



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:55 AM UTC

PDB ID : 7LJS / pdb_00007ljs
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

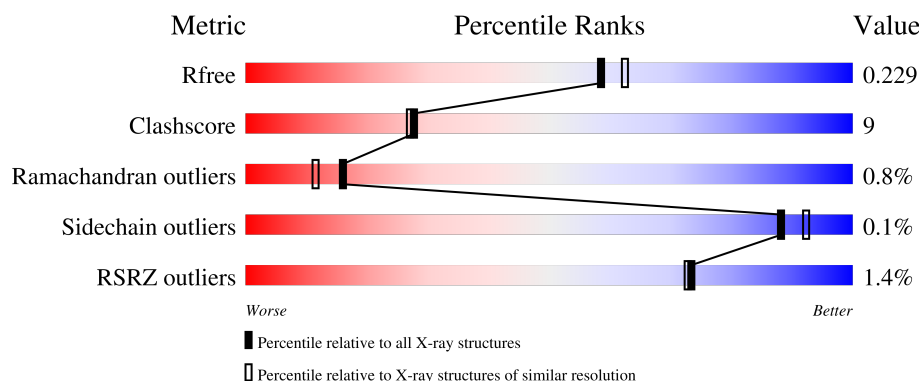
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 ≥ 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	0% 79% 18% ..
1	B	1025	0% 79% 17% ..
1	C	1025	2% 78% 19% ..
1	D	1025	0% 79% 17% ..

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	-
5	Y3G	A	1107	-	X	-	-
5	Y3G	B	1107	-	X	-	-
5	Y3G	C	1107	-	X	-	-
5	Y3G	D	1107	-	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.

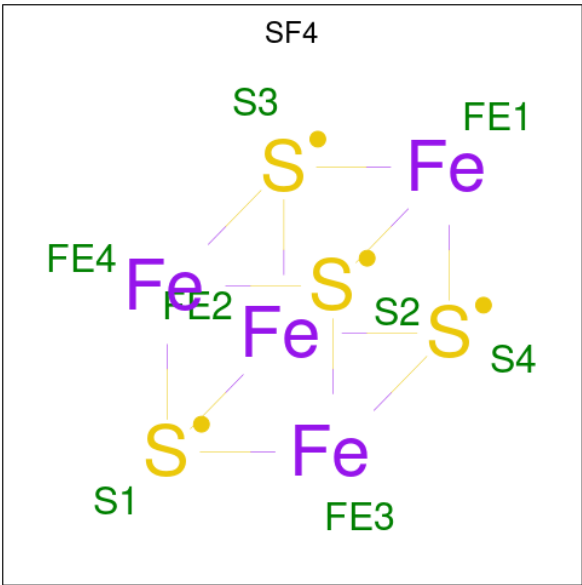
- Molecule 1 is a protein called Dihydropyrimidine dehydrogenase [NADP(+)].

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 (CCD ID: SF4) (formula: Fe₄S₄).



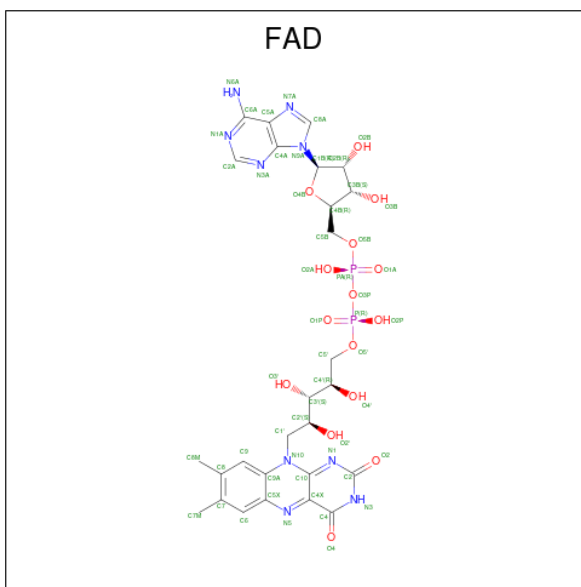
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

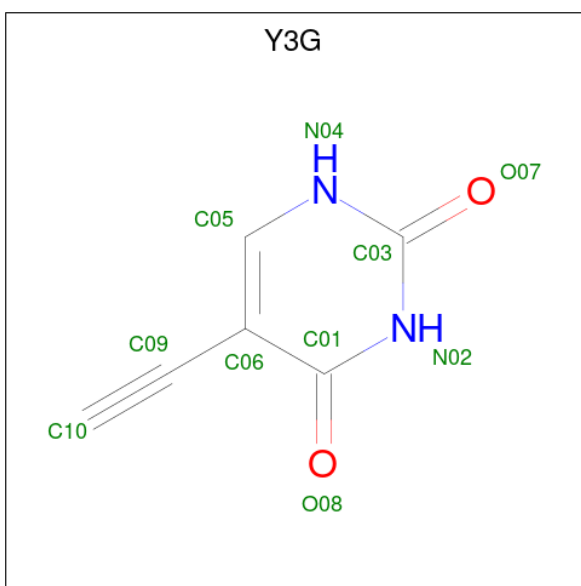
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- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system with atoms labeled N1, N3, N5, N10, C2, C4, C5A, C6, C7, C8, C9, C10, and C4A. The ring is substituted with a ribityl chain at the N10 position. The ribityl chain consists of a ribitol moiety (C1, C2, C3, C4) with hydroxyl groups at C2 and C4, and a phosphate group at C3. The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms: one double-bonded (O1P), and three single-bonded (O2P, O3P, O4P). The structure is rendered in a 3D perspective with wedge and dash bonds to indicate stereochemistry.

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 5-ethynylpyrimidine-2,4(1H,3H)-dione (CCD ID: Y3G) (formula: $\text{C}_6\text{H}_4\text{N}_2\text{O}_2$) (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		

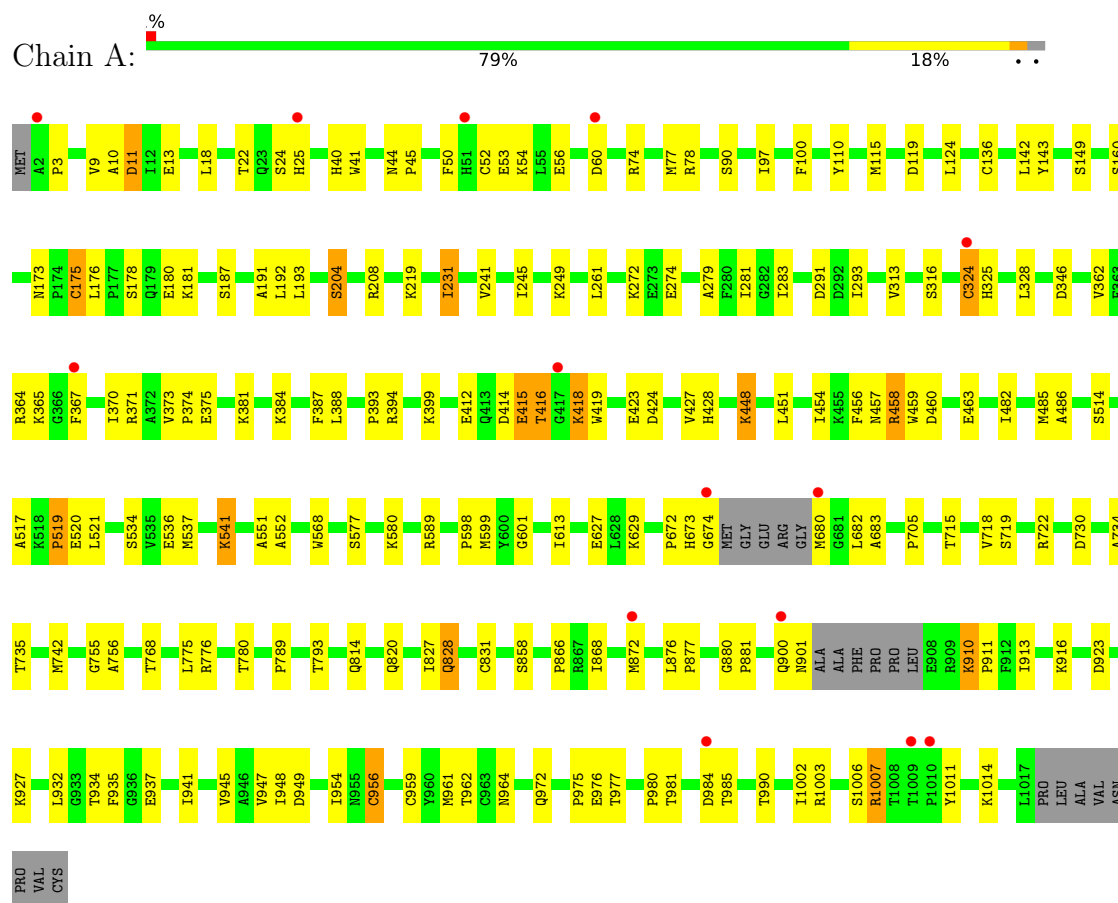
- Molecule 6 is water.

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		

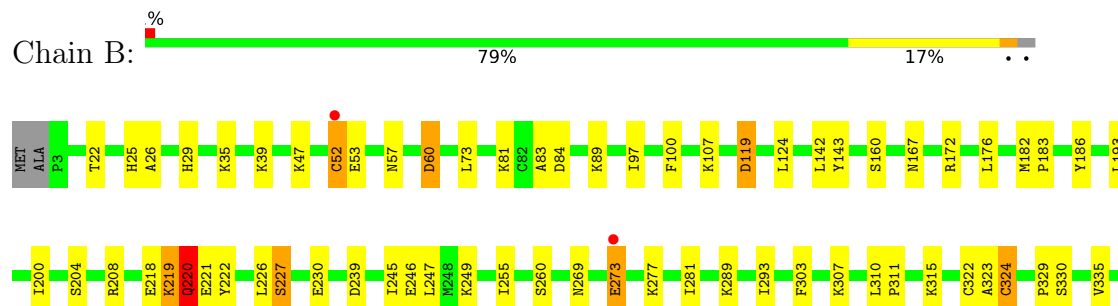
3 Residue-property plots

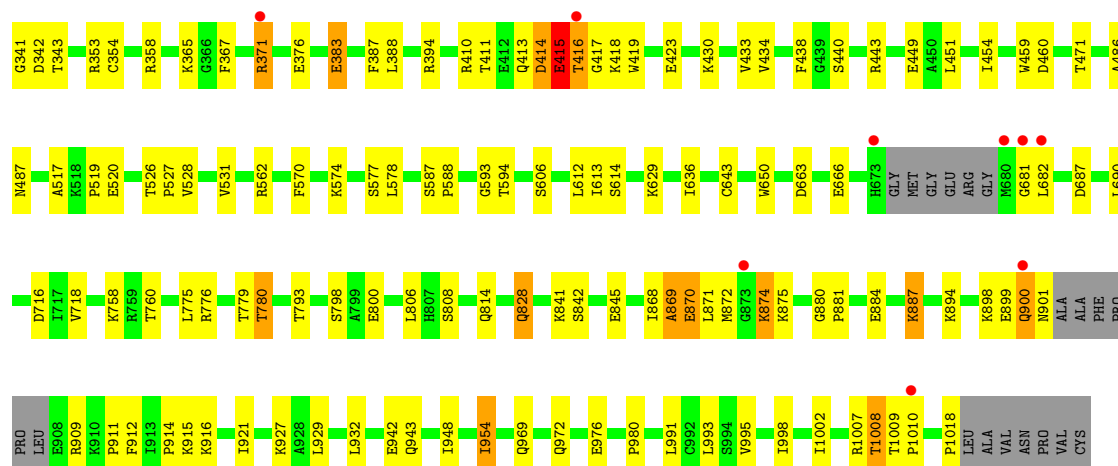
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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(+)]

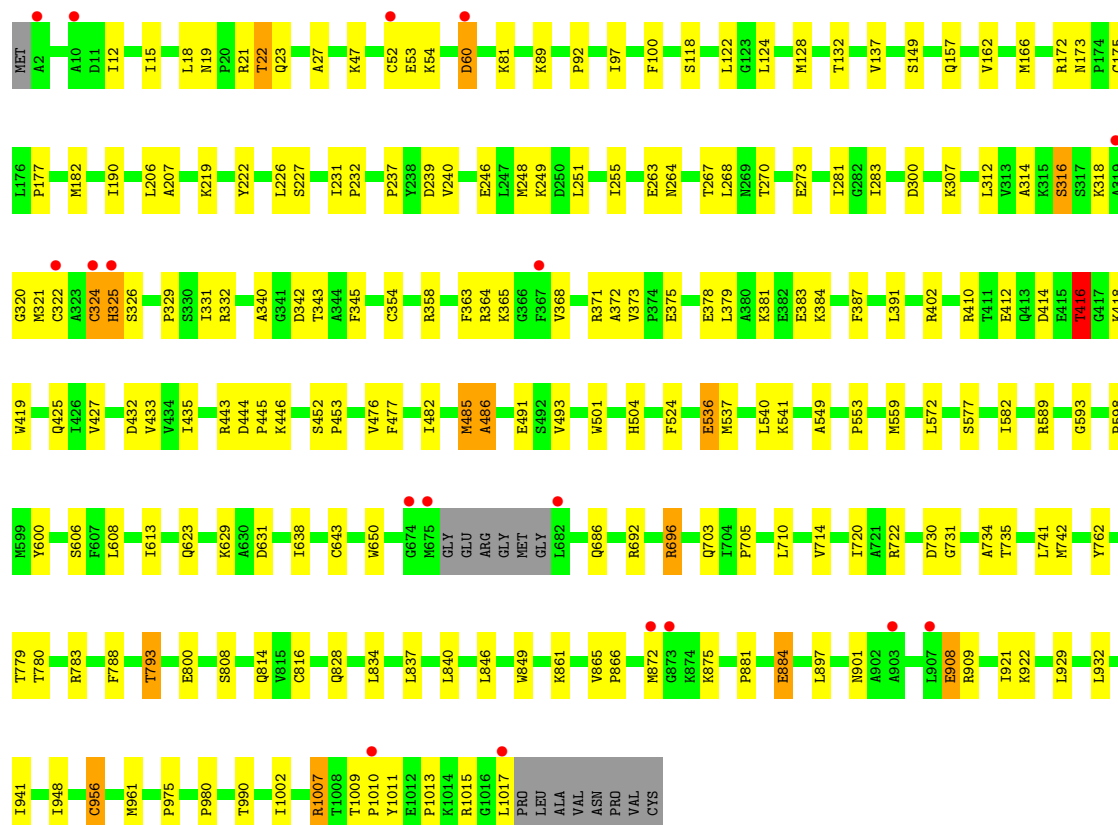
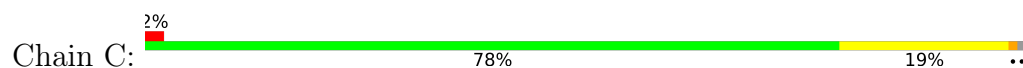


• Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]

