123.20	115.14
3	A	1105	FMN	C4-N3-C2	8.14	122.02	115.14
3	D	1105	FMN	C4-N3-C2	7.87	121.79	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	FMN	C4A-C4-N3	-6.95	113.92	123.43
5	A	1107	Y3G	C01-N02-C03	6.87	120.94	115.14
4	A	1106	FAD	C4X-C4-N3	-6.83	114.10	123.43
3	A	1105	FMN	C4-C4A-C10	6.77	124.43	119.95
4	D	1106	FAD	C4X-C4-N3	-6.67	114.30	123.43
4	B	1106	FAD	C4X-C4-N3	-6.49	114.55	123.43
5	D	1107	Y3G	C06-C05-N04	-6.46	113.74	123.42
4	C	1106	FAD	C4X-C4-N3	-6.30	114.81	123.43
3	D	1105	FMN	C1'-N10-C10	6.22	123.98	118.41
5	B	1107	Y3G	C01-N02-C03	6.19	120.37	115.14
3	D	1105	FMN	C4A-C4-N3	-5.77	115.54	123.43
3	B	1105	FMN	C5A-C9A-N10	5.59	121.76	117.72
5	C	1107	Y3G	C06-C05-N04	-5.53	115.12	123.42
5	B	1107	Y3G	C06-C05-N04	-5.23	115.58	123.42
3	B	1105	FMN	C4A-C4-N3	-5.22	116.30	123.43
3	D	1105	FMN	C10-C4A-N5	5.00	124.71	121.26
4	B	1106	FAD	C10-C4X-N5	4.94	124.67	121.26
4	D	1106	FAD	C10-C4X-N5	4.92	124.66	121.26
4	C	1106	FAD	C4-C4X-C10	-4.77	116.80	119.95
4	D	1106	FAD	C4-C4X-C10	-4.69	116.85	119.95
3	C	1105	FMN	C10-C4A-N5	-4.65	118.05	121.26
4	C	1106	FAD	C10-C4X-N5	4.57	124.42	121.26
3	D	1105	FMN	C4-C4A-N5	-4.55	113.39	118.60
3	D	1105	FMN	C5A-C9A-N10	4.21	120.76	117.72
3	C	1105	FMN	O3'-C3'-C4'	-4.19	98.70	108.81
3	B	1105	FMN	C1'-N10-C10	4.15	122.12	118.41
4	A	1106	FAD	C4-C4X-C10	-4.07	117.26	119.95
3	D	1105	FMN	C4A-C10-N10	-4.05	116.14	120.30
4	D	1106	FAD	C4X-C10-N10	-3.90	116.30	120.30
3	C	1105	FMN	C4-C4A-C10	3.80	122.47	119.95
4	C	1106	FAD	C1'-N10-C9A	3.78	121.27	118.29
3	A	1105	FMN	C4-C4A-N5	-3.72	114.34	118.60
5	A	1107	Y3G	N04-C03-N02	-3.65	125.53	128.43
4	A	1106	FAD	O2'-C2'-C1'	-3.56	101.03	109.59
4	A	1106	FAD	C1'-N10-C9A	3.53	121.07	118.29
3	C	1105	FMN	C5A-C9A-N10	3.47	120.23	117.72
3	B	1105	FMN	C8M-C8-C7	-3.43	113.70	120.74
4	A	1106	FAD	P-O3P-PA	3.39	144.46	132.83
3	D	1105	FMN	C1'-N10-C9A	-3.35	115.65	118.29
4	B	1106	FAD	C4X-C10-N10	-3.30	116.91	120.30
4	D	1106	FAD	C1'-N10-C9A	3.26	120.86	118.29
4	A	1106	FAD	C10-C4X-N5	3.25	123.51	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1106	FAD	C4X-C10-N10	-3.25	116.97	120.30
3	C	1105	FMN	C4-N3-C2	3.24	117.88	115.14
3	B	1105	FMN	O3P-P-O2P	3.23	119.97	107.64
4	B	1106	FAD	C4-C4X-C10	-3.15	117.86	119.95
4	B	1106	FAD	C1'-N10-C9A	3.13	120.76	118.29
3	B	1105	FMN	C9A-N10-C10	-3.12	117.82	121.91
3	A	1105	FMN	C5A-C9A-N10	3.04	119.92	117.72
5	B	1107	Y3G	N04-C03-N02	-3.01	126.03	128.43
3	D	1105	FMN	C4-C4A-C10	2.92	121.89	119.95
3	B	1105	FMN	O2P-P-O1P	-2.91	99.30	110.68
4	B	1106	FAD	O3B-C3B-C4B	-2.89	102.70	111.05
3	D	1105	FMN	O4'-C4'-C5'	-2.86	103.50	109.92
3	C	1105	FMN	O3P-P-O2P	2.80	118.34	107.64
3	A	1105	FMN	O3P-P-O2P	2.73	118.08	107.64
4	B	1106	FAD	O2P-P-O1P	2.73	125.72	112.24
3	B	1105	FMN	C10-C4A-N5	2.67	123.10	121.26
3	D	1105	FMN	O3P-P-O5'	-2.65	99.69	106.73
4	A	1106	FAD	C4X-C10-N10	-2.65	117.58	120.30
3	A	1105	FMN	C4A-C10-N10	-2.55	117.68	120.30
5	D	1107	Y3G	C05-N04-C03	2.52	119.51	115.36
3	A	1105	FMN	O2'-C2'-C3'	2.49	115.15	109.10
3	D	1105	FMN	O3'-C3'-C4'	-2.48	102.82	108.81
4	A	1106	FAD	O5B-PA-O1A	-2.46	99.45	109.07
3	C	1105	FMN	C4A-N5-C5A	2.44	119.21	116.77
4	A	1106	FAD	C5A-C6A-N6A	2.43	124.04	120.35
4	D	1106	FAD	O4'-C4'-C3'	-2.38	103.30	109.10
5	C	1107	Y3G	C05-N04-C03	2.38	119.28	115.36
3	C	1105	FMN	C4A-C4-N3	-2.37	120.19	123.43
4	D	1106	FAD	O3'-C3'-C2'	-2.35	103.13	108.81
3	C	1105	FMN	O3P-P-O1P	2.35	119.88	110.68
3	A	1105	FMN	O4'-C4'-C5'	2.35	115.19	109.92
3	A	1105	FMN	O2P-P-O5'	-2.34	100.50	106.73
4	B	1106	FAD	P-O3P-PA	2.31	140.76	132.83
4	C	1106	FAD	O2P-P-O1P	2.26	123.41	112.24
3	B	1105	FMN	C8M-C8-C9	2.26	125.74	120.34
5	A	1107	Y3G	C06-C05-N04	-2.25	120.05	123.42
4	D	1106	FAD	O2P-P-O1P	2.25	123.34	112.24
5	B	1107	Y3G	C05-N04-C03	2.17	118.94	115.36
3	B	1105	FMN	C7M-C7-C8	-2.17	116.29	120.74
4	C	1106	FAD	C5A-C6A-N6A	2.17	123.64	120.35
4	B	1106	FAD	O2P-P-O5'	2.15	117.74	107.75
4	C	1106	FAD	P-O3P-PA	2.11	140.07	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1106	FAD	C5A-C6A-N6A	2.10	123.55	120.35
3	D	1105	FMN	C8M-C8-C7	-2.10	116.43	120.74
3	A	1105	FMN	O4'-C4'-C3'	2.07	114.13	109.10
5	C	1107	Y3G	N04-C03-N02	-2.06	126.80	128.43
4	A	1106	FAD	O2A-PA-O1A	2.05	122.37	112.24
3	B	1105	FMN	C4A-N5-C5A	-2.04	114.73	116.77
3	C	1105	FMN	C7M-C7-C6	-2.03	115.48	120.34

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1106	FAD	PA-O3P-P-O5'
3	B	1105	FMN	O3'-C3'-C4'-O4'
3	B	1105	FMN	O3'-C3'-C4'-C5'
3	B	1105	FMN	C2'-C3'-C4'-O4'
4	B	1106	FAD	P-O3P-PA-O1A
4	B	1106	FAD	PA-O3P-P-O5'
3	A	1105	FMN	C4'-C5'-O5'-P
3	C	1105	FMN	C4'-C5'-O5'-P
3	D	1105	FMN	C4'-C5'-O5'-P
4	B	1106	FAD	P-O3P-PA-O2A
3	B	1105	FMN	C4'-C5'-O5'-P
3	C	1105	FMN	O3'-C3'-C4'-O4'
4	A	1106	FAD	O4B-C4B-C5B-O5B
3	D	1105	FMN	O3'-C3'-C4'-C5'
4	D	1106	FAD	PA-O3P-P-O5'
4	B	1106	FAD	O4B-C4B-C5B-O5B
4	A	1106	FAD	P-O3P-PA-O2A
4	C	1106	FAD	O4B-C4B-C5B-O5B
4	D	1106	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1106	FAD	2	0
2	A	1101	SF4	2	0
4	A	1106	FAD	2	0
5	B	1107	Y3G	2	0
5	A	1107	Y3G	1	0

