



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:11 AM UTC

PDB ID : 1H7X / pdb_00001h7x
Title : Dihydropyrimidine dehydrogenase (DPD) from pig, ternary complex of a mutant enzyme (C671A), NADPH and 5-fluorouracil
Authors : Dobritsch, D.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2001-01-19
Resolution : 2.01 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

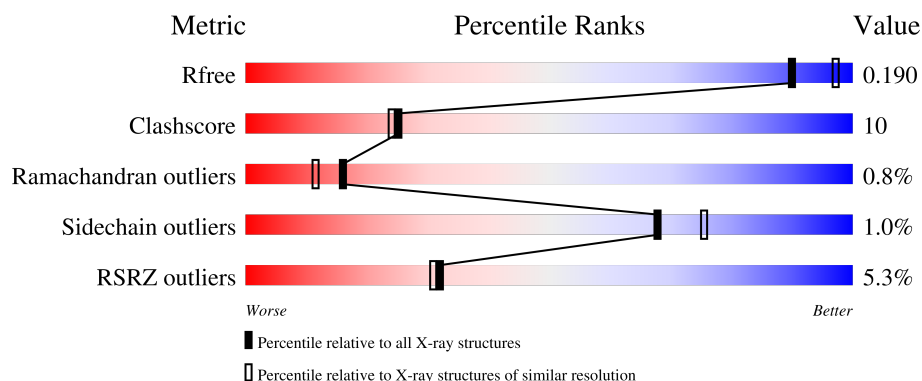
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	4% 80% 18% ..
1	B	1025	5% 80% 18% ..
1	C	1025	6% 80% 17% ..
1	D	1025	5% 81% 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	B	1027	-	-	X	-
2	SF4	D	1027	-	-	X	-
5	NDP	A	1032	X	-	-	-
5	NDP	B	1032	X	-	-	-
5	NDP	C	1032	X	-	-	-
5	NDP	D	1032	X	-	-	-
6	URF	B	1033	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36037 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.

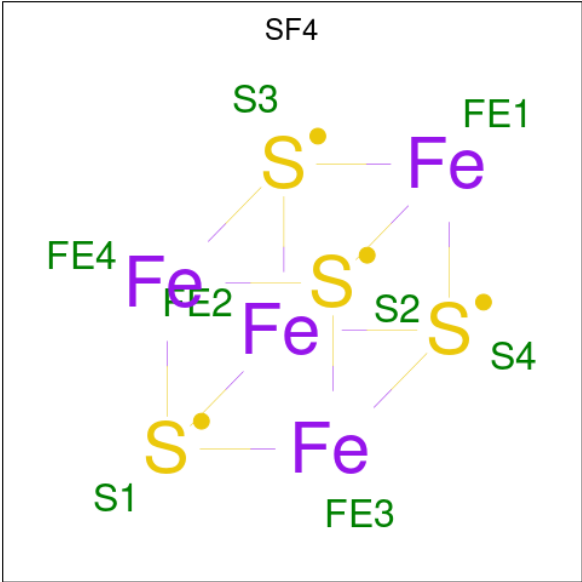
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	124	0	0
			7749	4913	1314	1467	55			
1	B	1019	Total	C	N	O	S	95	0	0
			7769	4927	1317	1470	55			
1	C	1019	Total	C	N	O	S	44	0	0
			7769	4927	1317	1470	55			
1	D	1019	Total	C	N	O	S	110	0	0
			7769	4927	1317	1470	55			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
A	671	ALA	CYS	engineered mutation	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
B	671	ALA	CYS	engineered mutation	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
C	671	ALA	CYS	engineered mutation	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943
D	671	ALA	CYS	engineered mutation	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



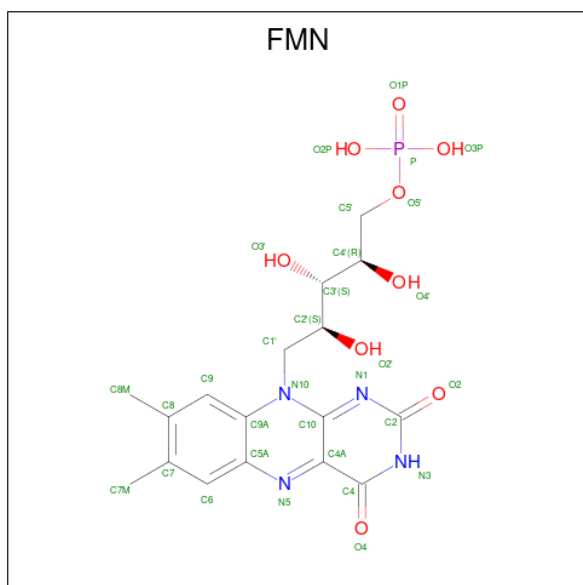
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

Continued on next page...

Continued from previous page...