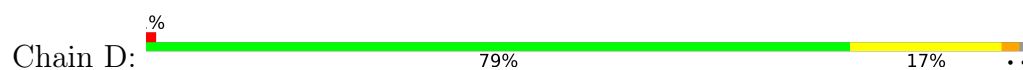


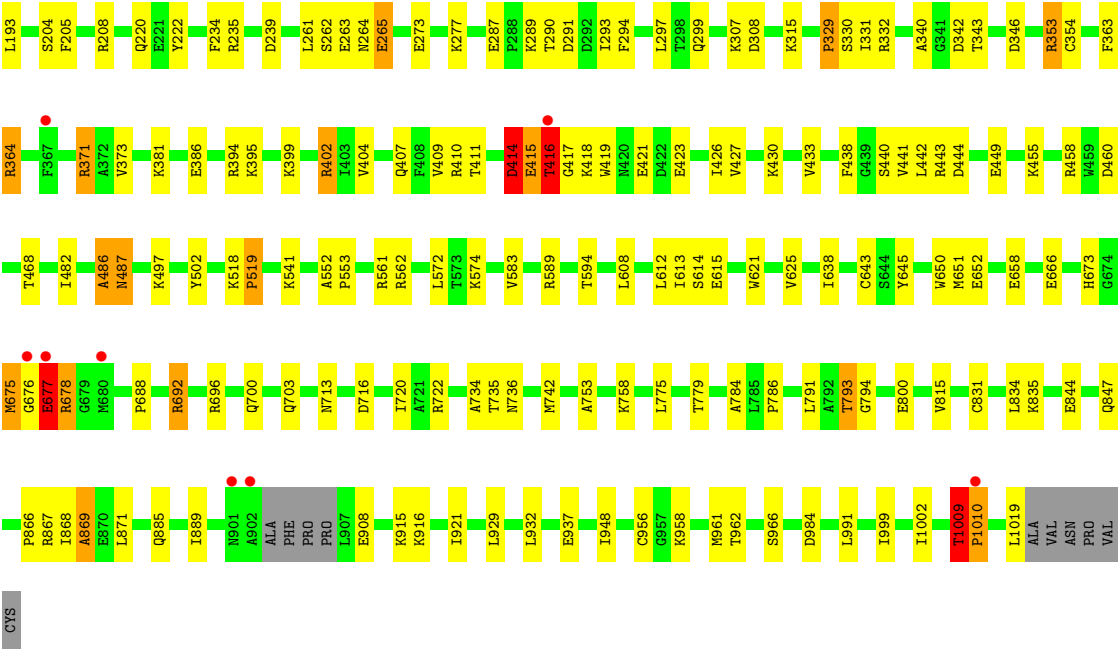


● Molecule 1: Dihydropyrimidine dehydrogenase [NADP(+)]



● 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, α , β , γ	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) 77.3 (45.62-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.172 , 0.229 0.173 , 0.229	Depositor DCC
R_{free} test set	10692 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.34	18/7849 (0.2%)	1.29	30/10635 (0.3%)
1	B	1.35	25/7865 (0.3%)	1.29	24/10655 (0.2%)
1	C	1.42	30/7945 (0.4%)	1.30	22/10772 (0.2%)
1	D	1.45	37/7936 (0.5%)	1.33	31/10754 (0.3%)
All	All	1.39	110/31595 (0.3%)	1.30	107/42816 (0.2%)

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 (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	519	PRO	N-CD	-20.26	1.19	1.47
1	D	265	GLU	CG-CD	11.10	1.79	1.52
1	C	60	ASP	CB-CG	9.68	1.76	1.52
1	D	60	ASP	CB-CG	8.62	1.73	1.52
1	D	984	ASP	CB-CG	7.99	1.72	1.52
1	A	956	CYS	CB-SG	7.90	2.07	1.81
1	D	265	GLU	CB-CG	7.87	1.76	1.52
1	B	60	ASP	CB-CG	7.69	1.71	1.52
1	B	371	ARG	CG-CD	7.40	1.74	1.52
1	D	487	ASN	CB-CG	7.05	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	LYS	CE-NZ	7.02	1.70	1.49
1	B	371	ARG	CD-NE	6.85	1.55	1.46
1	D	342	ASP	CG-OD2	6.73	1.38	1.25
1	D	800	GLU	CG-CD	6.71	1.68	1.52
1	C	703	GLN	CG-CD	6.70	1.68	1.52
1	D	2	ALA	CA-C	6.56	1.66	1.52
1	A	448	LYS	CG-CD	6.49	1.72	1.52
1	C	300	ASP	CG-OD1	6.43	1.37	1.25
1	A	927	LYS	CB-CG	6.42	1.71	1.52
1	D	455	LYS	CG-CD	6.37	1.71	1.52
1	C	828	GLN	CD-NE2	6.35	1.46	1.33
1	C	435	ILE	CG1-CD1	-6.29	1.27	1.51
1	D	184	GLU	CD-OE1	6.28	1.37	1.25
1	D	703	GLN	CD-NE2	6.23	1.46	1.33
1	A	828	GLN	CG-CD	6.18	1.67	1.52
1	C	956	CYS	CB-SG	6.18	2.01	1.81
1	C	828	GLN	CG-CD	6.09	1.67	1.52
1	D	265	GLU	CD-OE2	6.01	1.36	1.25
1	B	60	ASP	CA-CB	5.98	1.63	1.53
1	D	958	LYS	CG-CD	5.96	1.70	1.52
1	D	364	ARG	CG-CD	5.96	1.70	1.52
1	B	239	ASP	CG-OD2	5.96	1.36	1.25
1	C	536	GLU	CD-OE2	5.95	1.36	1.25
1	D	692	ARG	CZ-NH2	5.93	1.41	1.33
1	D	11	ASP	CG-OD1	5.92	1.36	1.25
1	A	324	CYS	CB-SG	5.90	2.00	1.81
1	A	984	ASP	CB-CG	5.89	1.66	1.52
1	B	666	GLU	CD-OE2	5.81	1.36	1.25
1	D	115	MET	SD-CE	5.80	1.94	1.79
1	D	561	ARG	CZ-NH1	5.77	1.40	1.32
1	D	703	GLN	CD-OE1	5.72	1.34	1.23
1	A	680	MET	CG-SD	5.71	1.95	1.80
1	C	375	GLU	CD-OE2	5.70	1.36	1.25
1	C	446	LYS	CE-NZ	5.70	1.66	1.49
1	A	580	LYS	CE-NZ	5.67	1.66	1.49
1	D	541	LYS	CD-CE	5.67	1.69	1.52
1	C	696	ARG	CZ-NH1	5.65	1.40	1.32
1	B	353	ARG	CZ-NH1	5.64	1.40	1.32
1	B	277	LYS	CE-NZ	5.63	1.66	1.49
1	D	956	CYS	CB-SG	5.61	1.99	1.81
1	A	536	GLU	CD-OE1	5.60	1.35	1.25
1	A	589	ARG	CZ-NH2	5.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	ASP	CA-CB	5.54	1.62	1.53
1	C	486	ALA	CA-CB	-5.54	1.45	1.53
1	D	107	LYS	CE-NZ	5.53	1.66	1.49
1	C	875	LYS	CD-CE	5.52	1.69	1.52
1	D	589	ARG	CZ-NH2	5.52	1.40	1.33
1	D	60	ASP	CG-OD1	5.50	1.35	1.25
1	C	800	GLU	CD-OE1	5.49	1.35	1.25
1	B	800	GLU	CB-CG	-5.48	1.36	1.52
1	D	371	ARG	CZ-NH2	5.47	1.40	1.33
1	B	143	TYR	CZ-OH	5.44	1.49	1.38
1	B	342	ASP	CG-OD2	5.44	1.35	1.25
1	D	74	ARG	CZ-NH1	5.42	1.40	1.32
1	D	308	ASP	CG-OD2	5.42	1.35	1.25
1	D	346	ASP	CG-OD1	5.41	1.35	1.25
1	B	884	GLU	CG-CD	5.39	1.65	1.52
1	A	11	ASP	CG-OD2	5.38	1.35	1.25
1	C	307	LYS	CG-CD	5.36	1.68	1.52
1	B	758	LYS	CE-NZ	5.35	1.65	1.49
1	C	884	GLU	CD-OE2	5.35	1.35	1.25
1	D	315	LYS	CE-NZ	5.35	1.65	1.49
1	B	909	ARG	CZ-NH1	5.34	1.40	1.32
1	C	249	LYS	CG-CD	5.30	1.68	1.52
1	C	324	CYS	CB-SG	5.28	1.98	1.81
1	A	460	ASP	CB-CG	5.27	1.65	1.52
1	C	908	GLU	CB-CG	5.24	1.68	1.52
1	C	884	GLU	CD-OE1	5.24	1.35	1.25
1	A	60	ASP	CB-CG	5.23	1.65	1.52
1	A	313	VAL	CB-CG2	5.23	1.69	1.52
1	B	246	GLU	CB-CG	5.23	1.68	1.52
1	D	342	ASP	CG-OD1	5.21	1.35	1.25
1	B	246	GLU	CD-OE2	5.21	1.35	1.25
1	B	884	GLU	CD-OE2	5.21	1.35	1.25
1	D	402	ARG	CZ-NH1	5.21	1.40	1.32
1	C	703	GLN	CB-CG	5.18	1.68	1.52
1	B	874	LYS	CB-CG	5.17	1.68	1.52
1	B	119	ASP	CB-CG	5.14	1.65	1.52
1	C	21	ARG	CZ-NH1	5.14	1.40	1.32
1	C	263	GLU	CG-CD	5.13	1.64	1.52
1	C	175	CYS	CB-SG	5.13	1.98	1.81
1	D	119	ASP	CG-OD2	5.12	1.35	1.25
1	B	376	GLU	CD-OE2	5.11	1.35	1.25
1	A	910	LYS	CG-CD	5.10	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	ASP	CG-OD2	5.10	1.35	1.25
1	B	487	ASN	CB-CG	5.09	1.64	1.52
1	B	969	GLN	CD-NE2	5.08	1.44	1.33
1	C	1002	ILE	CG1-CD1	5.08	1.71	1.51
1	A	77	MET	SD-CE	5.06	1.92	1.79
1	B	371	ARG	CB-CG	5.06	1.67	1.52
1	C	589	ARG	CZ-NH2	5.06	1.40	1.33
1	A	110	TYR	CZ-OH	5.05	1.48	1.38
1	C	793	THR	CA-CB	5.05	1.62	1.53
1	C	19	ASN	CB-CG	5.03	1.64	1.52
1	B	716	ASP	CG-OD2	5.02	1.34	1.25
1	D	167	ASN	CB-CG	-5.02	1.39	1.52
1	D	815	VAL	CB-CG1	5.02	1.69	1.52
1	D	54	LYS	CD-CE	5.01	1.67	1.52
1	B	273	GLU	CD-OE2	5.01	1.34	1.25
1	D	60	ASP	CA-CB	5.01	1.61	1.53

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	CYS	CA-CB-SG	-10.15	91.05	114.40
1	D	60	ASP	CA-CB-CG	9.03	121.63	112.60
1	B	52	CYS	CA-CB-SG	-9.01	93.67	114.40
1	C	909	ARG	CA-C-N	-8.39	106.09	122.70
1	C	909	ARG	C-N-CA	-8.39	106.09	122.70
1	B	780	THR	OG1-CB-CG2	-7.92	93.46	109.30
1	D	1010	PRO	CA-C-N	-7.67	112.22	122.42
1	D	1010	PRO	C-N-CA	-7.67	112.22	122.42
1	C	219	LYS	CD-CE-NZ	-7.63	87.47	111.90
1	C	21	ARG	CA-C-N	-7.57	110.88	122.09
1	C	21	ARG	C-N-CA	-7.57	110.88	122.09
1	D	265	GLU	CB-CG-CD	7.32	125.04	112.60
1	D	414	ASP	CA-C-N	-7.24	110.88	122.24
1	D	414	ASP	C-N-CA	-7.24	110.88	122.24
1	B	371	ARG	CA-CB-CG	7.03	128.15	114.10
1	D	115	MET	CG-SD-CE	6.93	116.15	100.90
1	D	54	LYS	CB-CG-CD	6.88	127.13	111.30
1	A	599	MET	CA-CB-CG	-6.88	100.35	114.10
1	A	981	THR	CA-CB-CG2	-6.47	99.50	110.50
1	A	954	ILE	CB-CG1-CD1	-6.45	100.26	113.80
1	D	562	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	A	324	CYS	CA-CB-SG	6.34	128.98	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1007	ARG	CG-CD-NE	-6.28	98.19	112.00
1	D	984	ASP	CA-C-N	-6.12	111.31	122.38
1	D	984	ASP	C-N-CA	-6.12	111.31	122.38
1	B	220	GLN	N-CA-C	6.08	123.74	110.80
1	B	1008	THR	CA-C-N	6.06	136.59	121.80
1	B	1008	THR	C-N-CA	6.06	136.59	121.80
1	D	172	ARG	CB-CG-CD	-5.94	97.64	111.30
1	B	874	LYS	CB-CG-CD	5.80	124.63	111.30
1	A	514	SER	CA-C-N	-5.78	114.73	122.77
1	A	514	SER	C-N-CA	-5.78	114.73	122.77
1	C	446	LYS	CD-CE-NZ	5.78	130.39	111.90
1	A	674	GLY	N-CA-C	5.78	130.05	113.30
1	A	231	ILE	CB-CG1-CD1	-5.77	101.68	113.80
1	B	293	ILE	CB-CG1-CD1	-5.76	101.71	113.80
1	B	414	ASP	CA-C-N	5.75	132.53	121.54
1	B	414	ASP	C-N-CA	5.75	132.53	121.54
1	B	887	LYS	CB-CG-CD	-5.67	98.26	111.30
1	B	371	ARG	CG-CD-NE	5.62	124.37	112.00
1	B	486	ALA	CA-C-N	-5.60	114.43	122.67
1	B	486	ALA	C-N-CA	-5.60	114.43	122.67
1	D	22	THR	CA-CB-OG1	-5.60	101.21	109.60
1	D	794	GLY	N-CA-C	-5.60	99.92	113.18
1	A	977	THR	CA-CB-CG2	5.58	119.99	110.50
1	D	486	ALA	CA-C-N	-5.56	113.56	122.62
1	D	486	ALA	C-N-CA	-5.56	113.56	122.62
1	D	867	ARG	CA-C-N	-5.54	111.99	121.97
1	D	867	ARG	C-N-CA	-5.54	111.99	121.97
1	A	22	THR	CA-C-N	-5.49	113.31	122.64
1	A	22	THR	C-N-CA	-5.49	113.31	122.64
1	A	204	SER	CA-C-N	-5.46	112.00	120.31
1	A	204	SER	C-N-CA	-5.46	112.00	120.31
1	A	680	MET	CA-C-N	5.44	132.07	121.41
1	A	680	MET	C-N-CA	5.44	132.07	121.41
1	B	383	GLU	CA-CB-CG	-5.43	103.23	114.10
1	D	329	PRO	CA-C-N	-5.43	113.65	122.34
1	D	329	PRO	C-N-CA	-5.43	113.65	122.34
1	D	60	ASP	N-CA-CB	5.40	117.95	110.17
1	A	78	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	C	384	LYS	CD-CE-NZ	-5.34	94.80	111.90
1	D	793	THR	OG1-CB-CG2	-5.34	98.62	109.30
1	D	416	THR	CA-C-N	5.33	131.22	121.85
1	D	416	THR	C-N-CA	5.33	131.22	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	780	THR	OG1-CB-CG2	-5.32	98.66	109.30
1	B	371	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	220	GLN	N-CA-CB	-5.28	101.57	110.49
1	D	519	PRO	CA-N-CD	5.28	119.39	112.00
1	D	265	GLU	N-CA-C	-5.24	99.63	110.80
1	C	541	LYS	CB-CG-CD	5.23	123.32	111.30
1	A	831	CYS	CA-CB-SG	-5.22	102.39	114.40
1	C	372	ALA	CA-C-N	-5.22	112.47	122.13
1	C	372	ALA	C-N-CA	-5.22	112.47	122.13
1	A	755	GLY	CA-C-N	-5.21	109.33	121.52
1	A	755	GLY	C-N-CA	-5.21	109.33	121.52
1	B	414	ASP	N-CA-C	5.19	113.73	108.75
1	C	485	MET	CG-SD-CE	-5.18	89.50	100.90
1	C	22	THR	OG1-CB-CG2	-5.18	98.94	109.30
1	D	11	ASP	CB-CG-OD2	-5.16	106.52	118.40
1	B	828	GLN	CB-CG-CD	5.15	121.35	112.60
1	A	50	PHE	CA-C-N	-5.14	114.60	122.62
1	A	50	PHE	C-N-CA	-5.14	114.60	122.62
1	C	149	SER	CA-CB-OG	-5.13	100.83	111.10
1	A	1007	ARG	CG-CD-NE	-5.13	100.71	112.00
1	B	459	TRP	CA-CB-CG	-5.10	103.91	113.60
1	C	598	PRO	CA-C-N	5.08	129.45	122.84
1	C	598	PRO	C-N-CA	5.08	129.45	122.84
1	B	322	CYS	CA-C-N	5.08	131.23	121.54
1	B	322	CYS	C-N-CA	5.08	131.23	121.54
1	B	798	SER	CA-C-N	-5.07	113.48	120.28
1	B	798	SER	C-N-CA	-5.07	113.48	120.28
1	D	594	THR	OG1-CB-CG2	-5.07	99.17	109.30
1	A	768	THR	OG1-CB-CG2	-5.05	99.19	109.30
1	A	722	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	C	1013	PRO	CA-C-N	-5.03	114.42	121.72
1	C	1013	PRO	C-N-CA	-5.03	114.42	121.72
1	A	482	ILE	CB-CG1-CD1	-5.03	103.24	113.80
1	D	353	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	C	316	SER	CA-C-N	-5.03	114.45	122.29
1	C	316	SER	C-N-CA	-5.03	114.45	122.29
1	A	715	THR	CA-C-N	-5.02	114.94	122.47
1	A	715	THR	C-N-CA	-5.02	114.94	122.47
1	A	742	MET	CA-C-N	-5.02	114.43	121.56
1	A	742	MET	C-N-CA	-5.02	114.43	121.56
1	C	703	GLN	CB-CG-CD	5.02	121.13	112.60
1	D	53	GLU	CA-C-N	-5.02	114.33	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	GLU	C-N-CA	-5.02	114.33	121.50