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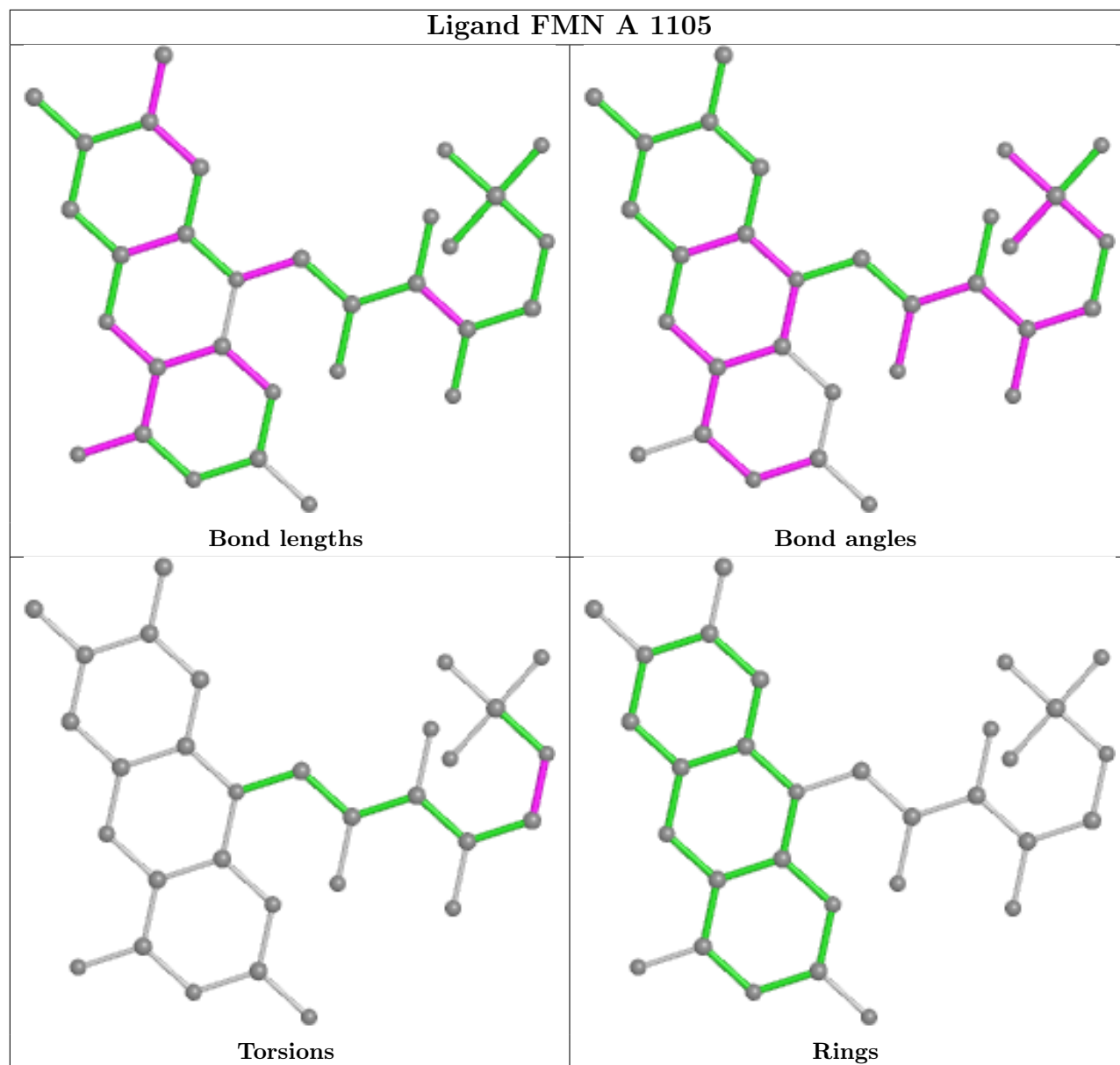
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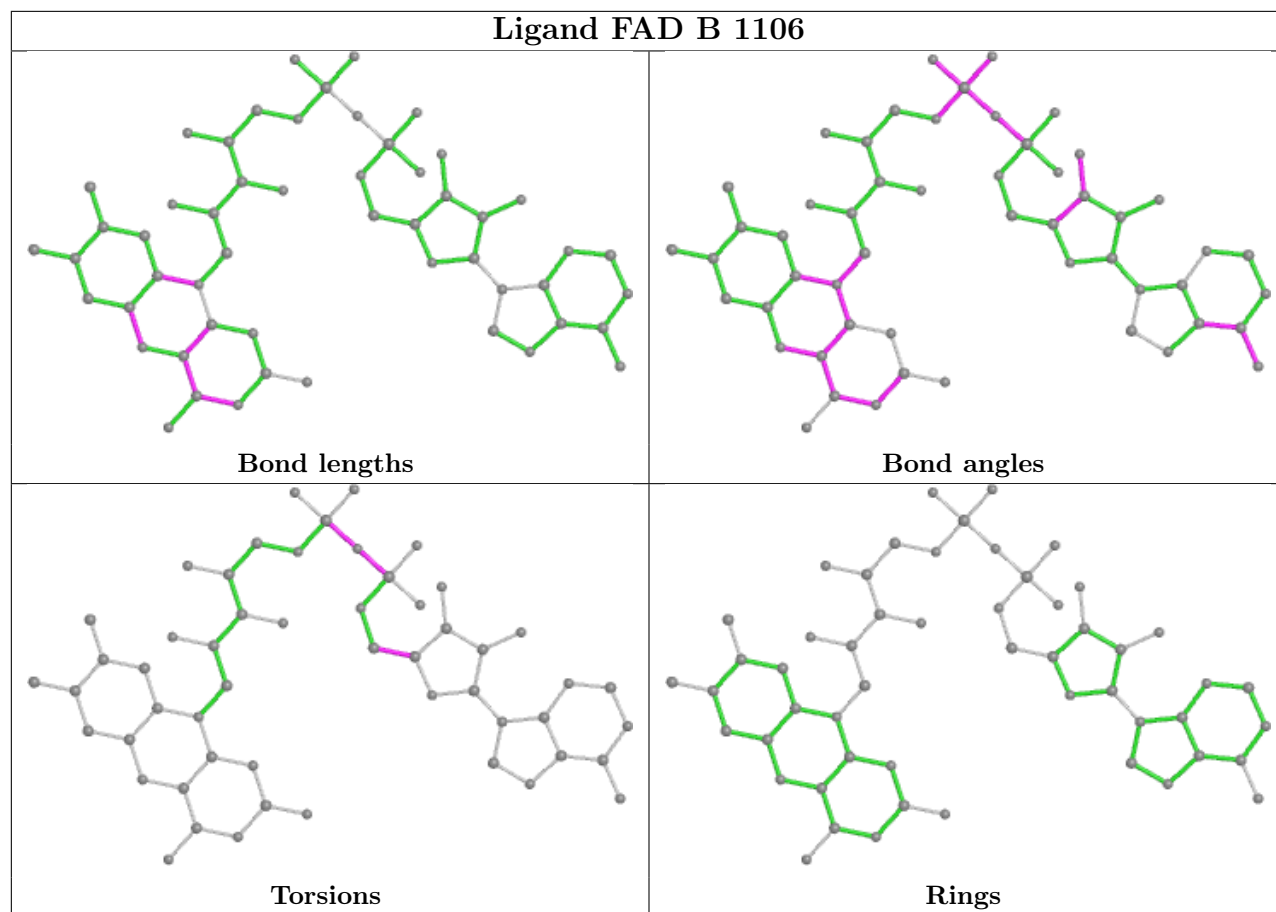
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1107	Y3G	2	0
4	D	1106	FAD	1	0
2	C	1101	SF4	1	0
5	D	1107	Y3G	1	0
3	D	1105	FMN	4	0
2	B	1101	SF4	1	0
4	C	1106	FAD	1	0
3	C	1105	FMN	2	0

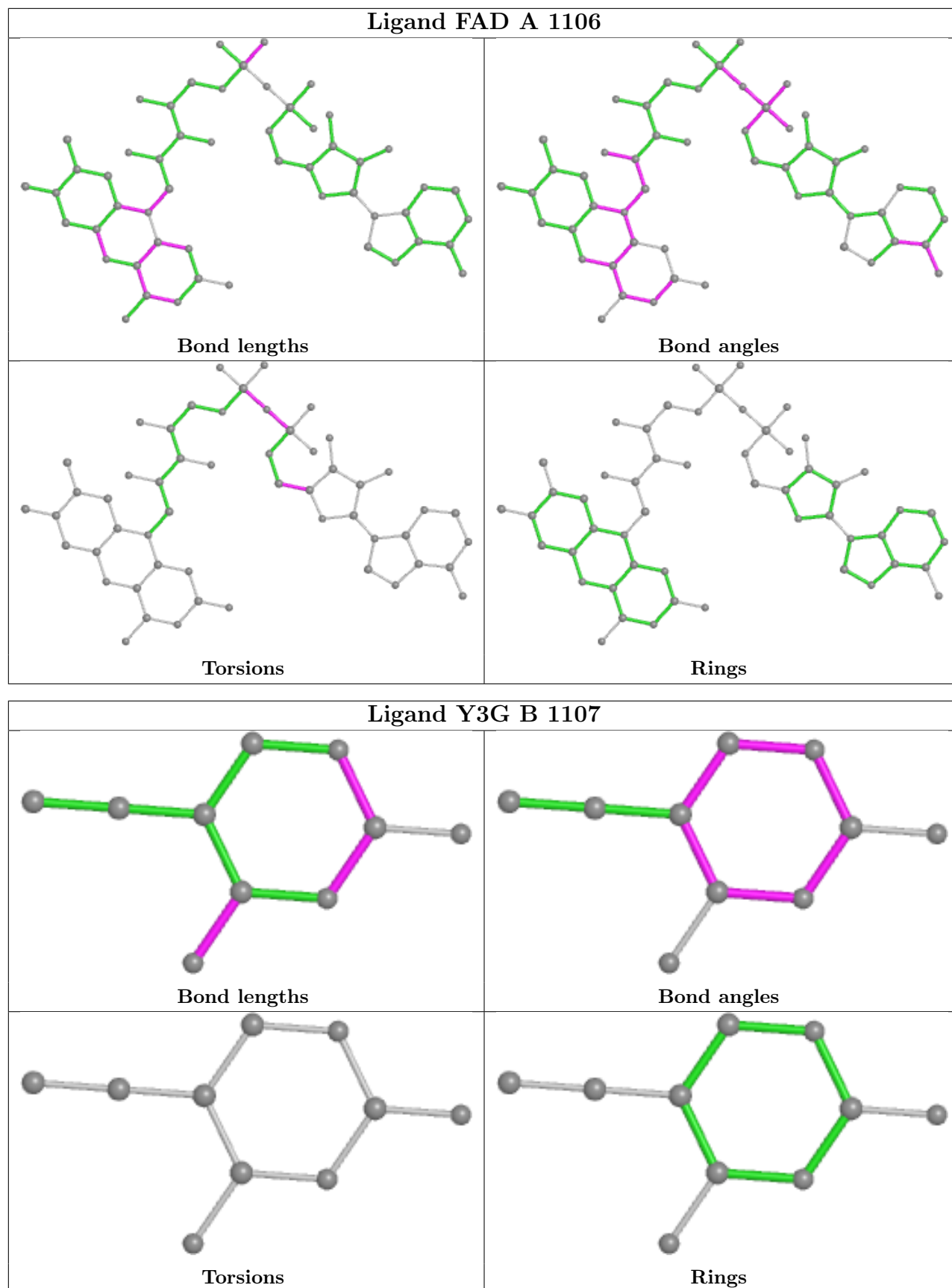
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