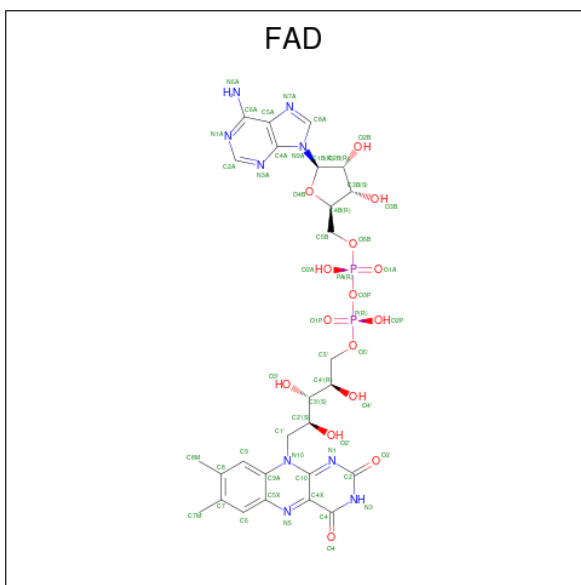
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



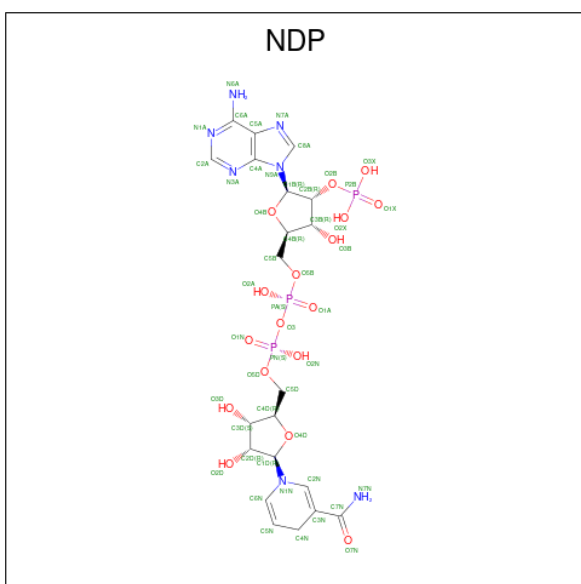
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



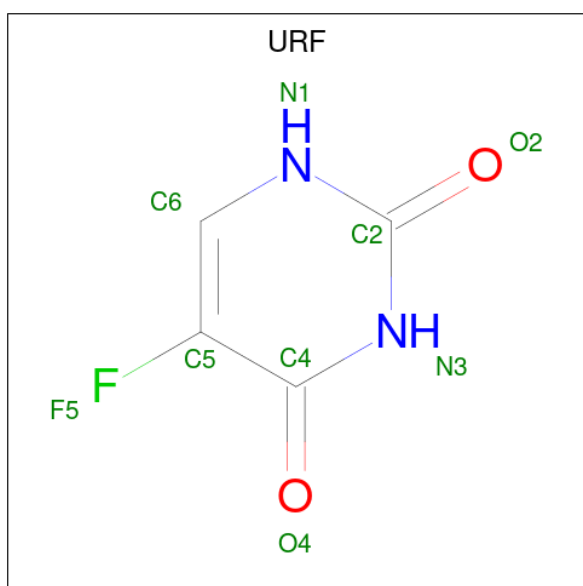
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	9	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	9	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is 5-FLUOROURACIL (CCD ID: URF) (formula: $C_4H_3FN_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
6	B	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
6	C	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
6	D	1	Total	C	F	N	O	0	0
			9	4	1	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1052	Total	O	0	0
			1052	1052		
7	B	1048	Total	O	0	0
			1048	1048		

Continued on next page...

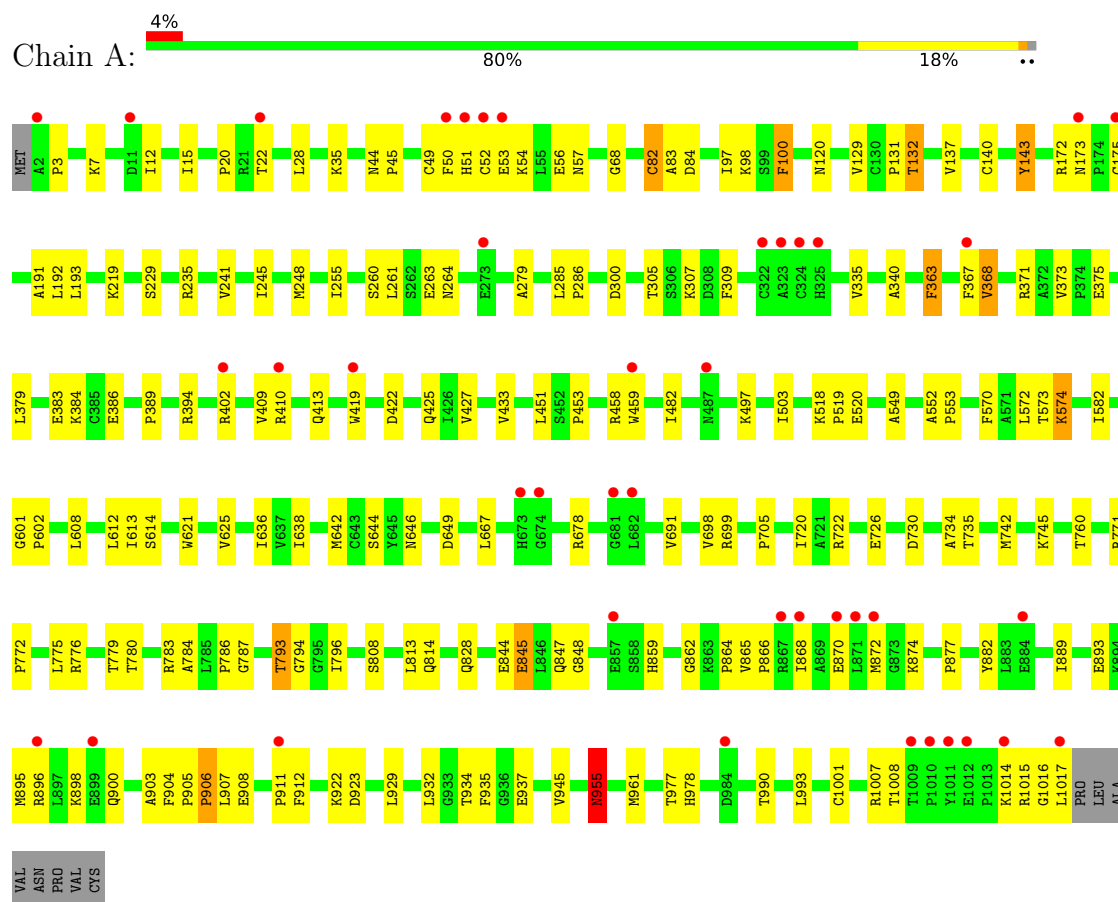
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1096	Total 1096	O 1096	0	0
7	D	1093	Total 1093	O 1093	0	0