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7678	0	7707	130	0
1	B	7688	0	7715	154	1
1	C	7741	0	7767	166	0
1	D	7750	0	7781	152	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	1	0
3	D	31	0	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	53	0	31	1	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	24	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	561	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 (561) 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:C:60:ASP:CG	1:C:60:ASP:CB	1.76	1.57
1:D:265:GLU:CG	1:D:265:GLU:CB	1.76	1.56
1:D:265:GLU:CG	1:D:265:GLU:CD	1.79	1.54
1:A:541:LYS:NZ	1:A:541:LYS:CE	1.70	1.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:222:TYR:OH	6:C:1209:HOH:O	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:415:GLU:C	1:B:417:GLY:H	2.00	0.70
1:C:322:CYS:SG	1:C:324:CYS:HB2	2.32	0.70
1:D:13:GLU:CD	6:D:1215:HOH:O	2.34	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:C:881:PRO:HA	1:C:884:GLU:HG3	1.77	0.67
1:B:60:ASP:OD1	1:B:894:LYS:NZ	2.21	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:399:LYS:HD2	1:D:404:VAL:HG21	1.78	0.65
1:B:943:GLN:HB2	1:B:1007:ARG:HD3	1.77	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:395:LYS:HE2	1:D:407:GLN:OE1	1.97	0.64
1:C:128:MET:HE2	1:C:157:GLN:NE2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:D:180:GLU:H	1:D:180:GLU:CD	2.11	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:A:961:MET:HE1	1:B:81:LYS:O	2.04	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:B:841:LYS:NZ	6:B:1215:HOH:O	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:VAL:HG12	1:C:166:MET:HE3	1.86	0.57
1:D:415:GLU:C	1:D:417:GLY:N	2.62	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:C:608:LEU:HB2	1:C:742:MET:HE2	1.87	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:D:343:THR:HA	4:D:1106:FAD:HM72	1.87	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:C:762:TYR:HH	1:D:779[B]:THR:HG22	1.71	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:269:ASN:O	1:B:273:GLU:CD	2.49	0.55
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:C:485:MET:HE3	1:D:31:THR:HG22	1.88	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
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: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:A:394:ARG:HH22	1:A:423:GLU:CD	2.16	0.54
1:C:124:LEU:HG	1:C:240:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:272:LYS:NZ	6:A:1240:HOH:O	2.40	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:B:887:LYS:NZ	6:B:1228:HOH:O	2.37	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:C:137:VAL:HG12	6:C:1286:HOH:O	2.08	0.53
1:C:222:TYR:CZ	6:C:1209:HOH:O	2.60	0.53
1:B:415:GLU:C	1:B:417:GLY:N	2.63	0.52
1:C:861:LYS:NZ	6:C:1213:HOH:O	2.05	0.52
1:D:371:ARG:NH1	6:D:1212:HOH:O	2.20	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:D:395:LYS:HE2	1:D:407:GLN:CD	2.35	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
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:C:248:MET:HE1	1:C:255:ILE:HD11	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:164:LYS:NZ	1:D:239:ASP:OD2	2.26	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: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:C:22:THR:HG22	1:C:23:GLN:N	2.27	0.50
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: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:192:LEU:C	1:A:193:LEU:HD22	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:681:GLY:C	1:B:682:LEU:HD23	2.39	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:651:MET:HE3	1:D:700:GLN:HG3	1.96	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:C:320:GLY:O	1:C:321:MET:C	2.56	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:A:485:MET:HB3	1:A:485:MET:HE2	1.61	0.47
1:B:869:ALA:C	1:B:871:LEU:H	2.21	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
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: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:D:458:ARG:C	1:D:460:ASP:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:371:ARG:O	1:B:47:LYS:NZ	2.36	0.47
1:A:900:GLN:NE2	6:A:1264:HOH:O	2.47	0.47
1:C:553:PRO:O	1:C:559:MET:HE2	2.15	0.47
1:A:858:SER:HB3	1:A:949:ASP:OD2	2.15	0.46
1:B:587:SER:HA	1:B:588:PRO:C	2.40	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
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:537:MET:HE2	1:C:537:MET:HB3	1.76	0.45
1:C:452:SER:HA	1:C:453:PRO:HA	1.73	0.45
1:A:115:MET:HB2	1:A:115:MET:HE2	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:LYS:NZ	6:D:1257:HOH:O	2.50	0.45
1:C:81:LYS:O	1:D:961:MET:HE1	2.17	0.45
1:B:687:ASP:HB3	1:B:690:LEU:HD12	1.99	0.45
1:C:343:THR:HA	4:C:1106:FAD:HM72	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:219:LYS:O	1:B:220:GLN:C	2.59	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:320:GLY:C	1:C:322:CYS:N	2.72	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:316:SER:OG	1:C:326:SER:O	2.19	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: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:C:132:THR:HB	1:C:137:VAL:HG23	2.00	0.44
1:D:608:LEU:HB2	1:D:742:MET:HE2	1.99	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
1:D:583:VAL:HB	1:D:612:LEU:CD1	2.47	0.44
1:D:868:ILE:O	1:D:869:ALA:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:426:ILE:HD12	1:D:426:ILE:C	2.43	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:C	1:C:322:CYS:H	2.27	0.43
1:C:623:GLN:HB3	1:D:5:LEU:HD12	2.00	0.43
1:A:934:THR:OG1	1:A:937:GLU:OE2	2.30	0.43
1:B:182:MET:HE3	1:B:186:TYR:CD1	2.53	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: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:841:LYS:NZ	6:B:1218:HOH:O	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG12	1:A:11:ASP:H	1.84	0.42
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: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:B:343:THR:HA	4:B:1106:FAD:HM72	2.02	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: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:226:LEU:O	1:C:227:SER:C	2.61	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:182:MET:HE3	1:B:182:MET:HB3	1.88	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:B:394:ARG:HH21	1:B:423:GLU:CD	2.28	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:415:GLU:C	1:D:417:GLY:H	2.27	0.42
1:D:518:LYS:HA	1:D:519:PRO:HD2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:226:LEU:O	1:B:227:SER:C	2.62	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:100:PHE:CD1	1:A:100:PHE:C	2.98	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:B:387:PHE:C	1:B:388:LEU:HD23	2.45	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:83:ALA:O	1:B:84:ASP:C	2.62	0.41
1:B:107:LYS:HB3	6:B:1348:HOH:O	2.20	0.41
1:B:993:LEU:C	1:B:993:LEU:HD23	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LYS:HG3	1:A:456:PHE:CZ	2.56	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
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:C:961:MET:HE1	1:D:81:LYS:O	2.20	0.41
1:D:414:ASP:CG	1:D:416:THR:HB	2.46	0.41
1:D:1019:LEU:HD23	1:D:1019:LEU:HA	1.72	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: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: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:A:718:VAL:O	1:A:719:SER:C	2.65	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:9:VAL:O	1:A:10:ALA:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1003/1025 (98%)	955 (95%)	41 (4%)	7 (1%)	18	14
1	B	1003/1025 (98%)	942 (94%)	49 (5%)	12 (1%)	10	6
1	C	1017/1025 (99%)	972 (96%)	43 (4%)	2 (0%)	43	42
1	D	1017/1025 (99%)	964 (95%)	41 (4%)	12 (1%)	10	6
All	All	4040/4100 (98%)	3833 (95%)	174 (4%)	33 (1%)	16	11

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
1	A	416	THR
1	B	219	LYS

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Mol	Chain	Res	Type
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
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%)	841 (100%)	1 (0%)	88 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	845/854 (99%)	842 (100%)	3 (0%)	84	89
1	C	852/854 (100%)	850 (100%)	2 (0%)	87	92
1	D	851/854 (100%)	851 (100%)	0	100	100
All	All	3390/3416 (99%)	3384 (100%)	6 (0%)	88	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	519	PRO
1	B	460	ASP
1	B	932[A]	LEU
1	B	932[B]	LEU
1	C	932[A]	LEU
1	C	932[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	167	ASN
1	A	179	GLN
1	A	413	GLN
1	A	648	ASN
1	B	48	ASN
1	B	57	ASN
1	B	242	ASN
1	B	407	GLN
1	B	487	ASN
1	B	494	ASN
1	B	498	GLN
1	B	508	GLN
1	B	648	ASN
1	B	878	ASN
1	C	23	GLN
1	C	157	GLN
1	C	420	ASN
1	C	494	ASN
1	C	901	ASN
1	D	167	ASN
1	D	242	ASN

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Mol	Chain	Res	Type
1	D	420	ASN
1	D	635	ASN
1	D	878	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
2	SF4	B	1101	1	0,12,12	-	-	-		
2	SF4	B	1104	1	0,12,12	-	-	-		
2	SF4	D	1102	1	0,12,12	-	-	-		
4	FAD	A	1106	-	58,58,58	0.81	1 (1%)	85,89,89	0.85	5 (5%)
2	SF4	A	1103	1	0,12,12	-	-	-		
2	SF4	C	1102	1	0,12,12	-	-	-		
2	SF4	A	1102	1	0,12,12	-	-	-		
2	SF4	D	1104	1	0,12,12	-	-	-		
2	SF4	A	1101	1	0,12,12	-	-	-		
5	Y3G	B	1107	-	9,10,10	4.19	7 (77%)	12,13,13	4.57	7 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	1104	1	0,12,12	-	-	-		
5	Y3G	D	1107	-	9,10,10	5.07	5 (55%)	12,13,13	6.31	10 (83%)
2	SF4	D	1103	1	0,12,12	-	-	-		
2	SF4	C	1103	1	0,12,12	-	-	-		
3	FMN	C	1105	-	33,33,33	1.86	10 (30%)	48,50,50	1.84	14 (29%)
4	FAD	C	1106	-	58,58,58	0.86	3 (5%)	85,89,89	0.69	1 (1%)
5	Y3G	C	1107	-	9,10,10	4.24	4 (44%)	12,13,13	6.19	9 (75%)
2	SF4	D	1101	1	0,12,12	-	-	-		
5	Y3G	A	1107	-	9,10,10	4.62	5 (55%)	12,13,13	4.42	8 (66%)
3	FMN	A	1105	-	33,33,33	1.88	12 (36%)	48,50,50	1.69	16 (33%)
4	FAD	D	1106	-	58,58,58	0.98	3 (5%)	85,89,89	0.87	6 (7%)
2	SF4	B	1103	1	0,12,12	-	-	-		
2	SF4	C	1101	1	0,12,12	-	-	-		
2	SF4	C	1104	1	0,12,12	-	-	-		
4	FAD	B	1106	-	58,58,58	0.82	2 (3%)	85,89,89	0.98	4 (4%)
3	FMN	B	1105	-	33,33,33	1.69	3 (9%)	48,50,50	1.61	10 (20%)
2	SF4	B	1102	1	0,12,12	-	-	-		
3	FMN	D	1105	-	33,33,33	2.04	9 (27%)	48,50,50	1.73	12 (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
2	SF4	B	1101	1	-	-	0/6/5/5
2	SF4	B	1104	1	-	-	0/6/5/5
2	SF4	D	1102	1	-	-	0/6/5/5
4	FAD	A	1106	-	-	4/34/50/50	0/6/6/6
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	C	1102	1	-	-	0/6/5/5
2	SF4	A	1102	1	-	-	0/6/5/5
2	SF4	D	1104	1	-	-	0/6/5/5
2	SF4	A	1101	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
5	Y3G	D	1107	-	-	0/0/2/2	0/1/1/1
2	SF4	D	1103	1	-	-	0/6/5/5
2	SF4	C	1103	1	-	-	0/6/5/5
3	FMN	C	1105	-	-	2/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	C	1106	-	-	1/34/50/50	0/6/6/6
5	Y3G	C	1107	-	-	0/0/2/2	0/1/1/1
2	SF4	D	1101	1	-	-	0/6/5/5
5	Y3G	A	1107	-	-	0/0/2/2	0/1/1/1
3	FMN	A	1105	-	-	2/18/18/18	0/3/3/3
4	FAD	D	1106	-	-	1/34/50/50	0/6/6/6
2	SF4	B	1103	1	-	-	0/6/5/5
2	SF4	C	1101	1	-	-	0/6/5/5
2	SF4	C	1104	1	-	-	0/6/5/5
4	FAD	B	1106	-	-	4/34/50/50	0/6/6/6
3	FMN	B	1105	-	-	4/18/18/18	0/3/3/3
2	SF4	B	1102	1	-	-	0/6/5/5
3	FMN	D	1105	-	-	2/18/18/18	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1107	Y3G	O08-C01	11.57	1.45	1.23
5	A	1107	Y3G	O08-C01	9.84	1.42	1.23
5	C	1107	Y3G	O08-C01	9.37	1.41	1.23
5	B	1107	Y3G	O08-C01	8.10	1.38	1.23
5	A	1107	Y3G	O07-C03	7.43	1.39	1.23
5	D	1107	Y3G	O07-C03	7.39	1.39	1.23
5	B	1107	Y3G	O07-C03	7.21	1.38	1.23
5	C	1107	Y3G	O07-C03	6.36	1.36	1.23
3	B	1105	FMN	C4A-N5	5.53	1.42	1.30
3	C	1105	FMN	C4A-N5	5.10	1.41	1.30
3	A	1105	FMN	C4A-N5	5.09	1.41	1.30
3	D	1105	FMN	C9-C8	5.02	1.46	1.39
5	D	1107	Y3G	C09-C06	4.77	1.50	1.43
3	D	1105	FMN	C10-N1	4.22	1.41	1.33
3	D	1105	FMN	O2-C2	-4.08	1.16	1.24
5	A	1107	Y3G	C09-C06	4.00	1.49	1.43
4	C	1106	FAD	C4X-N5	3.84	1.39	1.30
3	B	1105	FMN	C1'-N10	3.68	1.56	1.47
3	B	1105	FMN	C10-N1	3.63	1.40	1.33
5	C	1107	Y3G	C06-C01	-3.53	1.38	1.44
5	C	1107	Y3G	C05-N04	-3.40	1.30	1.36
3	D	1105	FMN	C6-C7	3.37	1.44	1.39
3	D	1105	FMN	C4A-N5	3.34	1.38	1.30
3	A	1105	FMN	O4-C4	3.33	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	FAD	P-O2P	-3.33	1.39	1.55
3	C	1105	FMN	C1'-C2'	3.32	1.57	1.52
5	B	1107	Y3G	C01-N02	-3.28	1.32	1.38
4	D	1106	FAD	P-O2P	-3.21	1.40	1.55
5	B	1107	Y3G	C03-N02	-3.20	1.32	1.37
5	A	1107	Y3G	C05-N04	-3.18	1.31	1.36
3	D	1105	FMN	O4-C4	3.13	1.29	1.23
4	B	1106	FAD	P-O3P	3.03	1.62	1.59
3	A	1105	FMN	C9-C8	2.84	1.43	1.39
5	D	1107	Y3G	C05-N04	-2.76	1.31	1.36
3	C	1105	FMN	C9-C9A	2.75	1.44	1.39
3	C	1105	FMN	C8M-C8	2.67	1.56	1.51
5	A	1107	Y3G	C03-N04	-2.62	1.33	1.36
3	C	1105	FMN	C2-N1	2.58	1.42	1.36
5	D	1107	Y3G	C03-N02	-2.57	1.33	1.37
3	A	1105	FMN	C1'-C2'	2.57	1.56	1.52
5	B	1107	Y3G	C03-N04	-2.56	1.33	1.36
3	A	1105	FMN	C9A-C5A	-2.53	1.37	1.41
3	C	1105	FMN	C7M-C7	-2.53	1.46	1.51
3	C	1105	FMN	C9A-N10	-2.51	1.36	1.41
3	A	1105	FMN	C9-C9A	2.48	1.43	1.39
4	C	1106	FAD	P-O3P	-2.36	1.57	1.59
3	A	1105	FMN	C4A-C4	-2.35	1.35	1.44
5	B	1107	Y3G	C05-N04	-2.31	1.32	1.36
4	D	1106	FAD	PA-O3P	-2.28	1.57	1.59
3	D	1105	FMN	C6-C5A	2.27	1.43	1.40
3	A	1105	FMN	C4'-C3'	2.25	1.57	1.53
3	D	1105	FMN	C9-C9A	2.16	1.43	1.39
3	A	1105	FMN	C10-N1	2.16	1.37	1.33
3	D	1105	FMN	C7M-C7	2.15	1.55	1.51
3	A	1105	FMN	C8M-C8	2.15	1.55	1.51
4	D	1106	FAD	C4X-N5	2.15	1.35	1.30
3	A	1105	FMN	C9A-N10	-2.15	1.37	1.41
4	C	1106	FAD	PA-O3P	-2.12	1.57	1.59
3	C	1105	FMN	P-O2P	-2.08	1.47	1.54
3	C	1105	FMN	C10-N1	2.07	1.37	1.33
4	B	1106	FAD	C6-C5X	2.07	1.43	1.40
5	B	1107	Y3G	C06-C01	-2.03	1.41	1.44
3	C	1105	FMN	C1'-N10	2.02	1.52	1.47
3	A	1105	FMN	C5'-C4'	2.02	1.54	1.51