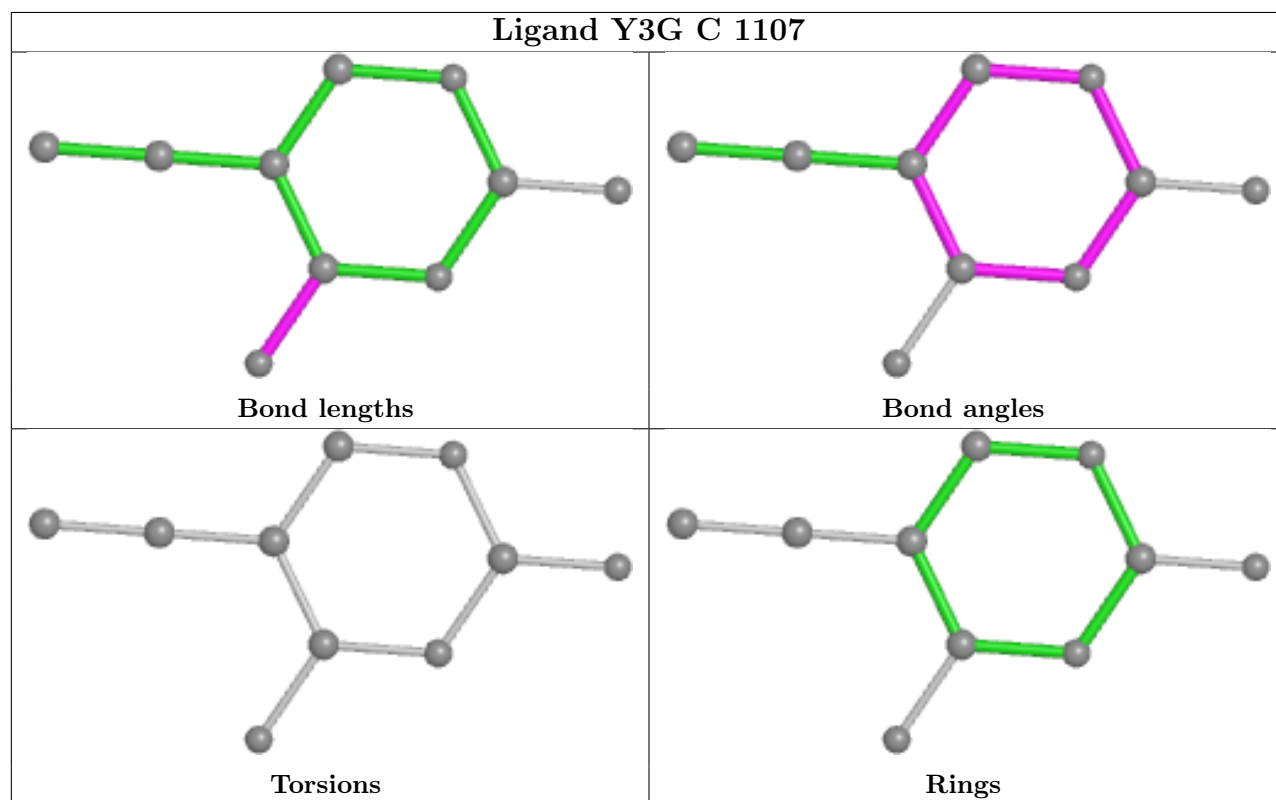
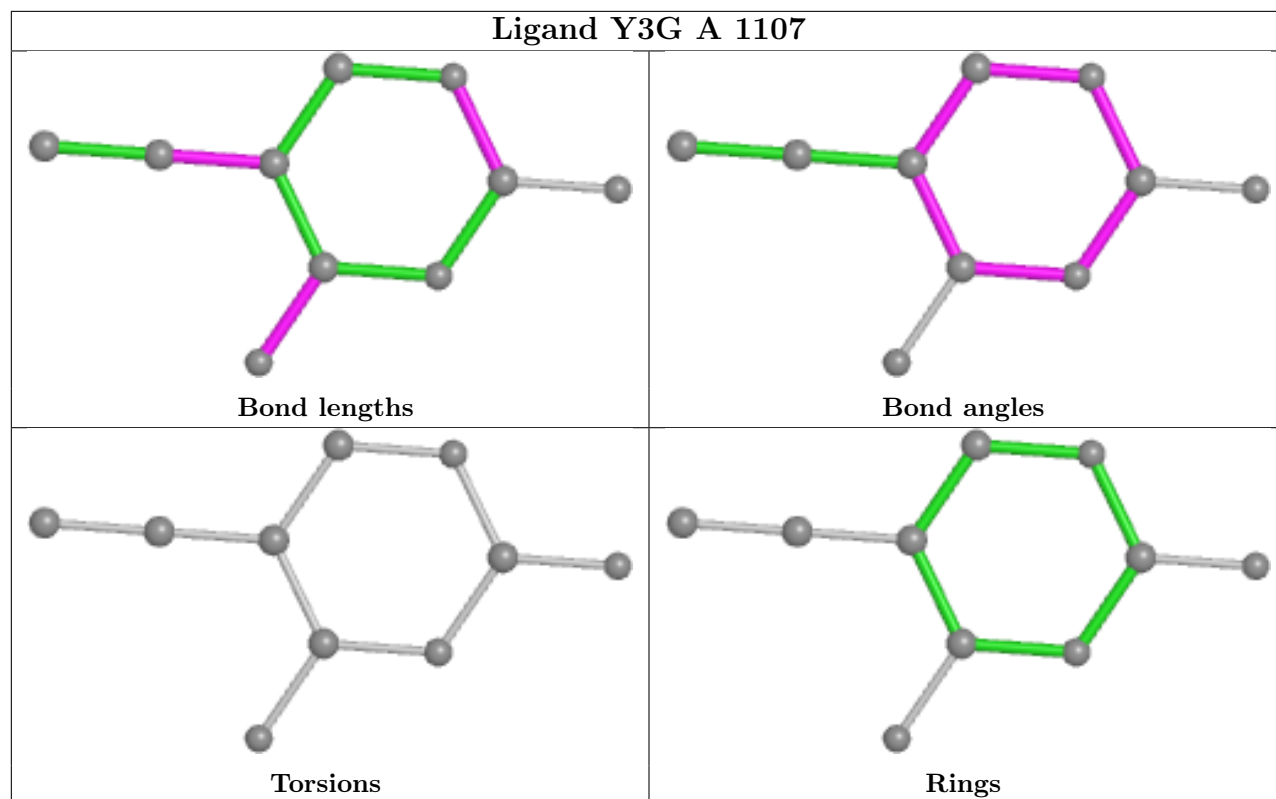