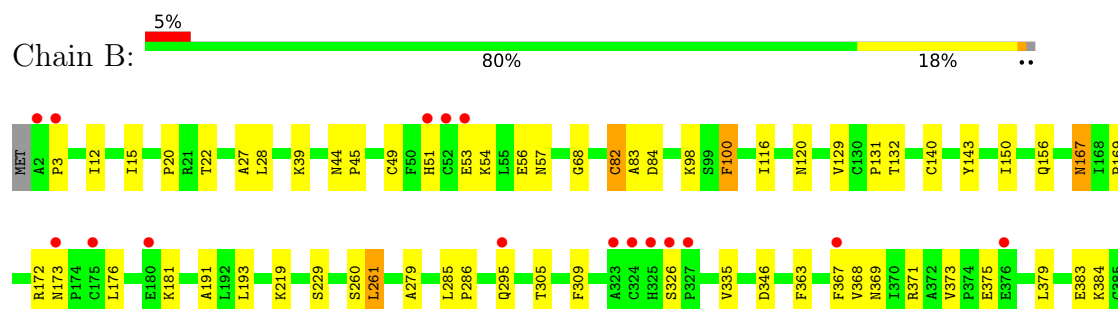
3 Residue-property plots [i](#)

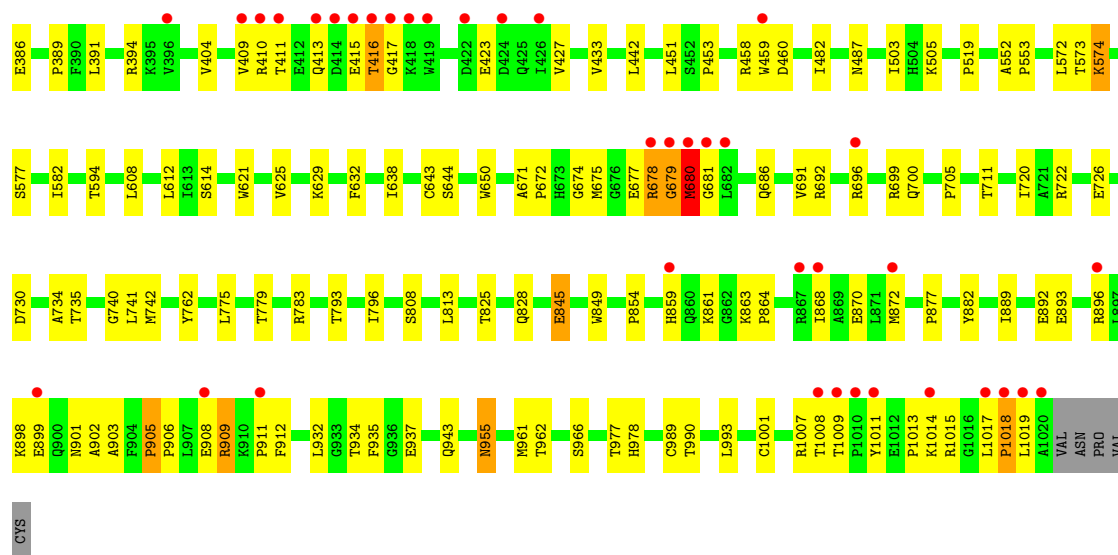
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