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1107	Y3G	N04-C03-N02	12.77	128.64	115.17
5	C	1107	Y3G	N04-C03-N02	11.02	126.80	115.17
5	B	1107	Y3G	N04-C03-N02	10.30	126.03	115.17
5	A	1107	Y3G	N04-C03-N02	9.82	125.53	115.17
5	C	1107	Y3G	O07-C03-N04	-9.75	112.74	122.79
5	D	1107	Y3G	O07-C03-N04	-8.98	113.53	122.79
5	C	1107	Y3G	O08-C01-C06	-8.56	114.58	125.12
5	D	1107	Y3G	O08-C01-C06	-7.90	115.39	125.12
5	D	1107	Y3G	C01-N02-C03	-7.76	115.68	126.37
5	C	1107	Y3G	C01-N02-C03	-7.69	115.78	126.37
5	D	1107	Y3G	C05-C06-C01	7.57	126.05	119.07
5	C	1107	Y3G	C05-C06-C01	7.28	125.78	119.07
5	B	1107	Y3G	C05-C06-C01	6.52	125.07	119.07
5	A	1107	Y3G	C05-N04-C03	-5.87	117.24	122.69
5	B	1107	Y3G	C05-C06-C09	-5.65	114.17	122.35
5	A	1107	Y3G	O07-C03-N04	-5.41	117.21	122.79
5	A	1107	Y3G	C05-C06-C09	-5.33	114.64	122.35
3	C	1105	FMN	O3'-C3'-C4'	-4.50	98.70	108.93
5	D	1107	Y3G	O08-C01-N02	4.39	128.37	120.11
3	A	1105	FMN	C4-C4A-C10	4.37	124.43	116.93
3	C	1105	FMN	C4-N3-C2	-4.37	117.88	125.64
5	B	1107	Y3G	C01-N02-C03	-4.36	120.37	126.37
5	C	1107	Y3G	O08-C01-N02	4.35	128.30	120.11
5	C	1107	Y3G	C09-C06-C01	-4.23	112.96	118.96
3	B	1105	FMN	C5A-C9A-N10	4.20	121.76	117.97
5	B	1107	Y3G	C05-N04-C03	-4.04	118.94	122.69
4	B	1106	FAD	O3P-P-O1P	-4.02	98.62	110.70
5	B	1107	Y3G	O07-C03-N04	-3.94	118.72	122.79
5	A	1107	Y3G	C01-N02-C03	-3.94	120.94	126.37
5	A	1107	Y3G	C05-C06-C01	3.76	122.53	119.07
5	B	1107	Y3G	O07-C03-N02	-3.73	115.23	121.86
5	C	1107	Y3G	C05-N04-C03	-3.68	119.28	122.69
3	D	1105	FMN	O2-C2-N3	-3.55	111.77	118.58
3	B	1105	FMN	C8M-C8-C9	3.50	125.74	119.57
3	D	1105	FMN	C4-C4A-N5	-3.49	113.39	118.21
3	B	1105	FMN	C8M-C8-C7	-3.46	113.70	120.76
5	D	1107	Y3G	C05-N04-C03	-3.43	119.51	122.69
3	C	1105	FMN	C10-C4A-N5	-3.31	118.05	124.81
3	B	1105	FMN	O3P-P-O2P	3.25	119.97	107.80
3	C	1105	FMN	C4-C4A-C10	3.23	122.47	116.93
3	A	1105	FMN	O2-C2-N3	-3.16	112.51	118.58
3	C	1105	FMN	O4-C4-C4A	-3.13	118.28	126.53
3	D	1105	FMN	C5A-C9A-N10	3.09	120.76	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1105	FMN	N3-C2-N1	3.05	125.98	119.50
3	C	1105	FMN	C4A-C10-N1	-3.00	117.23	124.59
5	D	1107	Y3G	C09-C06-C01	-2.96	114.75	118.96
3	B	1105	FMN	O2P-P-O1P	-2.96	99.30	110.83
3	D	1105	FMN	O4'-C4'-C5'	-2.94	103.50	109.99
4	B	1106	FAD	O3B-C3B-C4B	-2.92	102.70	111.08
3	D	1105	FMN	C4-C4A-C10	2.89	121.89	116.93
4	B	1106	FAD	O2P-P-O1P	2.85	125.72	112.44
3	C	1105	FMN	O3P-P-O2P	2.81	118.34	107.80
3	A	1105	FMN	C4-C4A-N5	-2.80	114.34	118.21
3	A	1105	FMN	O3P-P-O2P	2.74	118.08	107.80
3	C	1105	FMN	C4A-C4-N3	2.72	120.19	113.25
5	A	1107	Y3G	C09-C06-C01	2.72	122.82	118.96
3	D	1105	FMN	O3'-C3'-C4'	-2.69	102.82	108.93
3	D	1105	FMN	O3P-P-O5'	-2.68	99.69	106.67
4	D	1106	FAD	O4B-C1B-N9A	-2.66	102.98	108.09
3	D	1105	FMN	C9A-C5A-N5	-2.63	119.66	122.45
5	C	1107	Y3G	C06-C01-N02	2.63	117.07	114.14
3	A	1105	FMN	C8M-C8-C9	2.62	124.19	119.57
3	A	1105	FMN	N3-C2-N1	2.61	125.06	119.50
5	A	1107	Y3G	O07-C03-N02	-2.60	117.25	121.86
3	C	1105	FMN	C4A-C10-N10	2.57	120.16	116.48
3	D	1105	FMN	C1'-N10-C9A	-2.56	115.65	120.63
3	B	1105	FMN	C9-C9A-N10	-2.56	118.42	121.85
4	D	1106	FAD	O3'-C3'-C2'	-2.55	103.13	108.93
4	D	1106	FAD	O4'-C4'-C3'	-2.54	103.30	109.25
3	A	1105	FMN	O2'-C2'-C3'	2.52	115.15	109.25
3	C	1105	FMN	C5A-C9A-N10	2.51	120.23	117.97
4	D	1106	FAD	O3P-P-O1P	-2.51	103.17	110.70
3	A	1105	FMN	O4-C4-N3	2.42	124.67	120.11
4	A	1106	FAD	O5B-PA-O1A	-2.39	99.45	108.94
3	A	1105	FMN	O2P-P-O5'	-2.37	100.50	106.67
3	A	1105	FMN	O4'-C4'-C5'	2.36	115.19	109.99
4	C	1106	FAD	O2P-P-O1P	2.36	123.41	112.44
4	D	1106	FAD	O2P-P-O1P	2.34	123.34	112.44
3	C	1105	FMN	C7M-C7-C6	-2.32	115.48	119.57
3	C	1105	FMN	O3P-P-O1P	2.32	119.88	110.83
5	D	1107	Y3G	C05-C06-C09	-2.32	119.00	122.35
3	B	1105	FMN	O4-C4-C4A	-2.28	120.51	126.53
5	D	1107	Y3G	O07-C03-N02	-2.27	117.83	121.86
4	B	1106	FAD	O2P-P-O5'	2.24	117.74	107.57
4	A	1106	FAD	O2'-C2'-C1'	-2.23	101.03	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1106	FAD	C4'-C3'-C2'	2.19	117.21	113.57
3	B	1105	FMN	C7M-C7-C8	-2.19	116.29	120.76
3	B	1105	FMN	C7M-C7-C6	2.18	123.42	119.57
3	D	1105	FMN	C4-N3-C2	-2.17	121.79	125.64
4	A	1106	FAD	O3'-C3'-C4'	-2.17	104.01	108.93
3	A	1105	FMN	C5A-C9A-N10	2.16	119.92	117.97
4	A	1106	FAD	O2A-PA-O1A	2.13	122.37	112.44
3	D	1105	FMN	C8M-C8-C7	-2.12	116.43	120.76
3	A	1105	FMN	C9-C8-C7	-2.12	116.58	119.69
4	A	1106	FAD	O2A-PA-O3P	2.09	112.93	107.27
3	C	1105	FMN	C9-C8-C7	-2.09	116.61	119.69
3	A	1105	FMN	O4'-C4'-C3'	2.09	114.13	109.25
3	B	1105	FMN	C5A-N5-C4A	-2.08	114.73	118.09
3	A	1105	FMN	C4-N3-C2	-2.04	122.02	125.64
3	A	1105	FMN	C7M-C7-C6	-2.03	115.99	119.57
3	C	1105	FMN	C1'-C2'-C3'	2.01	115.11	109.66
3	A	1105	FMN	C10-N1-C2	-2.01	112.49	116.85

There are no chirality outliers.

All (20) 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'
4	A	1106	FAD	C2B-C1B-N9A-C8A
3	A	1105	FMN	C4'-C5'-O5'-P
4	B	1106	FAD	C2B-C1B-N9A-C8A
3	C	1105	FMN	O3'-C3'-C4'-O4'
3	D	1105	FMN	O3'-C3'-C4'-C5'
3	C	1105	FMN	C4'-C5'-O5'-P
3	D	1105	FMN	C4'-C5'-O5'-P
4	B	1106	FAD	P-O3P-PA-O2A
4	D	1106	FAD	PA-O3P-P-O5'
3	B	1105	FMN	C4'-C5'-O5'-P
3	A	1105	FMN	O3'-C3'-C4'-O4'
4	C	1106	FAD	C2B-C1B-N9A-C8A
4	A	1106	FAD	P-O3P-PA-O2A
4	A	1106	FAD	O4B-C4B-C5B-O5B

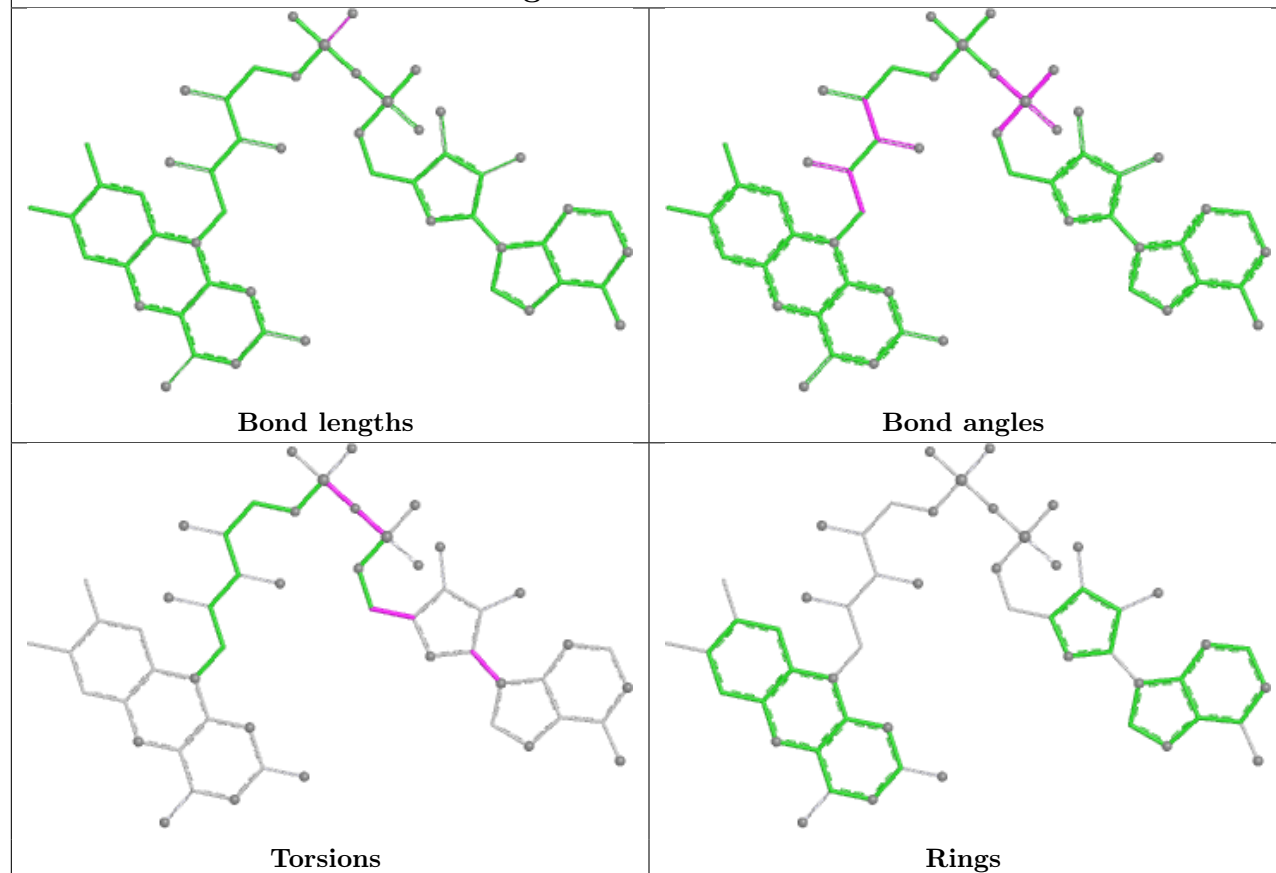
There are no ring outliers.