## Ligand FMN A 1105

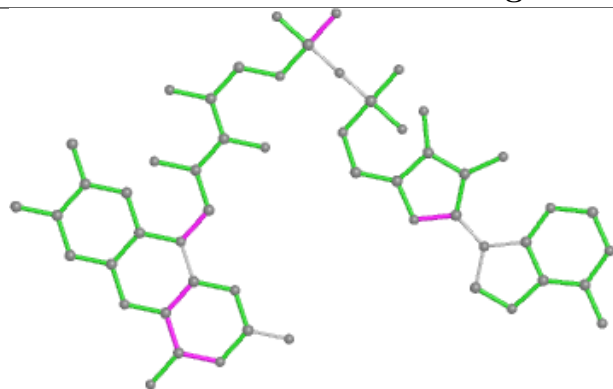




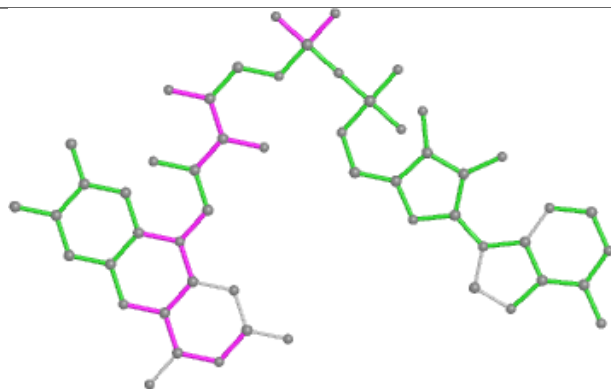




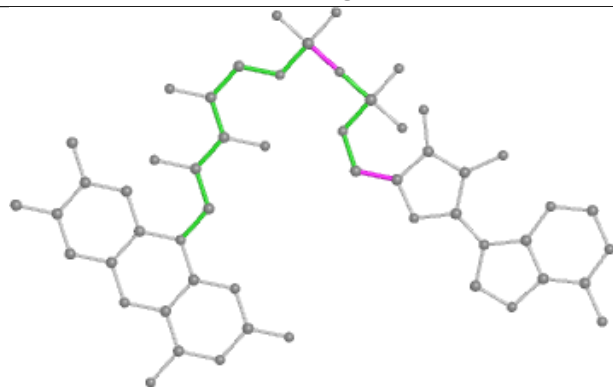
## Ligand FAD D 1106



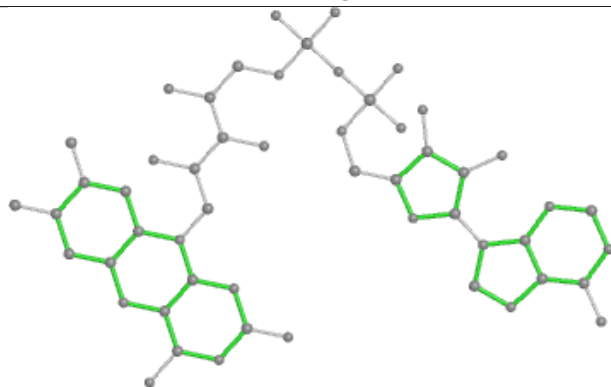
Bond lengths



Bond angles

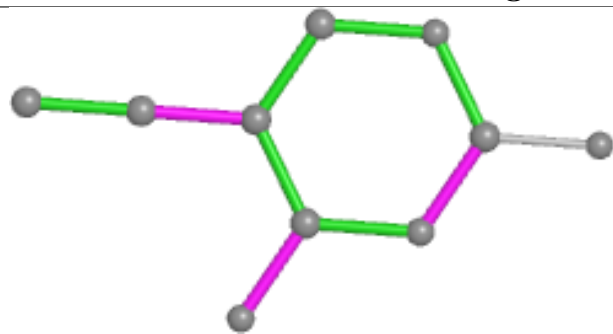


Torsions

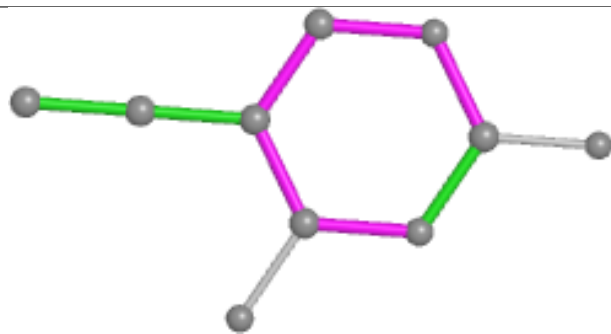


Rings

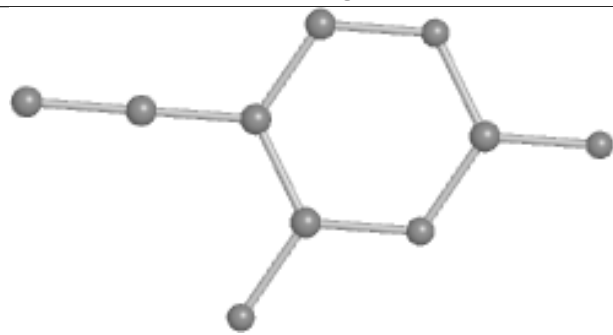
## Ligand Y3G D 1107



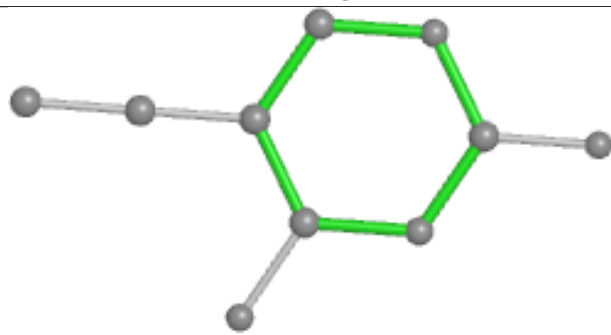
Bond lengths



Bond angles

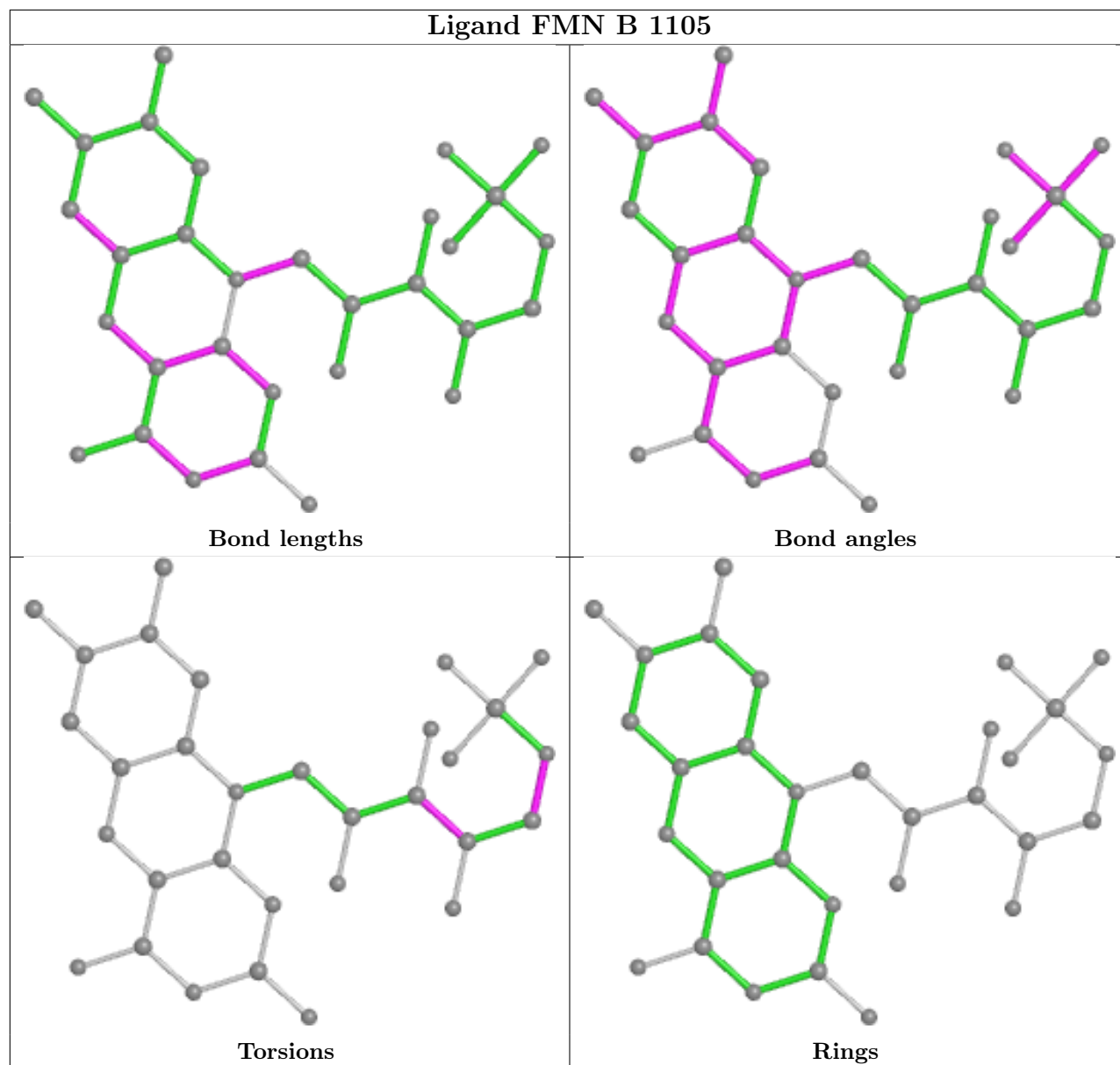


Torsions

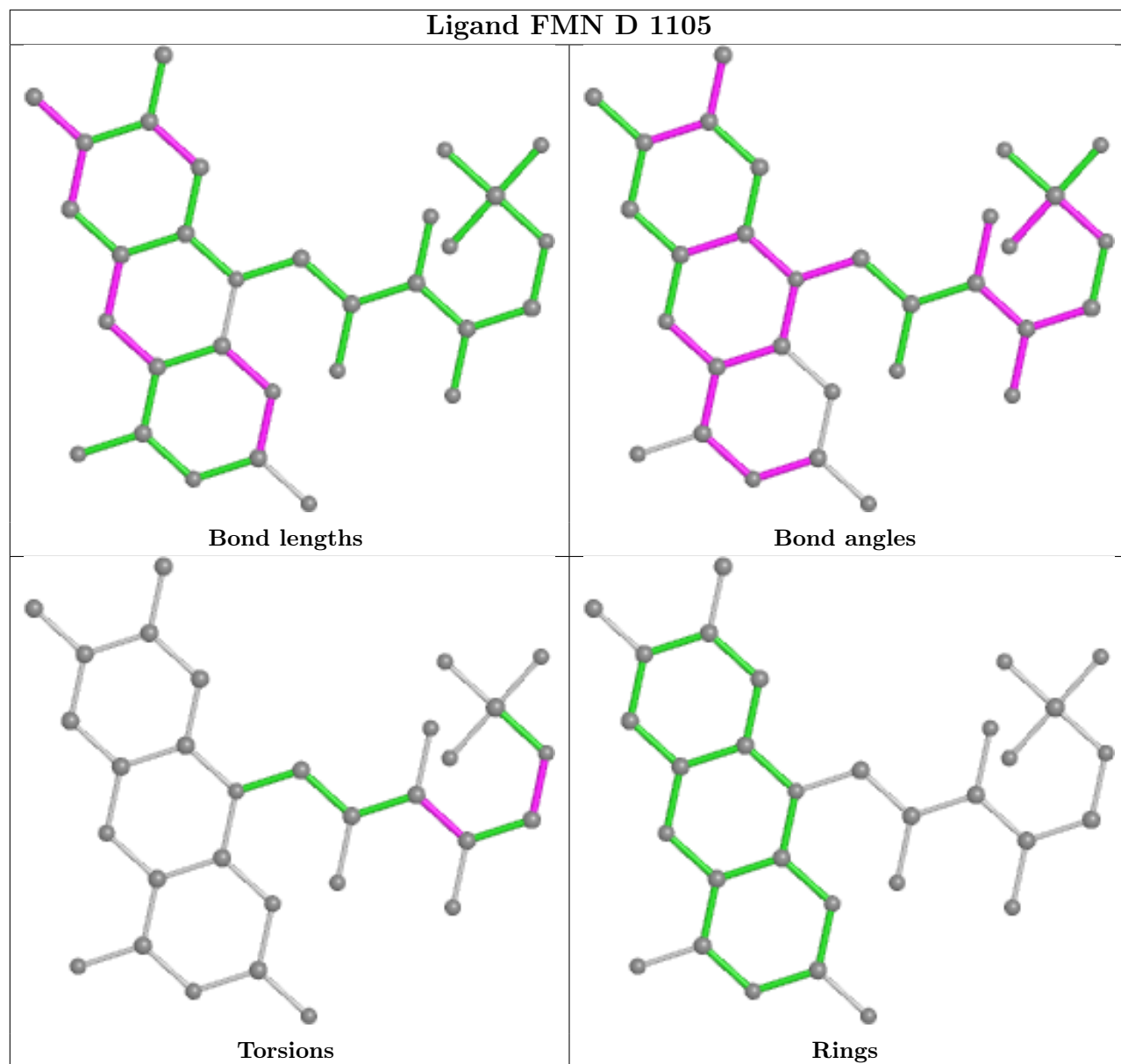


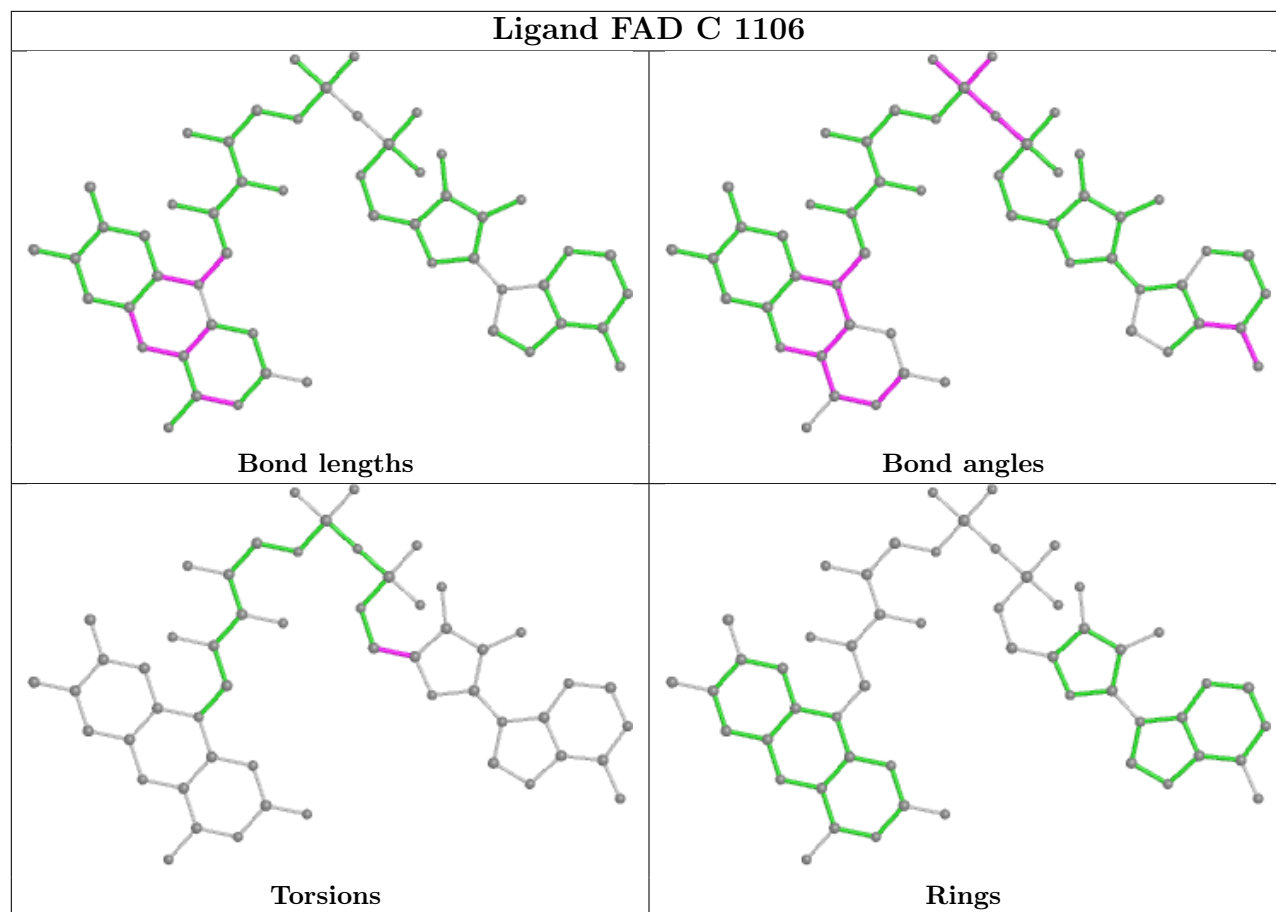
Rings

## Ligand FMN B 1105

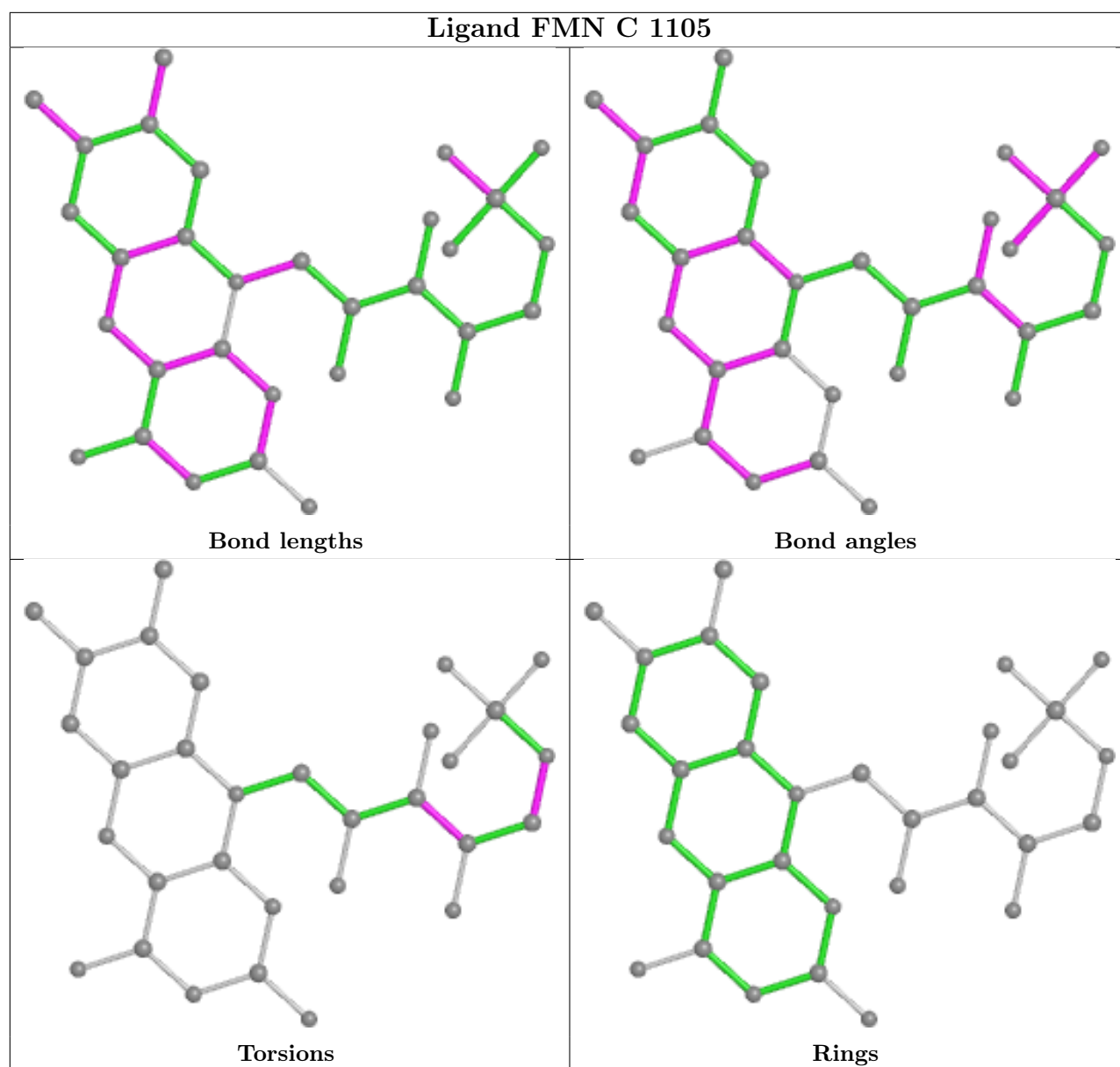


## Ligand FMN D 1105









## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	1005/1025 (98%)	-0.06	30 (2%)	50	49	18, 29, 49, 71	0
1	B	1004/1025 (97%)	-0.13	29 (2%)	51	50	19, 29, 48, 66	0
1	C	1010/1025 (98%)	-0.13	32 (3%)	47	46	17, 26, 46, 70	0
1	D	1014/1025 (98%)	-0.11	31 (3%)	49	48	16, 26, 44, 63	0
All	All	4033/4100 (98%)	-0.11	122 (3%)	50	49	16, 28, 47, 71	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	12.4
1	D	676	GLY	8.8
1	D	902	ALA	7.0
1	C	2	ALA	7.0
1	A	417	GLY	6.4
1	B	1010	PRO	6.0
1	A	1010	PRO	6.0
1	B	869	ALA	5.5
1	A	900	GLN	5.4
1	D	2	ALA	5.3
1	D	416	THR	5.3
1	B	416	THR	5.3
1	B	873	GLY	5.3
1	D	901	ASN	5.2
1	C	416	THR	5.0
1	A	324	CYS	5.0
1	C	324	CYS	4.9
1	C	675	MET	4.6
1	A	872	MET	4.5
1	B	900	GLN	4.3
1	C	674	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1009	THR	4.1
1	D	900	GLN	4.1
1	A	680	MET	4.1
1	D	867	ARG	4.0
1	D	907	LEU	3.8
1	C	52	CYS	3.7