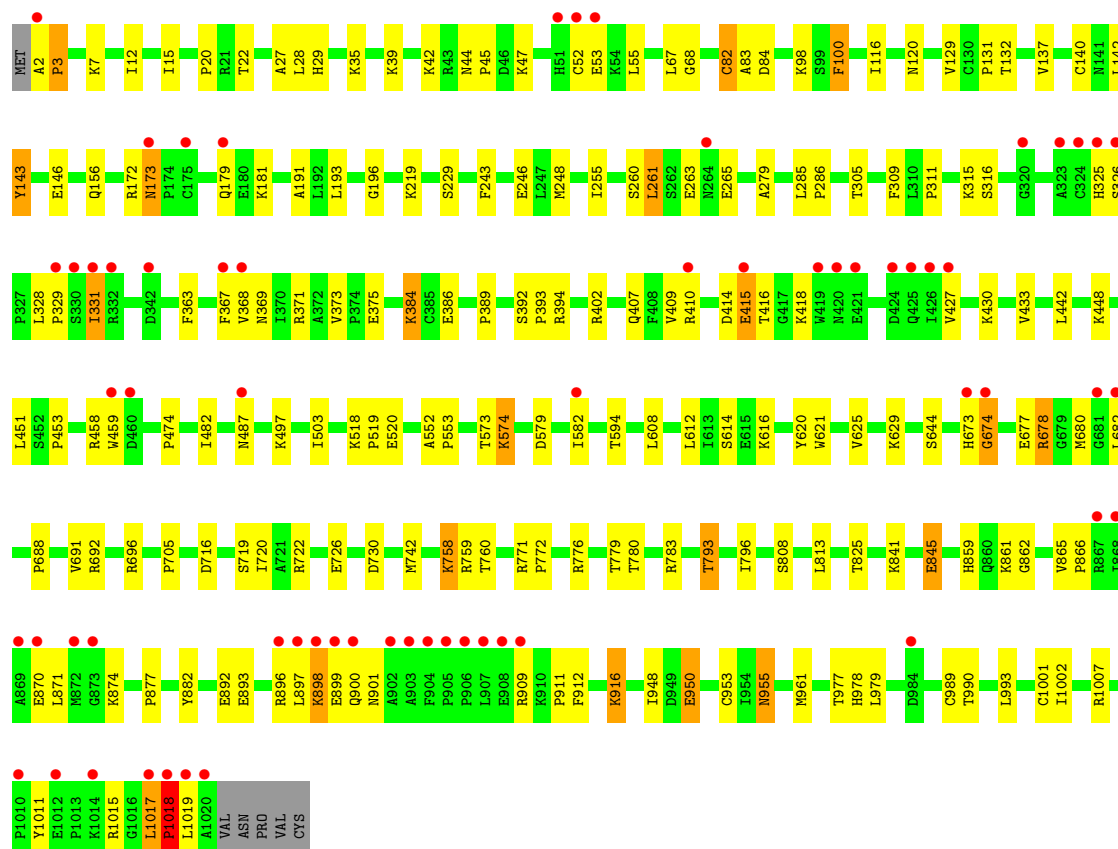


• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

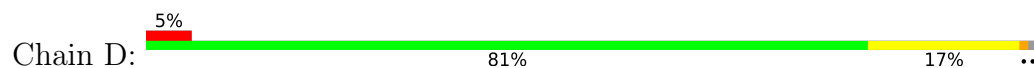


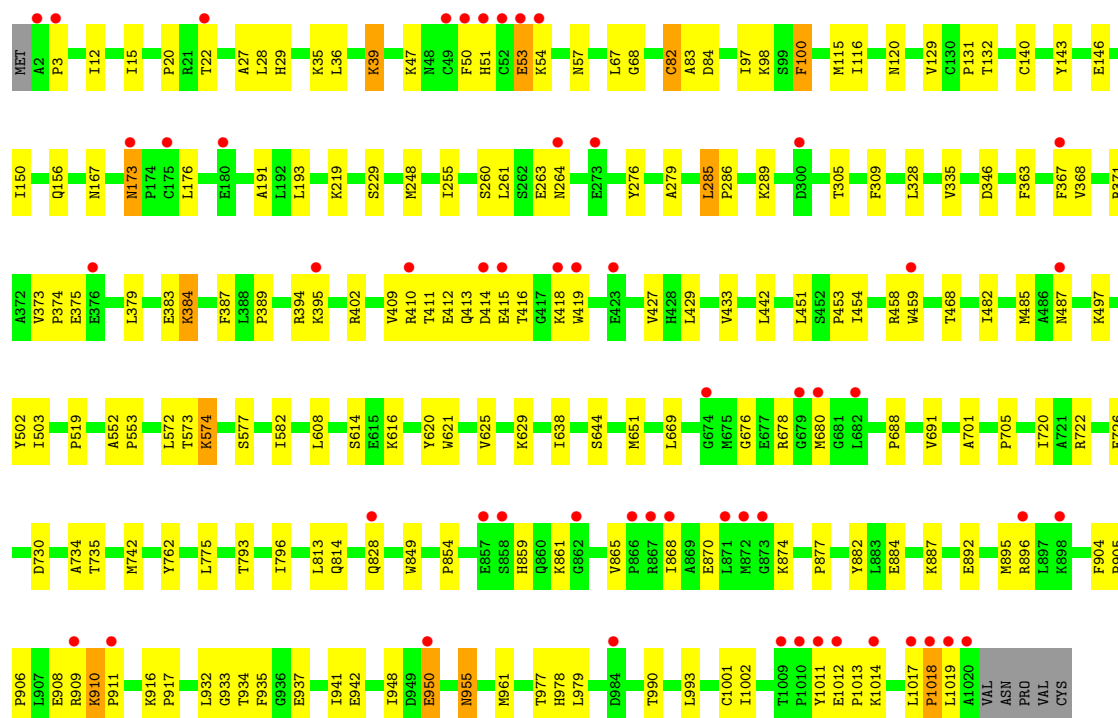


• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE



• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.95Å 159.29Å 163.57Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	25.08 – 2.01 25.08 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.6 (25.08-2.01) 98.9 (25.08-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.171 , 0.192 0.168 , 0.190	Depositor DCC
R_{free} test set	5418 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	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	0.95	EDS
Total number of atoms	36037	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: NDP, URF, FMN, SF4, 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	0.37	0/7910	0.91	24/10720 (0.2%)
1	B	0.37	0/7931	0.91	28/10750 (0.3%)
1	C	0.39	0/7931	0.91	26/10750 (0.2%)
1	D	0.37	0/7931	0.92	30/10750 (0.3%)
All	All	0.37	0/31703	0.91	108/42970 (0.3%)