13 monomers are involved in 20 short contacts:

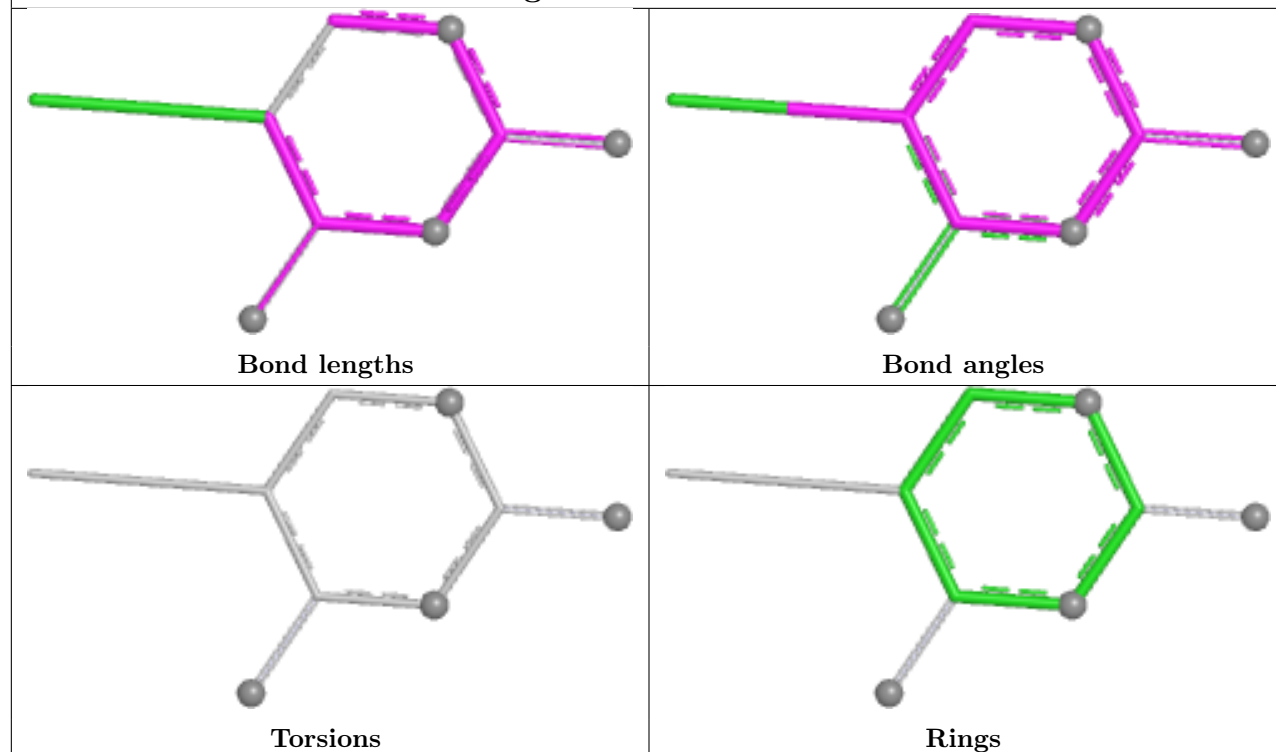
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	SF4	1	0
4	A	1106	FAD	1	0
2	A	1101	SF4	2	0
5	B	1107	Y3G	2	0
5	D	1107	Y3G	1	0
3	C	1105	FMN	1	0
4	C	1106	FAD	1	0
5	C	1107	Y3G	2	0
5	A	1107	Y3G	1	0
4	D	1106	FAD	1	0
2	C	1101	SF4	1	0
4	B	1106	FAD	2	0
3	D	1105	FMN	4	0

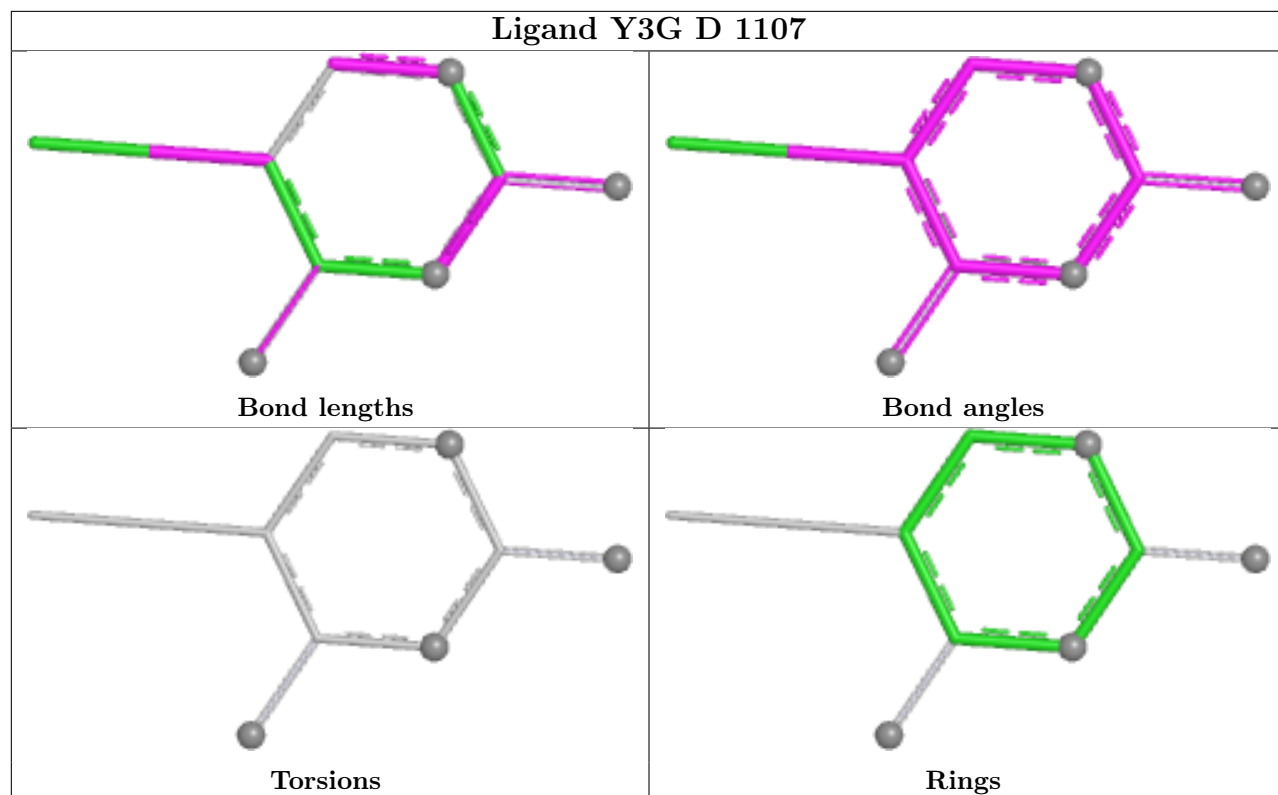
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD A 1106

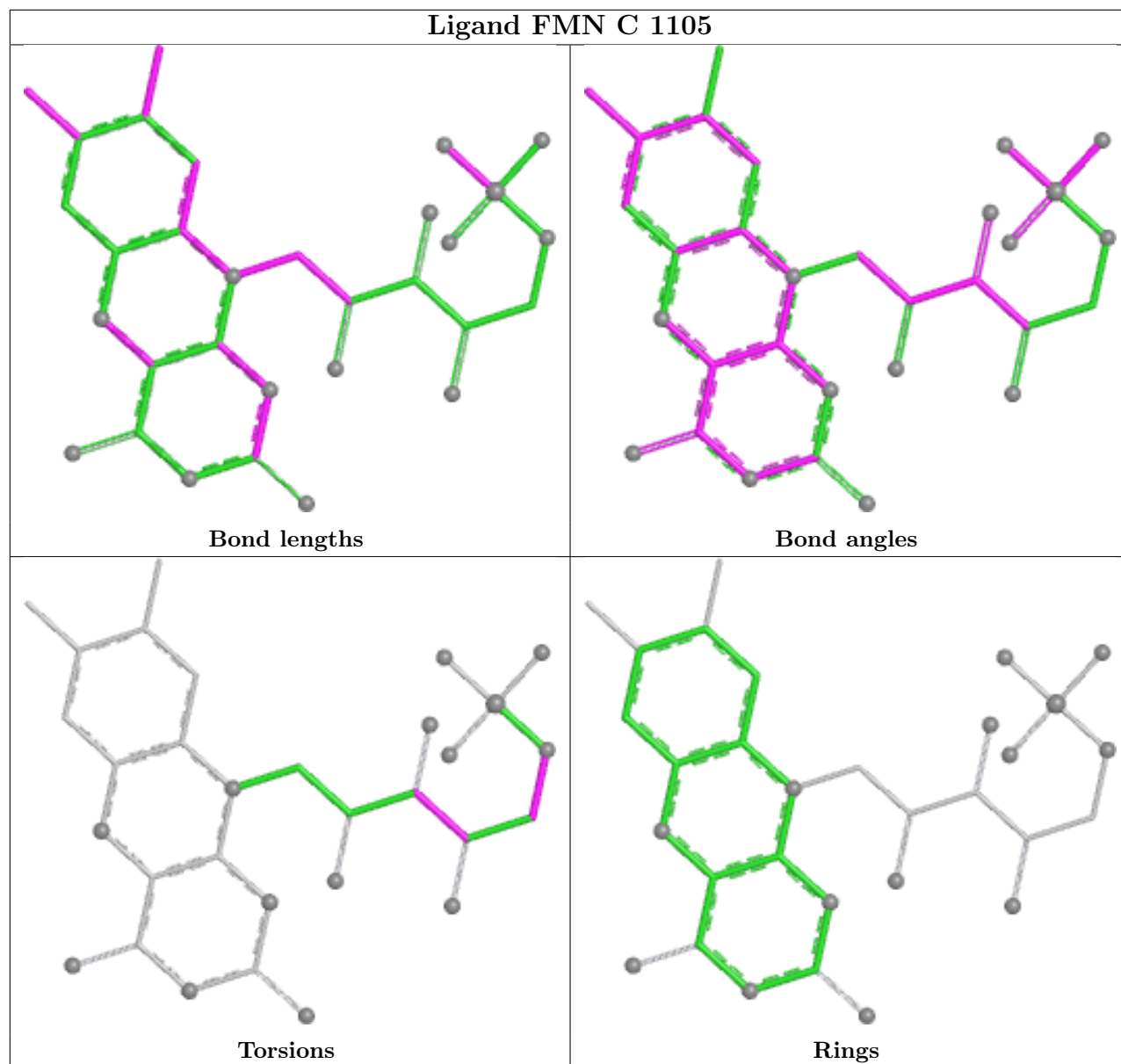


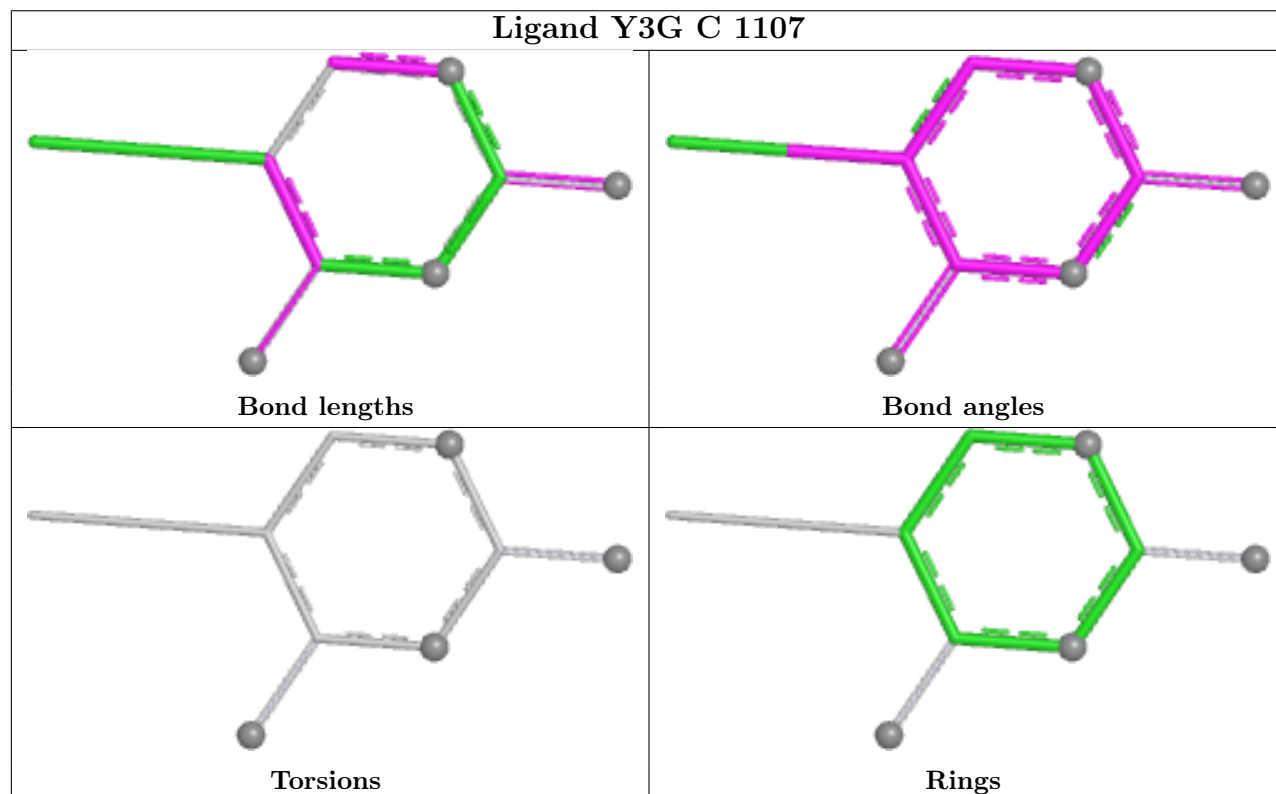
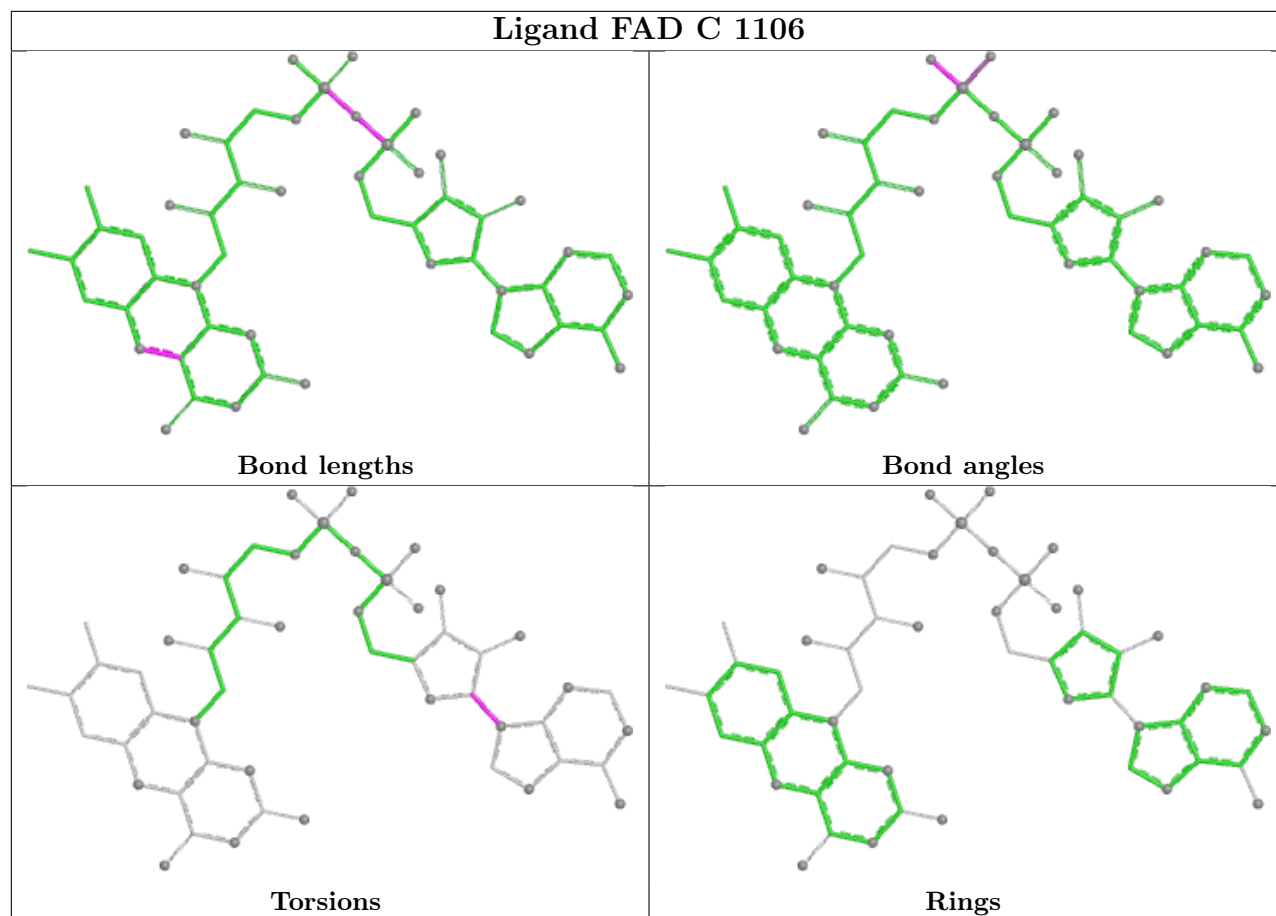
Ligand Y3G B 1107