1	A	416	THR	3.7
1	C	417	GLY	3.6
1	D	869	ALA	3.6
1	B	415	GLU	3.6
1	B	417	GLY	3.6
1	B	901	ASN	3.5
1	B	872	MET	3.5
1	D	908	GLU	3.5
1	A	415	GLU	3.5
1	A	869	ALA	3.5
1	D	873	GLY	3.5
1	C	415	GLU	3.5
1	B	673	HIS	3.4
1	C	325	HIS	3.4
1	D	51	HIS	3.4
1	B	52	CYS	3.3
1	C	1010	PRO	3.3
1	B	682	LEU	3.3
1	D	899	GLU	3.3
1	A	870	GLU	3.3
1	A	896	ARG	3.3
1	A	51	HIS	3.3
1	C	872	MET	3.3
1	C	907	LEU	3.3
1	D	870	GLU	3.2
1	D	414	ASP	3.2
1	C	869	ALA	3.2
1	B	899	GLU	3.1
1	C	908	GLU	3.1
1	D	868	ILE	3.1
1	C	867	ARG	3.1
1	C	414	ASP	3.1
1	B	175	CYS	3.1
1	C	682	LEU	3.0
1	B	273	GLU	3.0
1	C	60	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	908	GLU	2.9
1	B	868	ILE	2.9
1	D	459	TRP	2.9
1	C	873	GLY	2.8
1	B	867	ARG	2.8
1	B	180	GLU	2.8
1	B	1008	THR	2.7
1	D	1010	PRO	2.7
1	B	325	HIS	2.7
1	C	903	ALA	2.7
1	A	899	GLU	2.7
1	C	418	LYS	2.6
1	D	897	LEU	2.6
1	A	414	ASP	2.6
1	B	870	GLU	2.6
1	A	325	HIS	2.6
1	D	415	GLU	2.6
1	A	908	GLU	2.5
1	C	10	ALA	2.5
1	D	52	CYS	2.5
1	A	897	LEU	2.5
1	B	865	VAL	2.5
1	C	902	ALA	2.5
1	B	414	ASP	2.4
1	B	1009	THR	2.4
1	A	867	ARG	2.4
1	D	872	MET	2.4
1	A	868	ILE	2.4
1	A	984	ASP	2.4
1	D	858[A]	SER	2.3
1	C	868	ILE	2.3
1	B	874	LYS	2.3
1	A	175	CYS	2.3
1	C	870	GLU	2.3
1	D	418	LYS	2.2
1	D	888	LYS	2.2
1	D	136	CYS	2.2
1	C	326	SER	2.2
1	D	866	PRO	2.2
1	B	1011	TYR	2.2
1	C	51	HIS	2.2
1	D	50	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	51	HIS	2.2
1	A	418	LYS	2.1
1	A	179	GLN	2.1
1	A	892	GLU	2.1
1	A	901	ASN	2.1
1	C	367	PHE	2.1
1	A	367	PHE	2.1
1	C	424	ASP	2.1
1	B	897	LEU	2.0
1	D	181	LYS	2.0
1	A	322	CYS	2.0
1	C	331	ILE	2.0
1	A	864	PRO	2.0
1	D	1009	THR	2.0
1	C	865	VAL	2.0
1	C	910	LYS	2.0