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	905	PRO	N-CA-C	11.74	125.02	110.70
1	B	905	PRO	N-CA-C	10.38	123.37	110.70
1	B	285	LEU	CA-C-N	8.93	129.10	119.28
1	B	285	LEU	C-N-CA	8.93	129.10	119.28
1	D	904	PHE	N-CA-C	8.89	123.86	108.75
1	C	305	THR	N-CA-C	-8.83	96.74	110.42
1	D	305	THR	N-CA-C	-8.56	97.15	110.42
1	B	305	THR	N-CA-C	-8.48	97.28	110.42
1	A	305	THR	N-CA-C	-8.35	97.48	110.42
1	D	905	PRO	N-CA-C	-8.23	100.66	110.70
1	D	904	PHE	CA-C-N	-7.75	112.39	120.38
1	D	904	PHE	C-N-CA	-7.75	112.39	120.38
1	D	285	LEU	CA-C-N	7.58	127.62	119.28
1	D	285	LEU	C-N-CA	7.58	127.62	119.28
1	B	309	PHE	N-CA-C	7.47	119.33	111.03
1	B	955	ASN	N-CA-C	7.36	121.62	111.90
1	A	285	LEU	CA-C-N	7.35	127.36	119.28
1	A	285	LEU	C-N-CA	7.35	127.36	119.28
1	C	955	ASN	N-CA-C	7.20	121.41	111.90
1	D	574	LYS	N-CA-C	-7.15	100.42	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	955	ASN	N-CA-C	7.15	121.27	111.54
1	B	574	LYS	N-CA-C	-7.07	100.73	110.35
1	A	955	ASN	N-CA-C	7.05	121.21	111.90
1	D	309	PHE	N-CA-C	7.05	118.86	111.03
1	C	574	LYS	N-CA-C	-7.01	100.82	110.35
1	C	285	LEU	CA-C-N	6.97	126.94	119.28
1	C	285	LEU	C-N-CA	6.97	126.94	119.28
1	A	574	LYS	N-CA-C	-6.94	100.92	110.35
1	A	309	PHE	N-CA-C	6.93	118.72	111.03
1	D	229	SER	N-CA-C	6.72	119.61	111.82
1	A	82	CYS	N-CA-C	6.60	119.33	110.35
1	C	677	GLU	N-CA-C	6.55	117.78	108.74
1	D	82	CYS	N-CA-C	6.41	119.06	110.35
1	D	503	ILE	N-CA-C	-6.37	104.28	110.72
1	C	82	CYS	N-CA-C	6.32	119.41	110.50
1	B	82	CYS	N-CA-C	6.26	119.33	110.50
1	B	503	ILE	N-CA-C	-6.25	104.41	110.72
1	C	229	SER	N-CA-C	6.18	118.99	111.82
1	A	503	ILE	N-CA-C	-6.17	104.49	110.72
1	C	309	PHE	N-CA-C	6.15	117.86	111.03
1	C	143	TYR	N-CA-C	-6.15	105.04	112.54
1	C	120	ASN	CA-C-N	6.12	125.80	119.56
1	C	120	ASN	C-N-CA	6.12	125.80	119.56
1	A	68	GLY	N-CA-C	-5.99	103.11	112.58
1	B	129	VAL	N-CA-C	5.97	119.94	113.43
1	D	143	TYR	N-CA-C	-5.96	105.27	112.54
1	C	68	GLY	N-CA-C	-5.96	103.16	112.58
1	A	143	TYR	N-CA-C	-5.95	105.28	112.54
1	D	173	ASN	CA-C-N	5.93	125.80	119.28
1	D	173	ASN	C-N-CA	5.93	125.80	119.28
1	A	129	VAL	N-CA-C	5.92	119.89	113.43
1	B	143	TYR	N-CA-C	-5.86	105.23	112.38
1	C	503	ILE	N-CA-C	-5.85	104.81	110.72
1	D	129	VAL	N-CA-C	5.83	119.79	113.43
1	A	1016	GLY	CA-C-N	5.82	132.17	121.70
1	A	1016	GLY	C-N-CA	5.82	132.17	121.70
1	B	573	THR	N-CA-C	-5.80	102.72	110.55
1	B	68	GLY	N-CA-C	-5.77	103.46	112.58
1	D	1001	CYS	N-CA-C	-5.74	105.10	111.36
1	D	644	SER	N-CA-C	-5.73	102.44	110.35
1	C	129	VAL	N-CA-C	5.73	119.68	113.43
1	D	573	THR	N-CA-C	-5.73	102.82	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1001	CYS	N-CA-C	-5.73	105.12	111.36