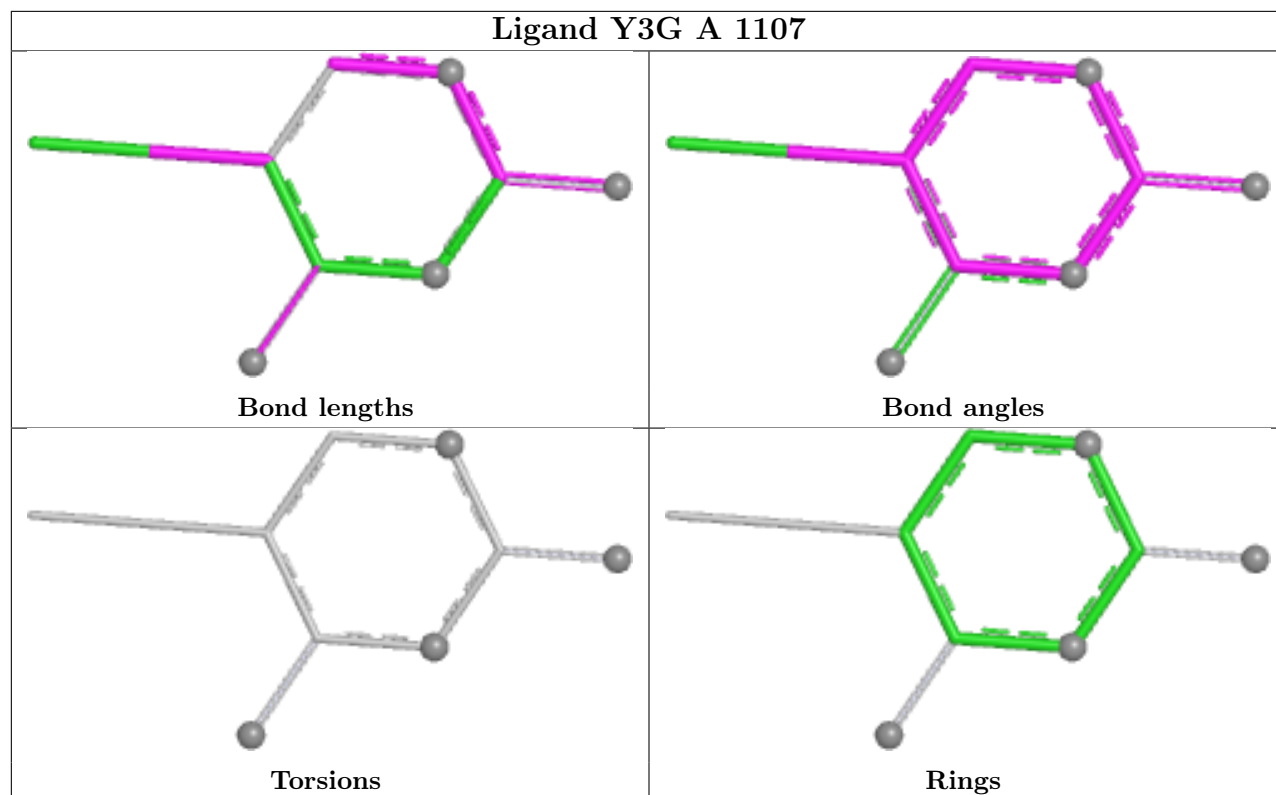




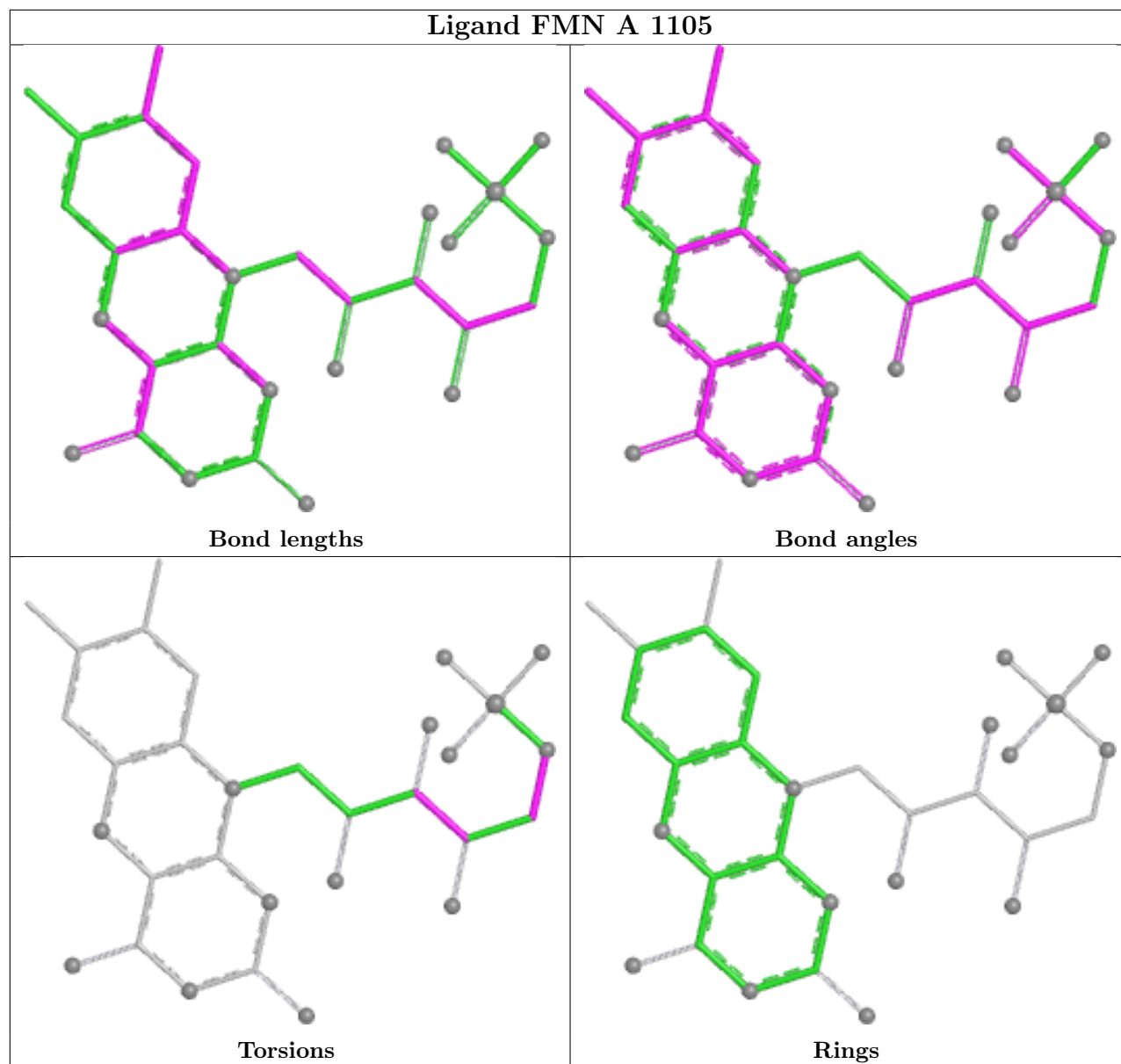
Ligand FMN C 1105

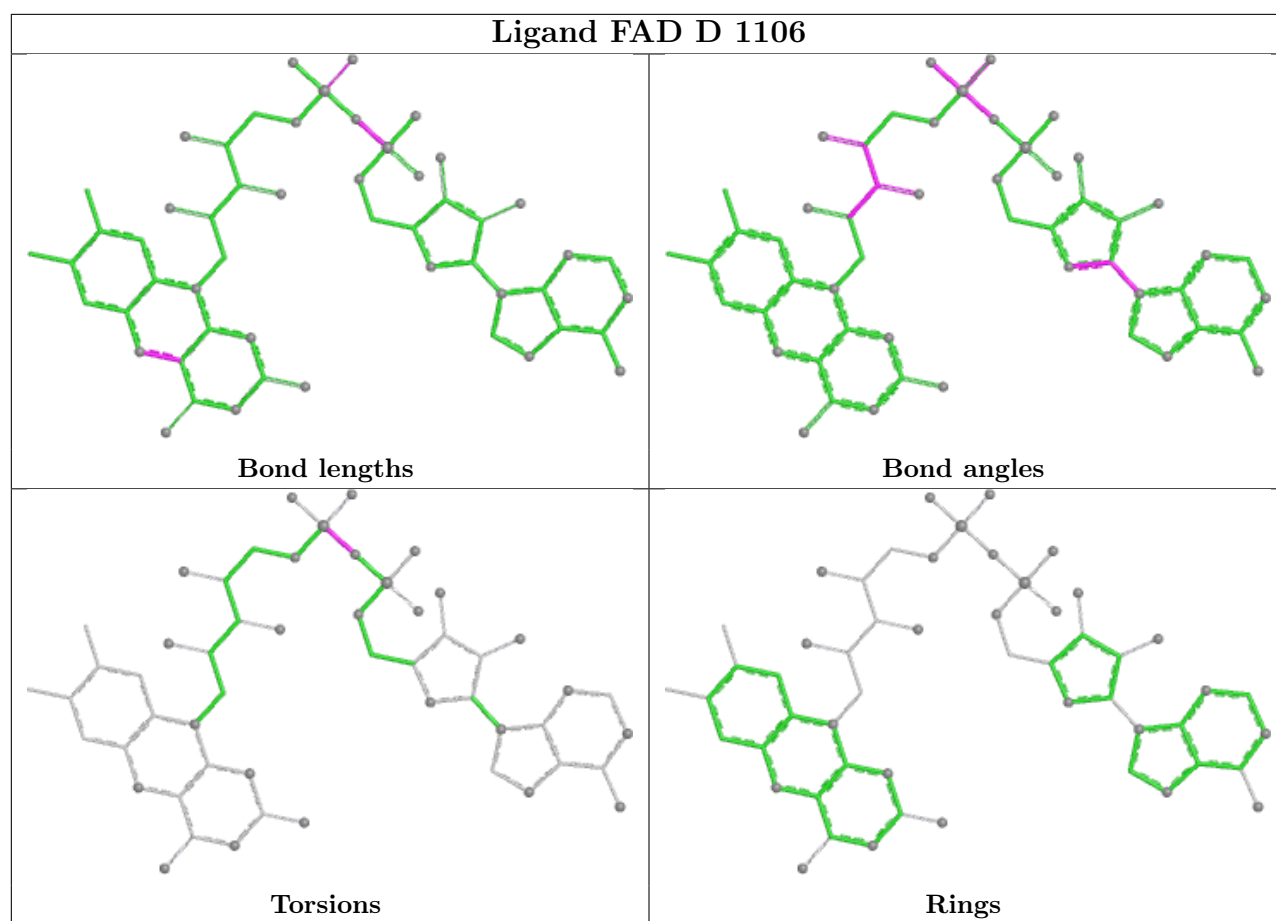


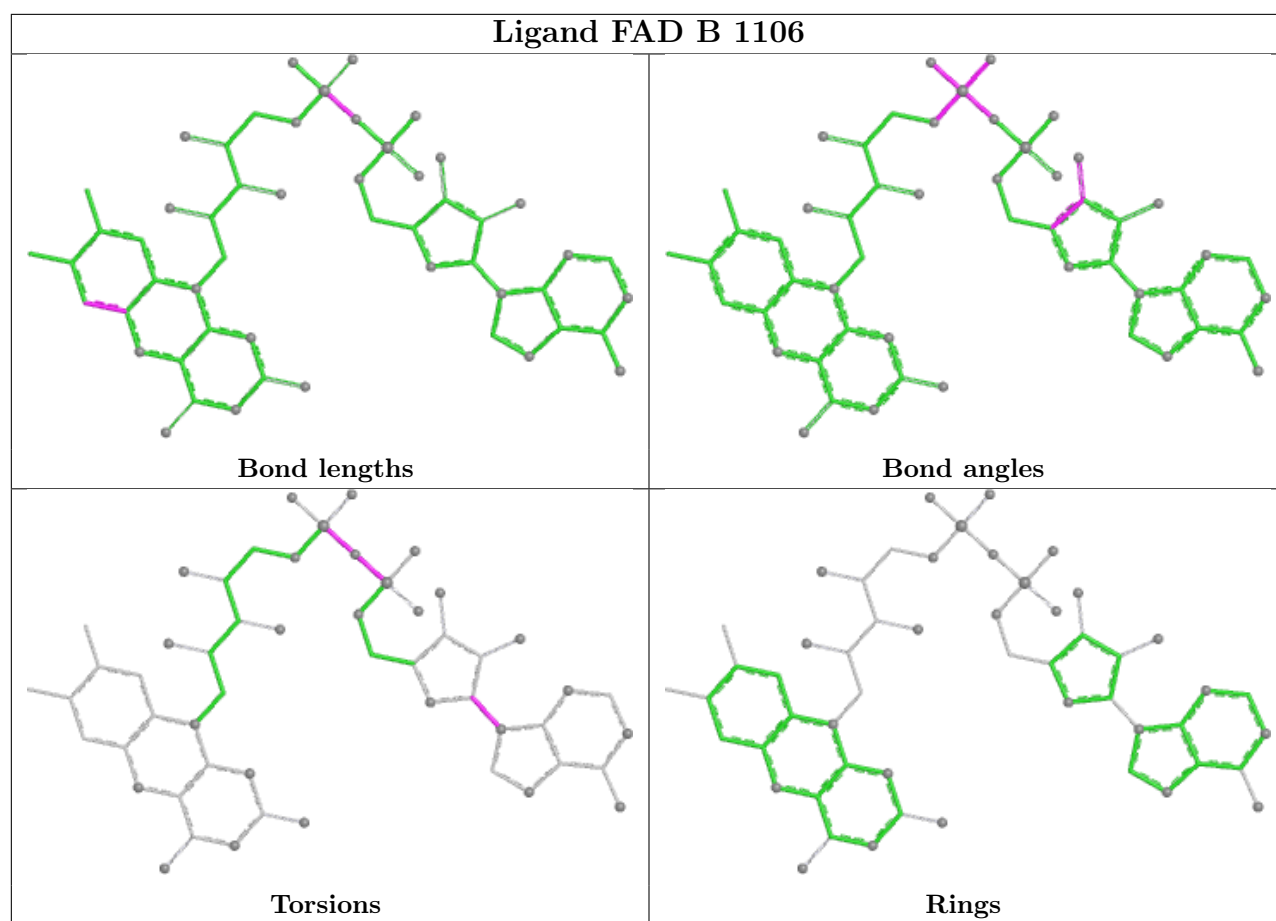


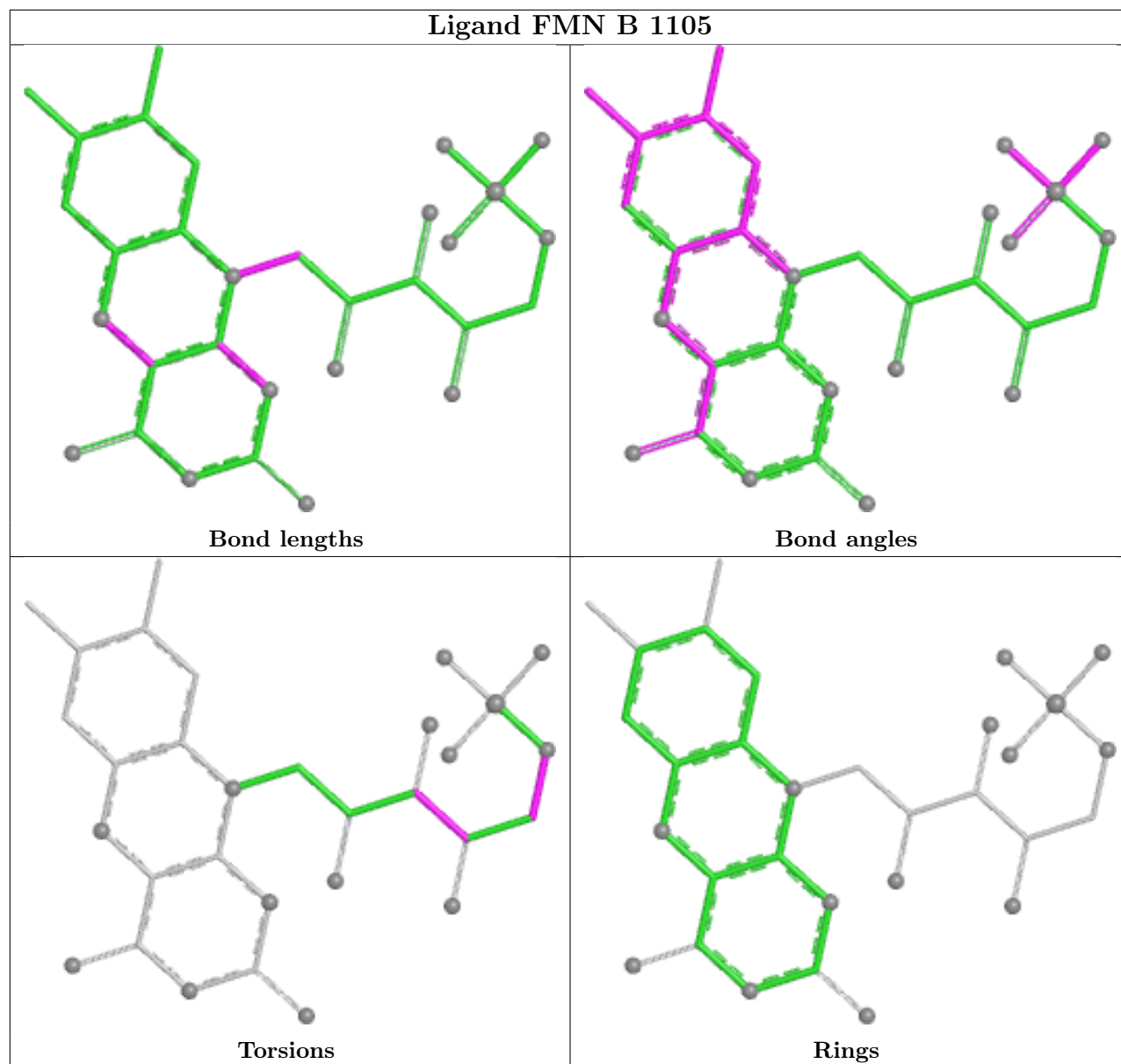


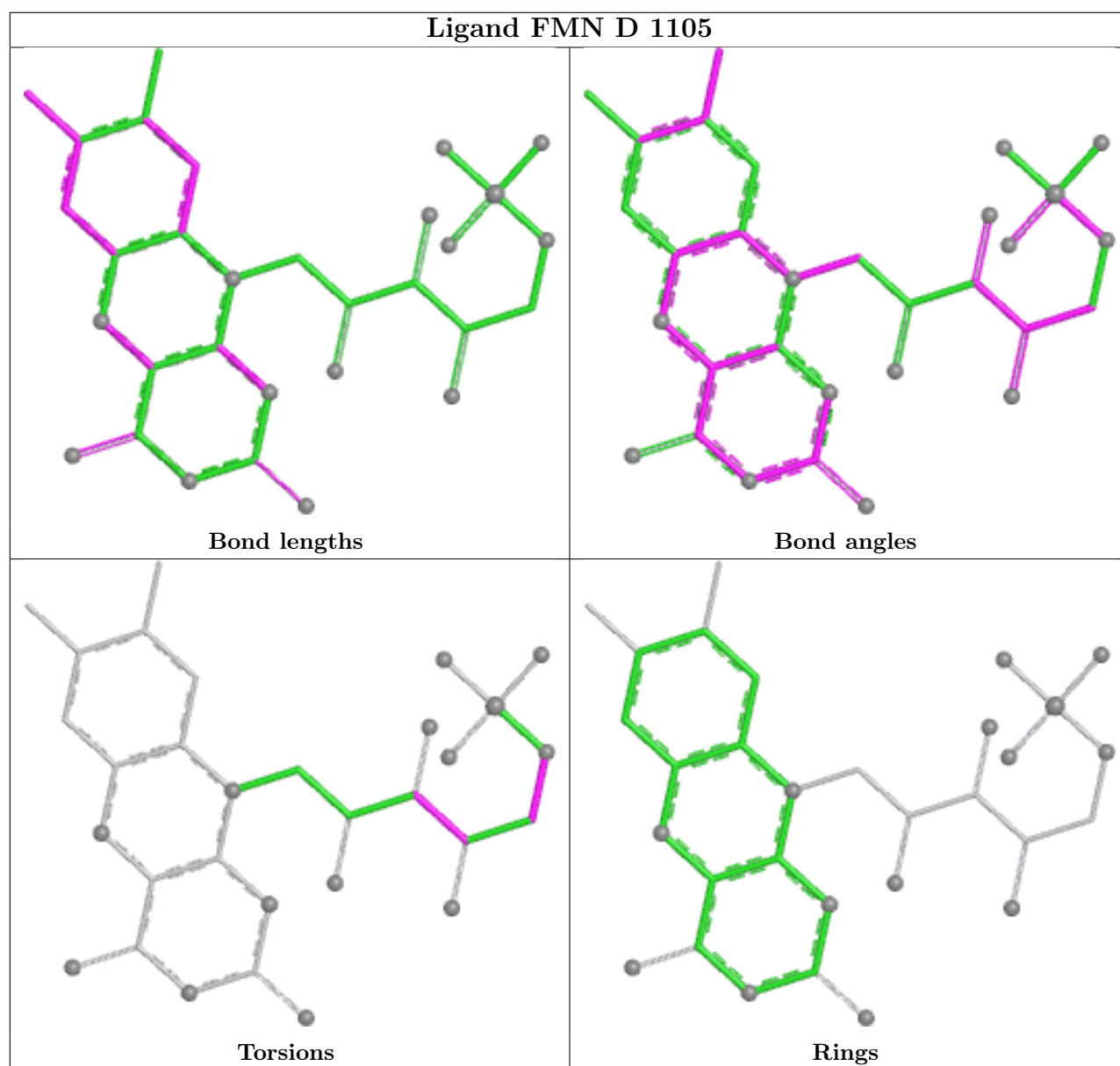
Ligand FMN A 1105











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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1005/1025 (98%)	-0.12	14 (1%) 73 73	17, 29, 49, 71	4 (0%)
1	B	1004/1025 (97%)	-0.16	11 (1%) 78 77	18, 29, 48, 66	5 (0%)
1	C	1010/1025 (98%)	-0.20	18 (1%) 67 67	14, 26, 46, 70	11 (1%)
1	D	1014/1025 (98%)	-0.20	12 (1%) 76 76	14, 26, 44, 63	7 (0%)
All	All	4033/4100 (98%)	-0.17	55 (1%) 73 73	14, 28, 47, 71	27 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	676	GLY	7.1
1	A	2	ALA	5.8
1	C	2	ALA	5.0
1	D	902	ALA	4.9
1	B	1010	PRO	4.8
1	B	273	GLU	4.3
1	D	2	ALA	4.0
1	A	680	MET	4.0
1	C	1017	LEU	3.6
1	B	416	THR	3.5
1	A	324	CYS	3.2
1	A	1010	PRO	3.2
1	C	324	CYS	3.2
1	D	416	THR	3.1
1	C	60	ASP	3.0
1	C	682	LEU	2.9
1	C	367	PHE	2.8
1	C	325	HIS	2.8
1	C	319	ALA	2.8
1	A	1009	THR	2.8
1	D	901	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	674	GLY	2.7
1	B	682	LEU	2.7
1	D	52	CYS	2.7
1	C	675	MET	2.7
1	B	52	CYS	2.7
1	A	900	GLN	2.6
1	A	984	ASP	2.6
1	A	417	GLY	2.6
1	D	1010	PRO	2.6
1	A	51	HIS	2.5
1	A	367	PHE	2.5
1	D	677	GLU	2.4
1	C	872	MET	2.4
1	C	52	CYS	2.4
1	B	873	GLY	2.4
1	D	680	MET	2.4
1	C	903	ALA	2.3
1	C	907	LEU	2.3
1	C	10	ALA	2.3
1	D	51	HIS	2.3
1	C	873	GLY	2.2
1	D	367	PHE	2.2
1	C	1010	PRO	2.2
1	D	60	ASP	2.2
1	A	25	HIS	2.1
1	B	673	HIS	2.1
1	A	872	MET	2.1
1	B	681	GLY	2.1
1	C	322	CYS	2.0
1	B	371	ARG	2.0
1	B	680	MET	2.0
1	B	900	GLN	2.0
1	A	60	ASP	2.0
1	A	674	GLY	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

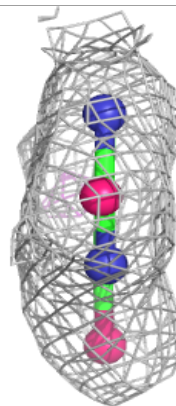