1	D	60	ASP	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 monosaccharides 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
2	SF4	B	1103	8/8	0.90	0.08	20,21,21,21	0
5	Y3G	D	1107	10/10	0.90	0.15	32,33,34,34	0
2	SF4	C	1103	8/8	0.91	0.08	17,18,18,18	0
2	SF4	A	1104	8/8	0.92	0.07	22,22,23,23	0
5	Y3G	B	1107	10/10	0.92	0.17	36,36,37,37	0
5	Y3G	C	1107	10/10	0.92	0.12	32,32,32,32	0

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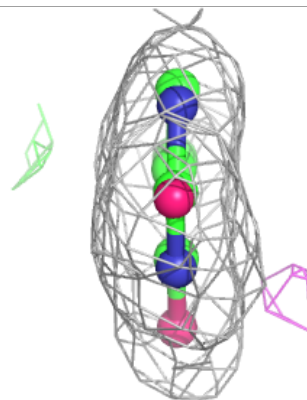
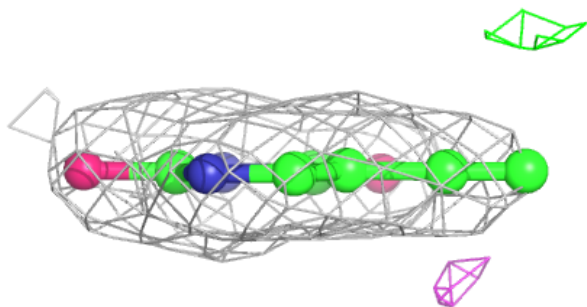
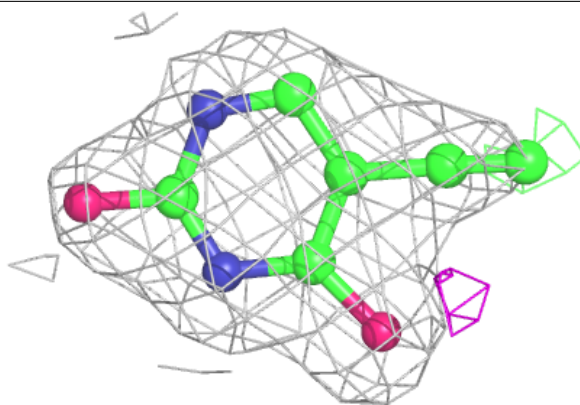
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SF4	B	1104	8/8	0.92	0.08	21,21,22,22	0
2	SF4	A	1103	8/8	0.93	0.07	19,20,20,21	0
2	SF4	B	1101	8/8	0.93	0.08	19,19,20,20	0
2	SF4	B	1102	8/8	0.93	0.08	17,17,17,18	0
2	SF4	C	1104	8/8	0.94	0.07	17,17,18,19	0
2	SF4	D	1103	8/8	0.94	0.08	18,19,20,20	0
5	Y3G	A	1107	10/10	0.94	0.11	39,39,40,40	0
2	SF4	C	1101	8/8	0.94	0.09	16,17,17,18	0
2	SF4	C	1102	8/8	0.94	0.09	16,16,17,17	0
2	SF4	A	1101	8/8	0.94	0.07	19,19,20,20	0
2	SF4	D	1102	8/8	0.95	0.10	15,16,17,17	0
2	SF4	D	1101	8/8	0.95	0.09	15,17,18,18	0
2	SF4	A	1102	8/8	0.96	0.09	17,18,18,18	0
2	SF4	D	1104	8/8	0.96	0.07	18,18,18,19	0
4	FAD	A	1106	53/53	0.97	0.10	22,24,24,24	0
4	FAD	B	1106	53/53	0.97	0.10	22,23,25,25	0
3	FMN	A	1105	31/31	0.97	0.12	22,22,23,23	0
4	FAD	D	1106	53/53	0.98	0.10	20,21,23,24	0
3	FMN	D	1105	31/31	0.98	0.12	17,18,18,18	0
3	FMN	B	1105	31/31	0.98	0.10	22,22,23,23	0
3	FMN	C	1105	31/31	0.98	0.12	18,19,21,22	0
4	FAD	C	1106	53/53	0.98	0.10	21,23,25,25	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.