1	D	120	ASN	CA-C-N	5.63	125.31	119.56
1	D	120	ASN	C-N-CA	5.63	125.31	119.56
1	B	261	LEU	N-CA-C	-5.63	99.95	108.67
1	C	1001	CYS	N-CA-C	-5.63	105.23	111.36
1	C	644	SER	N-CA-C	-5.60	102.63	110.35
1	D	68	GLY	N-CA-C	-5.58	103.77	112.58
1	A	132	THR	N-CA-C	5.57	118.07	111.33
1	A	872	MET	N-CA-C	5.55	118.23	109.96
1	C	384	LYS	N-CA-C	5.55	119.34	112.24
1	A	229	SER	N-CA-C	5.54	119.76	112.89
1	B	632	PHE	CA-C-N	5.54	125.37	119.28
1	B	632	PHE	C-N-CA	5.54	125.37	119.28
1	B	404	VAL	N-CA-C	-5.52	107.89	113.47
1	D	261	LEU	N-CA-C	-5.49	100.16	108.67
1	C	678	ARG	N-CA-C	-5.49	99.12	110.80
1	A	384	LYS	N-CA-C	5.47	119.24	112.24
1	C	263	GLU	N-CA-C	5.43	120.28	111.37
1	C	261	LEU	N-CA-C	-5.42	100.27	108.67
1	A	1001	CYS	N-CA-C	-5.40	105.48	111.36
1	A	644	SER	N-CA-C	-5.38	102.92	110.35
1	C	573	THR	N-CA-C	-5.38	103.29	110.55
1	D	678	ARG	N-CA-C	-5.38	106.72	113.28
1	B	384	LYS	N-CA-C	5.36	119.11	112.24
1	B	680	MET	N-CA-C	-5.36	105.19	112.26
1	B	286	PRO	N-CA-C	5.32	120.83	113.65
1	A	120	ASN	CA-C-N	5.31	124.98	119.56
1	A	120	ASN	C-N-CA	5.31	124.98	119.56
1	C	286	PRO	N-CA-C	5.30	120.81	113.65
1	B	594	THR	N-CA-C	-5.29	106.05	112.88
1	B	229	SER	N-CA-C	5.28	119.44	112.89
1	B	132	THR	N-CA-C	5.26	117.69	111.33
1	A	286	PRO	N-CA-C	5.26	120.75	113.65
1	A	573	THR	N-CA-C	-5.17	103.56	110.55
1	D	384	LYS	N-CA-C	5.17	118.86	112.24
1	B	120	ASN	CA-C-N	5.17	124.83	119.56
1	B	120	ASN	C-N-CA	5.17	124.83	119.56
1	B	644	SER	N-CA-C	-5.12	103.28	110.35
1	D	286	PRO	N-CA-C	5.12	120.56	113.65
1	B	674	GLY	N-CA-C	5.10	125.27	113.18
1	D	910	LYS	CA-C-N	5.10	125.10	119.90
1	D	910	LYS	C-N-CA	5.10	125.10	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	THR	N-CA-C	5.06	117.45	111.33
1	C	594	THR	N-CA-C	-5.02	106.41	112.88
1	C	196	GLY	CA-C-N	5.01	124.45	119.24
1	C	196	GLY	C-N-CA	5.01	124.45	119.24

There are no chirality outliers.

There are no planarity outliers.

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	7749	0	7775	167	0
1	B	7769	0	7798	160	1
1	C	7769	0	7798	170	0
1	D	7769	0	7798	184	1
2	A	32	0	0	2	0
2	B	32	0	0	2	0
2	C	32	0	0	1	0
2	D	32	0	0	3	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	C	31	0	19	0	0
3	D	31	0	19	1	0
4	A	53	0	31	2	0
4	B	53	0	31	2	0
4	C	53	0	31	0	0
4	D	53	0	31	1	0
5	A	48	0	26	1	0
5	B	48	0	26	3	0
5	C	48	0	26	1	0
5	D	48	0	26	7	0
6	A	9	0	3	0	0
6	B	9	0	3	0	0
6	C	9	0	3	0	0
6	D	9	0	3	0	0
7	A	1052	0	0	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1048	0	0	32	0
7	C	1096	0	0	26	0
7	D	1093	0	0	29	0
All	All	36037	0	31485	603	1

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 10.