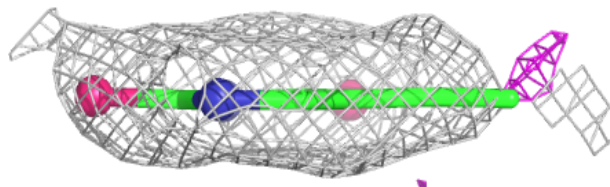
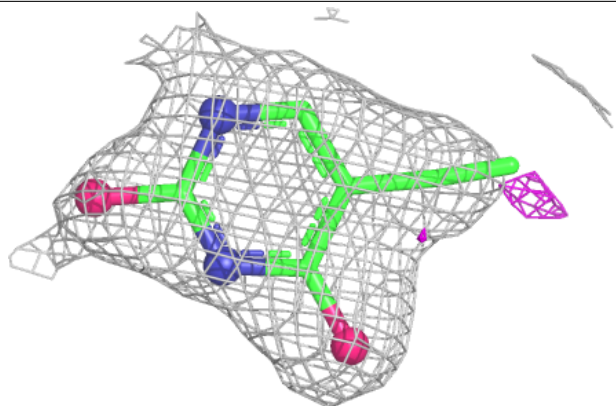
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	Y3G	B	1107	10/10	0.89	0.09	36,36,37,37	0
5	Y3G	D	1107	10/10	0.89	0.10	32,33,34,34	0
5	Y3G	C	1107	10/10	0.90	0.09	32,32,32,32	0
2	SF4	C	1103	8/8	0.90	0.07	17,18,18,18	0
5	Y3G	A	1107	10/10	0.91	0.09	39,39,40,40	0
2	SF4	B	1103	8/8	0.91	0.07	20,21,21,21	0
2	SF4	A	1104	8/8	0.92	0.08	22,22,23,23	0
2	SF4	B	1104	8/8	0.92	0.08	21,21,22,22	0
2	SF4	B	1102	8/8	0.92	0.07	17,17,17,18	0
2	SF4	D	1103	8/8	0.92	0.07	18,19,20,20	0
2	SF4	D	1104	8/8	0.93	0.07	18,18,18,19	0
2	SF4	A	1103	8/8	0.93	0.08	19,20,20,21	0
2	SF4	C	1104	8/8	0.93	0.06	17,17,18,19	0
2	SF4	D	1102	8/8	0.93	0.06	15,16,17,17	0
2	SF4	C	1102	8/8	0.93	0.06	16,16,17,17	0
2	SF4	A	1102	8/8	0.94	0.06	17,18,18,18	0
2	SF4	B	1101	8/8	0.94	0.07	19,19,20,20	0
2	SF4	D	1101	8/8	0.94	0.07	15,17,18,18	0
2	SF4	C	1101	8/8	0.94	0.06	16,17,17,18	0
2	SF4	A	1101	8/8	0.94	0.07	19,19,20,20	0
4	FAD	B	1106	53/53	0.96	0.06	22,23,25,25	0
3	FMN	D	1105	31/31	0.97	0.05	17,18,18,18	0
4	FAD	A	1106	53/53	0.97	0.06	22,24,24,24	0
3	FMN	A	1105	31/31	0.97	0.05	22,22,23,23	0
4	FAD	C	1106	53/53	0.97	0.06	21,23,25,25	0
3	FMN	C	1105	31/31	0.98	0.05	18,19,21,22	0
4	FAD	D	1106	53/53	0.98	0.05	20,21,23,24	0
3	FMN	B	1105	31/31	0.98	0.05	22,22,23,23	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.

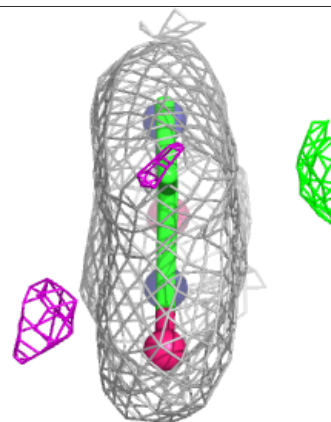
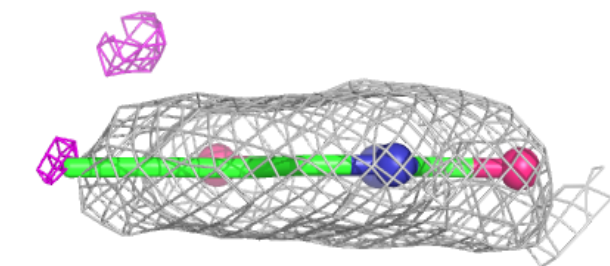
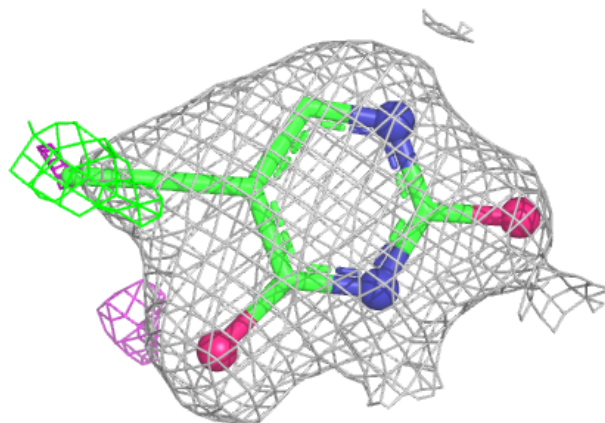
Electron density around Y3G B 1107:

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



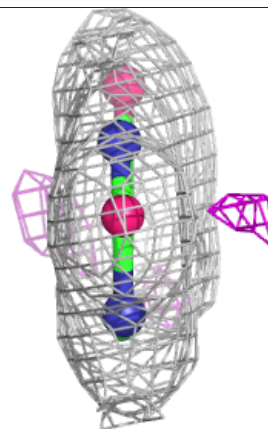
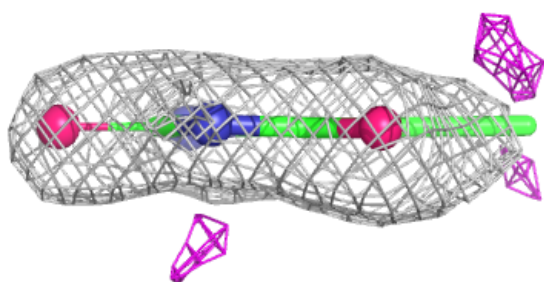
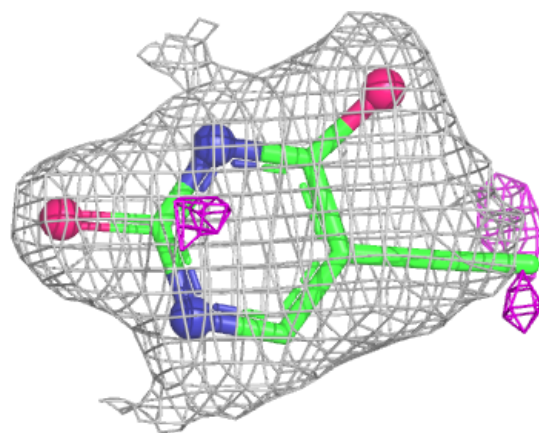
Electron density around Y3G D 1107:

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



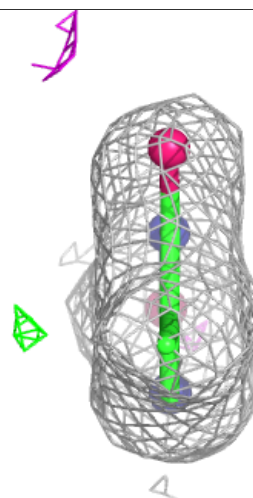
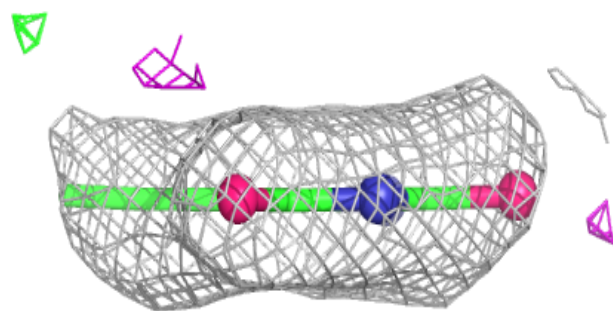
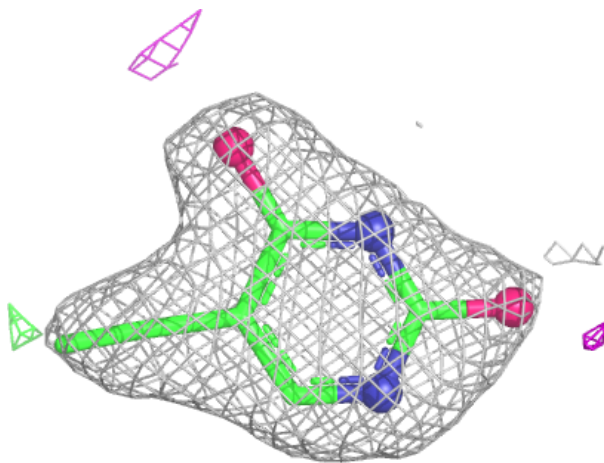
Electron density around Y3G C 1107:

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



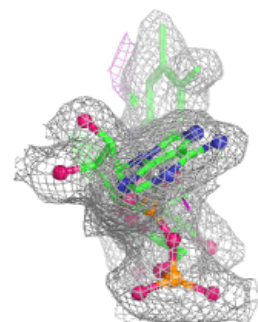
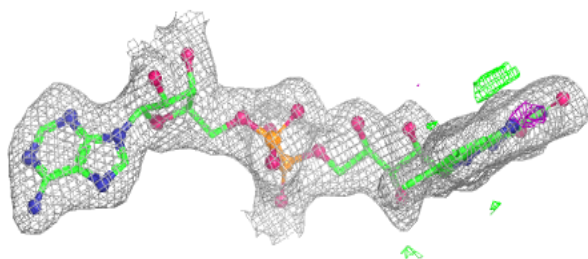
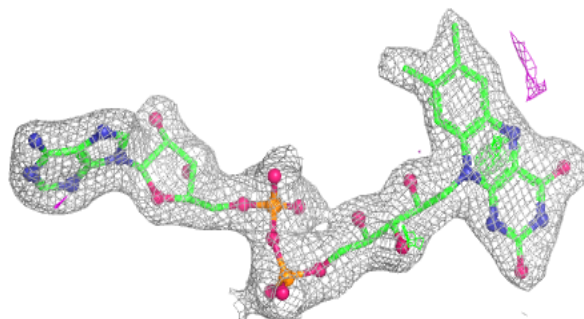
Electron density around Y3G A 1107:

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

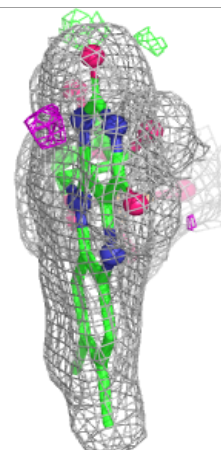
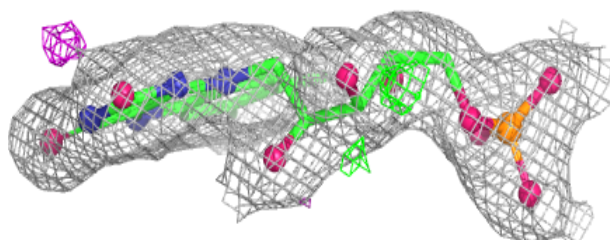
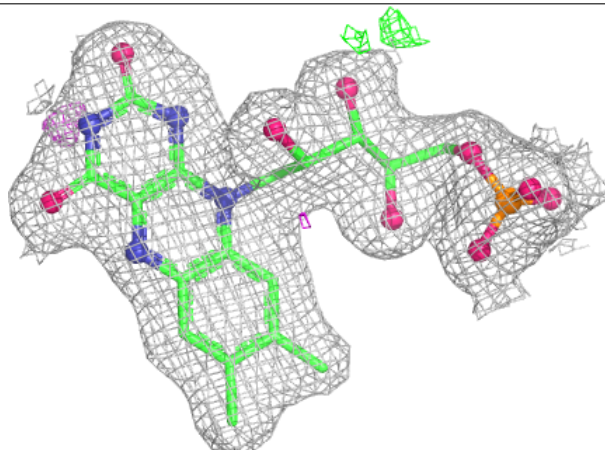


Electron density around FAD B 1106:

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

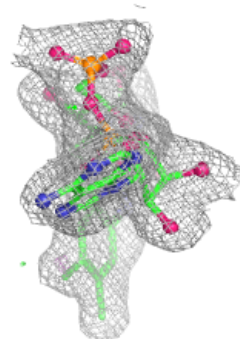
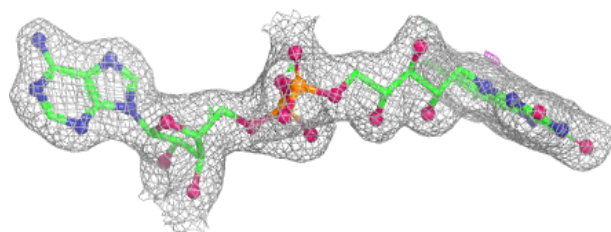
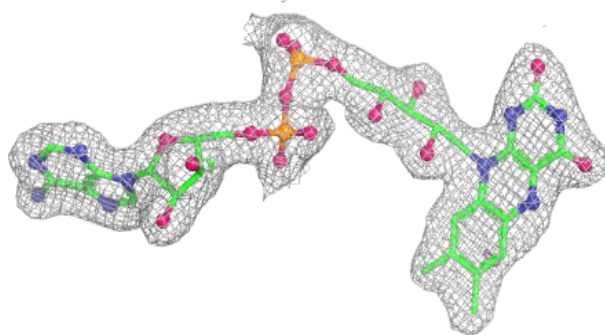
**Electron density around FMN D 1105:**

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



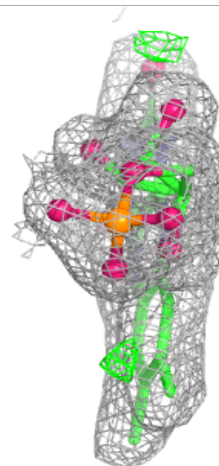
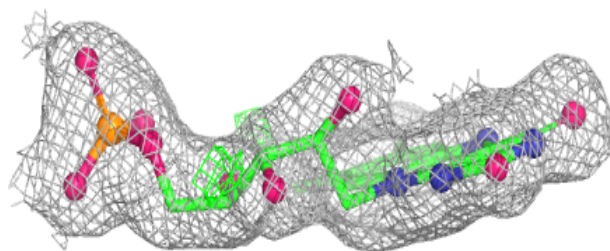
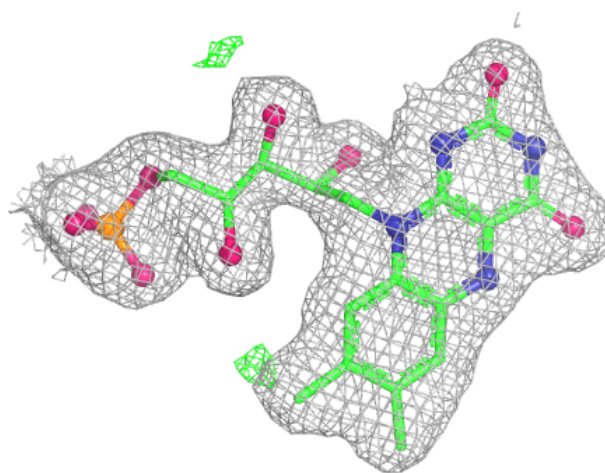
Electron density around FAD A 1106:

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



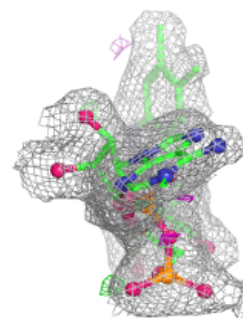
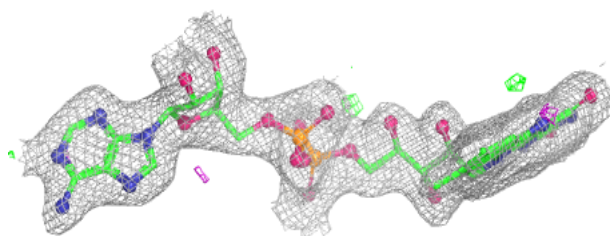
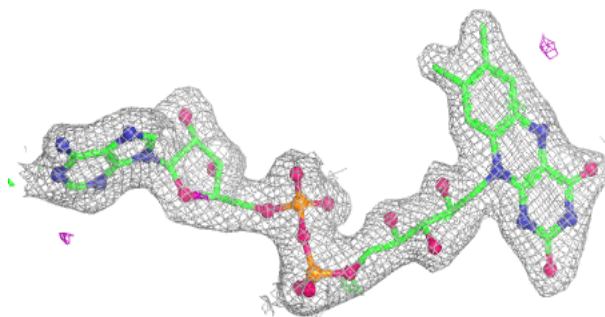
Electron density around FMN A 1105:

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



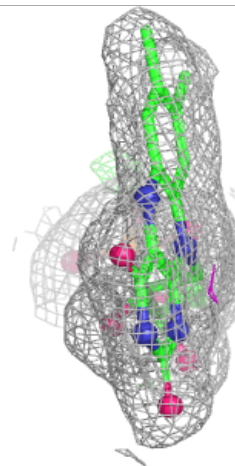
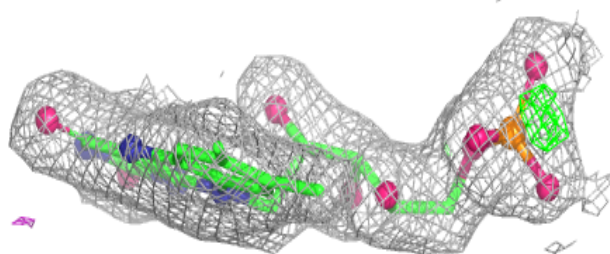
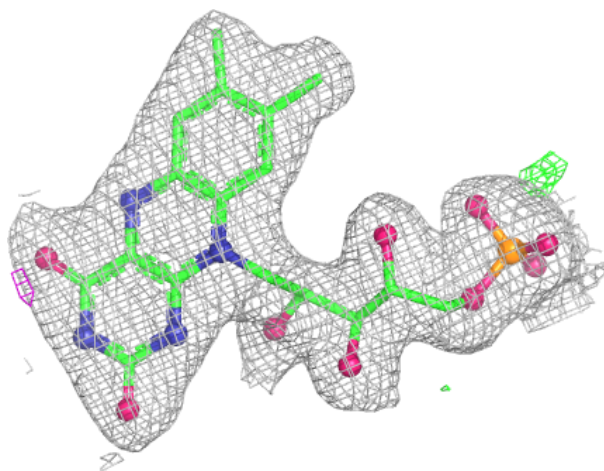
Electron density around FAD C 1106:

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



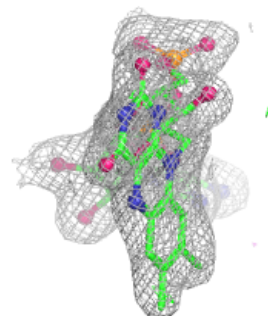
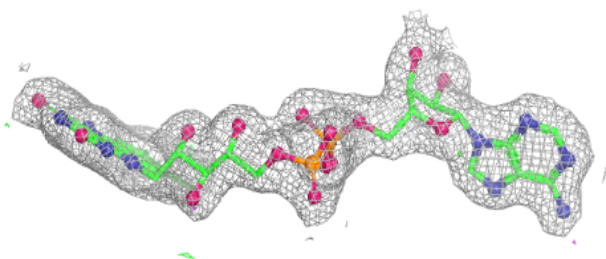
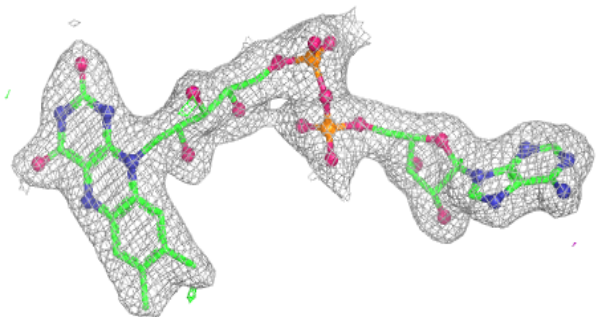
Electron density around FMN C 1105:

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



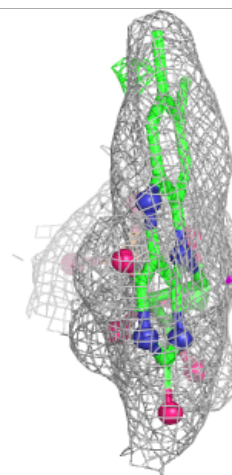
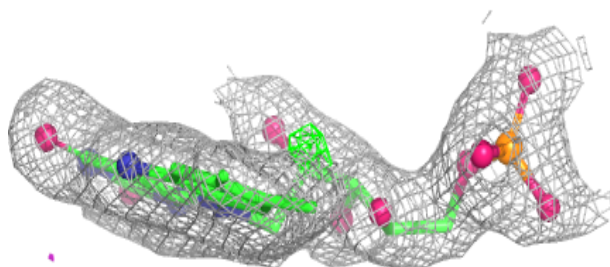
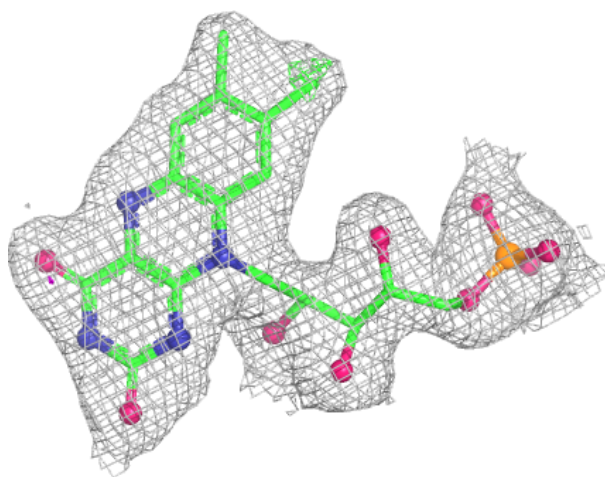
Electron density around FAD D 1106:

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



Electron density around FMN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.