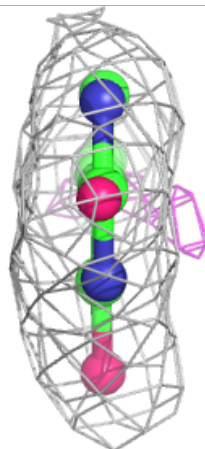
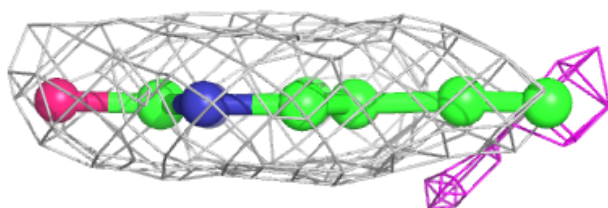
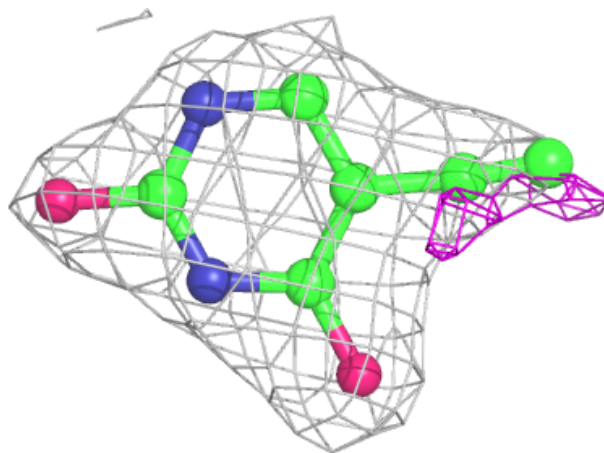
**Electron density around Y3G D 1107:**

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



**Electron density around Y3G B 1107:**

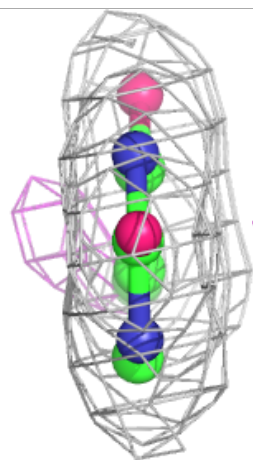
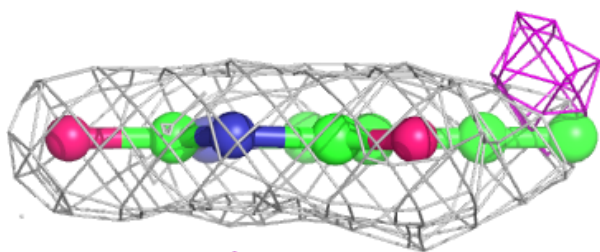
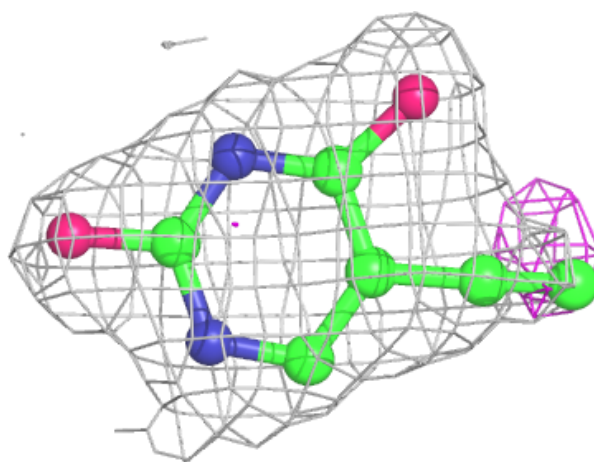
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





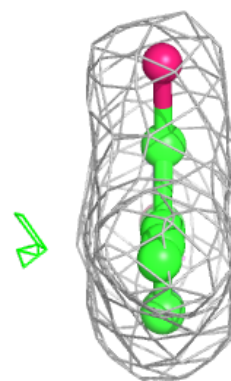
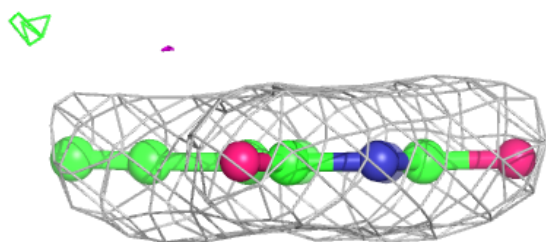
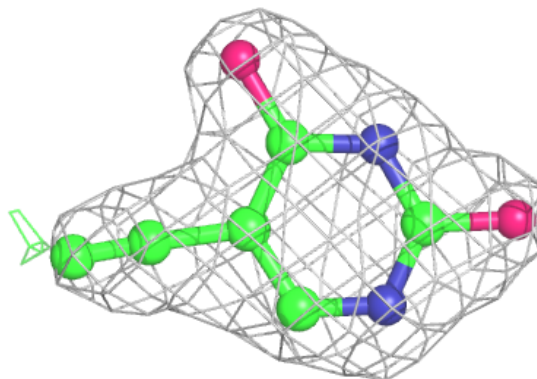
**Electron density around Y3G C 1107:**

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

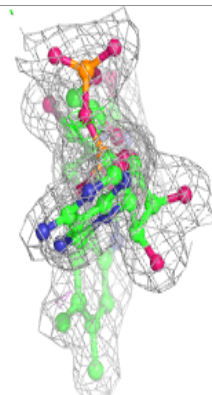
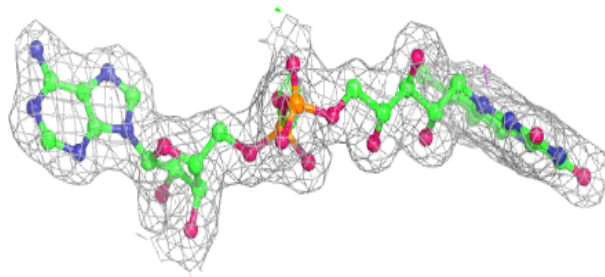
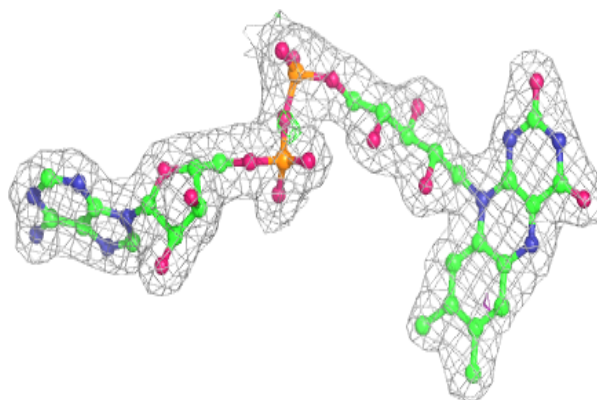


**Electron density around Y3G A 1107:**

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

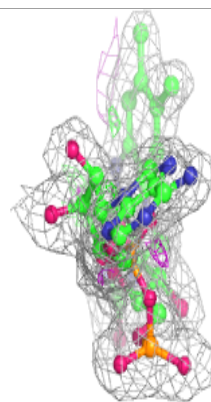
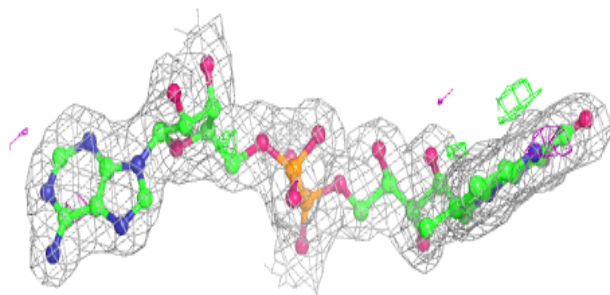
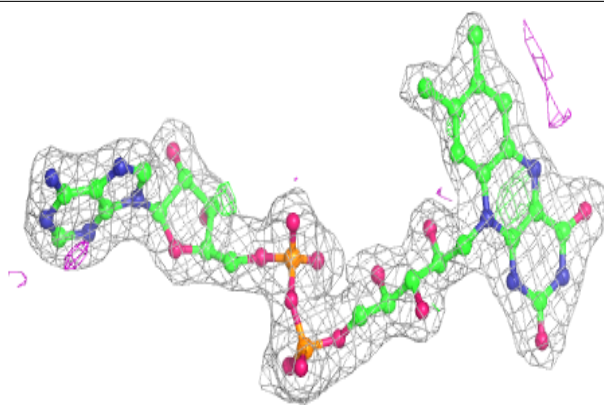
**Electron density around FAD A 1106:**

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



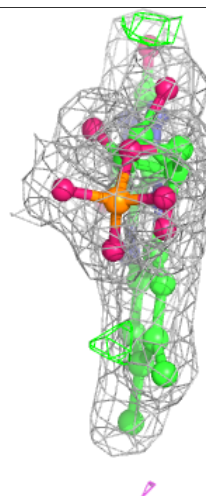
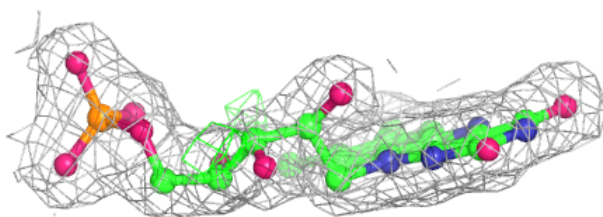
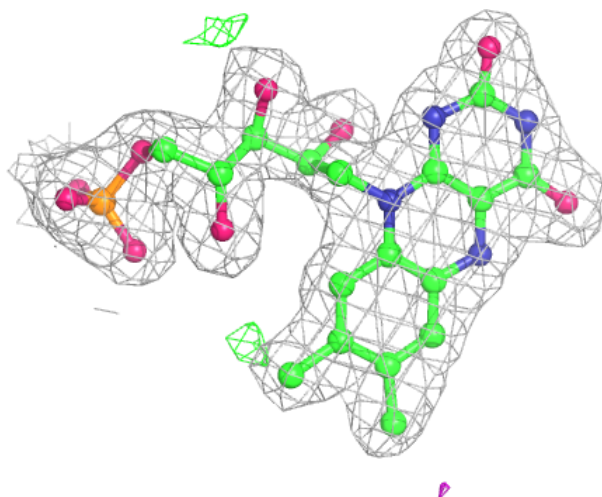
**Electron density around FAD B 1106:**