All (603) 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:D:22:THR:HG22	7:D:2056:HOH:O	1.62	0.96
1:A:410:ARG:HH21	1:B:427:VAL:HG21	1.30	0.96
1:A:410:ARG:NH2	1:B:427:VAL:HG21	1.81	0.95
1:A:923:ASP:OD1	1:D:937:GLU:HG2	1.67	0.93
1:A:1017:LEU:O	1:A:1017:LEU:HD12	1.68	0.93
1:A:1015:ARG:C	1:A:1017:LEU:H	1.78	0.92
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.40	0.85
1:A:410:ARG:HH21	1:B:427:VAL:CG2	1.90	0.85
1:A:173:ASN:HB2	7:A:2315:HOH:O	1.77	0.84
1:C:487:ASN:HD21	1:D:35:LYS:HZ1	1.26	0.83
1:D:487:ASN:O	5:D:1032:NDP:H2N	1.77	0.82
1:D:22:THR:HG23	7:D:2057:HOH:O	1.79	0.81
1:D:402:ARG:HH11	1:D:402:ARG:HB3	1.45	0.81
1:A:427:VAL:HG13	1:B:410:ARG:NH1	1.94	0.81
1:A:427:VAL:HG13	1:B:410:ARG:CZ	2.10	0.80
1:D:264:ASN:HB2	7:D:2412:HOH:O	1.79	0.80
1:D:680:MET:HE2	1:D:688:PRO:HD3	1.64	0.79
1:A:22:THR:HB	7:A:2049:HOH:O	1.81	0.78
1:C:1017:LEU:HD23	1:C:1018:PRO:HD2	1.65	0.78
1:D:51:HIS:HA	1:D:384:LYS:HG3	1.66	0.77
1:C:487:ASN:HD21	1:D:35:LYS:NZ	1.82	0.76
1:C:776:ARG:O	1:C:780:THR:HG23	1.86	0.76
1:B:458:ARG:HG2	1:B:459:TRP:CE3	2.21	0.75
1:B:896:ARG:HH11	1:B:896:ARG:HG2	1.51	0.75
7:A:2049:HOH:O	1:B:825:THR:HB	1.87	0.74
1:C:53:GLU:OE2	1:C:55:LEU:HD21	1.88	0.74
1:C:579:ASP:O	1:C:582:ILE:HG12	1.86	0.74
1:C:369:ASN:HA	1:D:50:PHE:HE1	1.51	0.73
1:C:427:VAL:HG13	1:D:410:ARG:CZ	2.18	0.73
1:C:260:SER:HB2	1:C:265:GLU:OE1	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ARG:HE	1:B:427:VAL:HG22	1.52	0.73
1:D:487:ASN:HB3	5:D:1032:NDP:C7N	2.18	0.73
1:D:1018:PRO:HD3	7:D:3069:HOH:O	1.88	0.73
1:A:371:ARG:HD3	7:A:3046:HOH:O	1.89	0.72
1:C:859:HIS:HD2	1:C:862:GLY:H	1.35	0.72
1:C:316:SER:HA	1:C:325:HIS:CD2	2.25	0.72
1:D:680:MET:HE2	1:D:688:PRO:CD	2.18	0.72
1:A:386:GLU:OE2	1:B:368:VAL:HG22	1.89	0.72
1:C:1017:LEU:CD2	1:C:1018:PRO:HD2	2.20	0.72
1:A:22:THR:HG22	7:A:2050:HOH:O	1.88	0.72
1:D:1011:TYR:CE2	1:D:1013:PRO:HG3	2.25	0.71
1:B:678:ARG:O	1:B:680:MET:N	2.23	0.70
1:A:50:PHE:CE2	1:B:369:ASN:HA	2.25	0.70
1:C:458:ARG:HH21	1:C:459:TRP:HH2	1.39	0.70
1:C:427:VAL:HG13	1:D:410:ARG:NH1	2.06	0.70
1:A:371:ARG:HH11	1:A:371:ARG:HG2	1.57	0.69
1:A:54:LYS:HE3	7:A:2115:HOH:O	1.93	0.68
1:D:909:ARG:HG3	7:D:2272:HOH:O	1.92	0.68
5:D:1032:NDP:O2N	5:D:1032:NDP:C4D	2.42	0.68
1:C:487:ASN:ND2	1:D:35:LYS:NZ	2.41	0.67
1:A:776:ARG:O	1:A:780:THR:HG23	1.94	0.67
1:A:1017:LEU:O	1:A:1017:LEU:CD1	2.43	0.67
1:C:1019:LEU:HD21	1:D:582:ILE:CD1	2.25	0.67
1:A:868:ILE:HD12	1:A:893:GLU:HB2	1.77	0.66
1:C:950:GLU:HG3	1:C:979:LEU:HD22	1.76	0.66
1:C:870:GLU:O	1:C:874:LYS:HD2	1.96	0.66
1:A:410:ARG:NH1	7:A:2542:HOH:O	2.20	0.66
1:A:458:ARG:HG2	1:A:459:TRP:CE3	2.31	0.66
1:D:36:LEU:HA	1:D:39:LYS:HE2	1.78	0.66
1:A:7:LYS:HE2	7:A:2009:HOH:O	1.95	0.65
1:C:371:ARG:HG2	1:C:371:ARG:HH11	1.61	0.65
1:D:1014:LYS:NZ	7:D:3061:HOH:O	2.27	0.65
1:A:410:ARG:NH2	1:B:427:VAL:CG2	2.54	0.65
1:D:458:ARG:HH21	1:D:459:TRP:HH2	1.43	0.65
1:A:787:GLY:HA3	1:D:942:GLU:OE2	1.97	0.65
1:D:487:ASN:HB3	5:D:1032:NDP:C3N	2.26	0.65
1:A:458:ARG:HD3	7:A:2577:HOH:O	1.95	0.65
1:B:678:ARG:O	1:B:679:GLY:C	2.38	0.65
1:B:893:GLU:OE1	1:B:896:ARG:NH2	2.30	0.65
1:D:328:LEU:HD12	7:D:2119:HOH:O	1.97	0.65
1:A:722:ARG:O	1:A:726:GLU:HG3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:O	1:A:874:LYS:HD3	1.98	0.64
1:C:52:CYS:HB2	1:C:384:LYS:HB2	1.79	0.64
1:A:54:LYS:NZ	1:A:895:MET:HG3	2.13	0.63
1:A:699:ARG:O	1:A:699:ARG:HD3	1.98	0.63
1:C:448:LYS:HD3	7:C:2589:HOH:O	1.97	0.63
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.79	0.63
1:D:722:ARG:O	1:D:726:GLU:HG3	1.98	0.63
1:B:722:ARG:O	1:B:726:GLU:HG3	1.99	0.63
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.33	0.62
1:C:990:THR:O	1:C:990:THR:HG22	1.99	0.62
7:C:2879:HOH:O	1:D:22:THR:CG2	2.46	0.62
1:B:678:ARG:O	1:B:680:MET:HE3	1.99	0.62
1:C:2:ALA:HB3	7:D:2747:HOH:O	1.99	0.62
1:C:369:ASN:HA	1:D:50:PHE:CE1	2.33	0.61
1:D:414:ASP:O	1:D:416:THR:N	2.32	0.61
1:D:379:LEU:O	1:D:383:GLU:HG3	2.01	0.61
1:D:402:ARG:HB3	1:D:402:ARG:NH1	2.14	0.61
1:D:934:THR:HG1	1:D:937:GLU:HG3	1.65	0.61
1:D:285:LEU:HD12	7:D:3081:HOH:O	2.00	0.61
1:B:394:ARG:HG3	1:B:409:VAL:HG13	1.82	0.61
1:A:582:ILE:HD11	1:B:1015:ARG:CZ	2.31	0.60
1:D:115:MET:HE2	1:D:828:GLN:NE2	2.15	0.60
1:A:990:THR:HG22	1:A:990:THR:O	2.01	0.60
1:C:179:GLN:HG3	7:C:2274:HOH:O	2.01	0.60
1:C:1007:ARG:CD	1:C:1011:TYR:HB2	2.31	0.60
1:A:896:ARG:HD2	7:A:2923:HOH:O	2.00	0.60
1:A:868:ILE:HG12	1:A:870:GLU:H	1.67	0.60
1:C:219:LYS:HG3	1:C:260:SER:OG	2.01	0.60
1:C:410:ARG:CZ	1:D:427:VAL:HG13	2.32	0.60
1:A:859:HIS:HD2	1:A:862:GLY:H	1.47	0.59
1:D:51:HIS:HD2	1:D:384:LYS:HB2	1.66	0.59
1:D:990:THR:HG22	1:D:990:THR:O	2.01	0.59
1:A:54:LYS:HZ1	1:A:895:MET:HG3	1.68	0.59
1:D:950:GLU:HG3	1:D:979:LEU:HD22	1.85	0.59
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.38	0.59
1:B:696:ARG:HD2	7:B:2763:HOH:O	2.02	0.59
1:C:845:GLU:HG3	1:C:912:PHE:CD1	2.37	0.59
1:A:410:ARG:NE	1:B:427:VAL:HG22	2.16	0.59
1:B:859:HIS:HE1	1:B:864:PRO:HG3	1.67	0.59
1:C:371:ARG:HG2	1:C:371:ARG:NH1	2.18	0.59
1:A:1007:ARG:NH2	7:A:3025:HOH:O	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:990:THR:HG22	1:B:990:THR:O	2.02	0.59
1:C:367:PHE:CZ	1:D:367:PHE:CE1	2.91	0.58
1:C:1015:ARG:CZ	1:D:582:ILE:HD11	2.33	0.58
1:D:289:LYS:HD2	7:D:2583:HOH:O	2.03	0.58
1:B:413:GLN:HE21	1:B:417:GLY:HA2	1.68	0.58
1:A:845:GLU:HG3	1:A:912:PHE:CE1	2.39	0.58
1:C:243:PHE:HD1	1:C:909:ARG:NH1	2.02	0.58
1:B:896:ARG:NH2	7:B:2915:HOH:O	2.36	0.58
1:A:219:LYS:HG3	1:A:260:SER:OG	2.02	0.57
1:A:12:ILE:O	1:A:15:ILE:HG22	2.04	0.57
1:A:57:