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



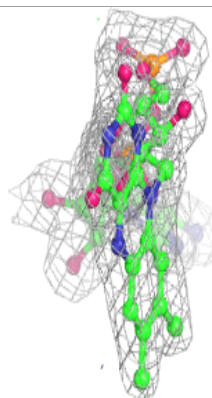
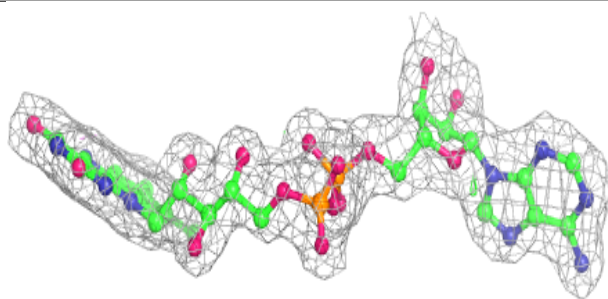
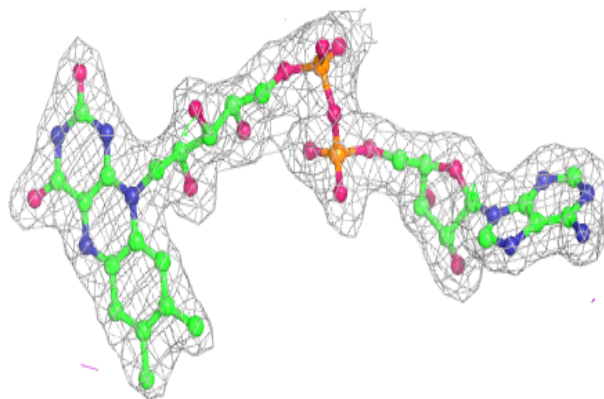
**Electron density around FMN A 1105:**

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

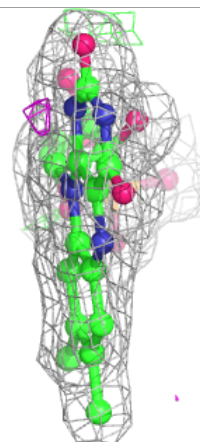
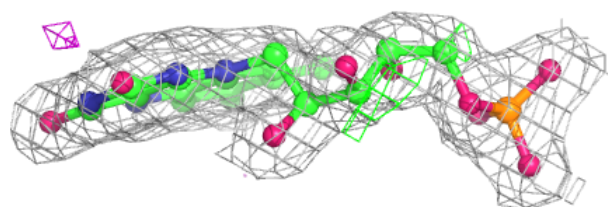
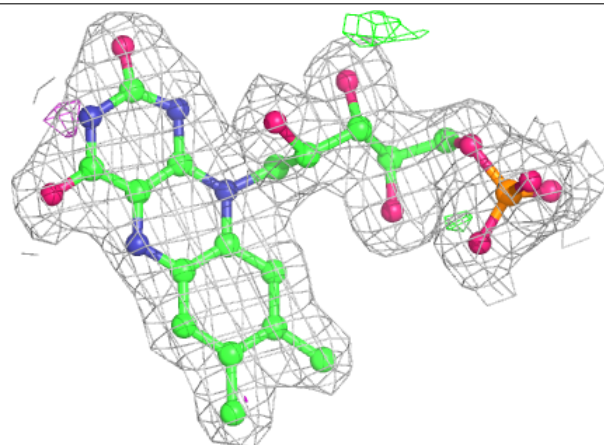


**Electron density around FAD D 1106:**

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

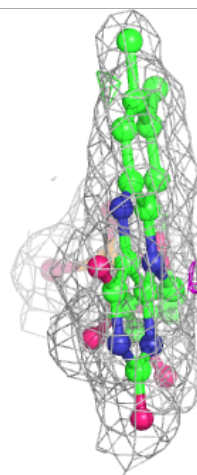
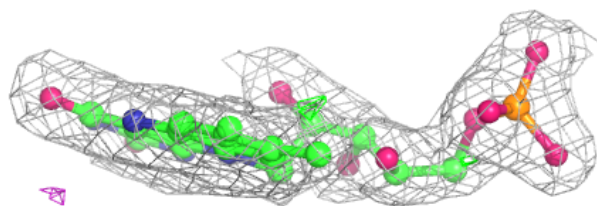
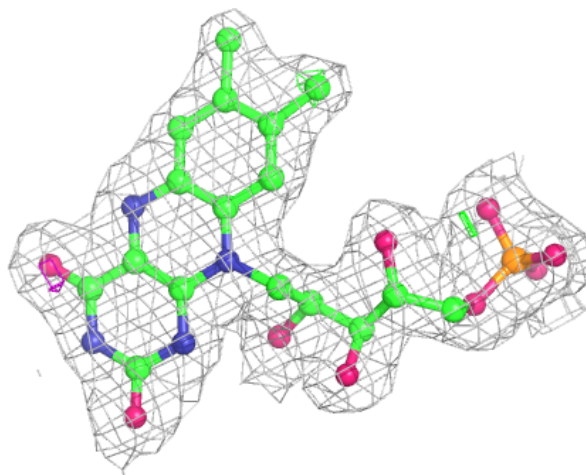
**Electron density around FMN D 1105:**

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



**Electron density around FMN B 1105:**

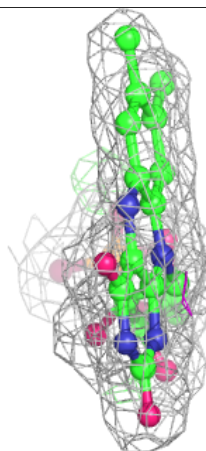
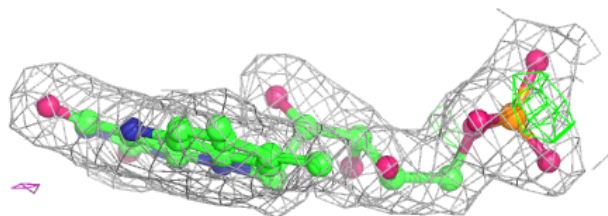
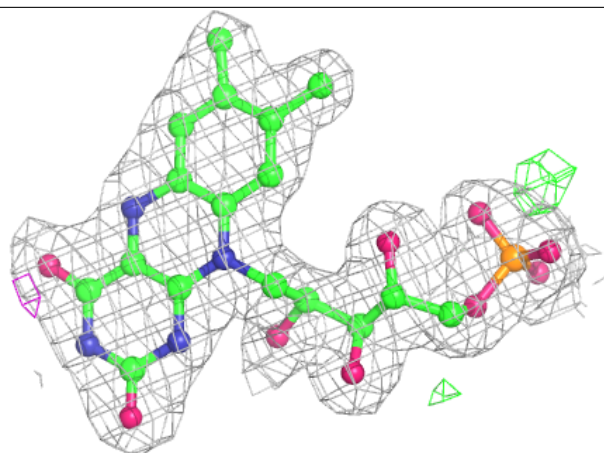
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



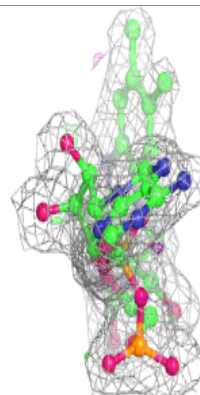
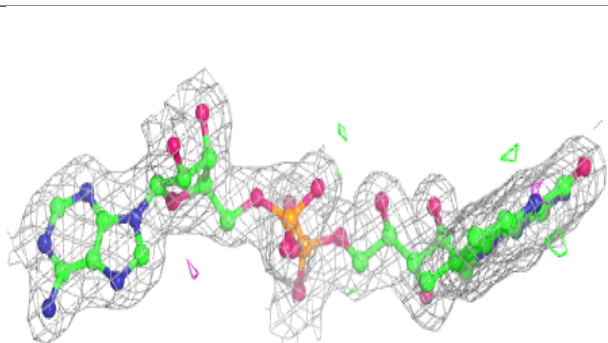
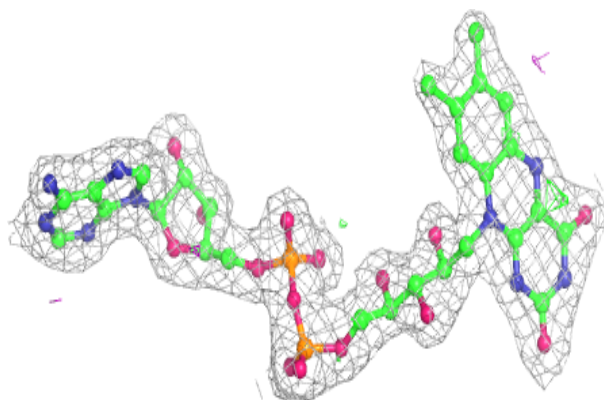


**Electron density around FMN C 1105:**

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

**Electron density around FAD C 1106:**

$2mF_o-DF_c$  (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.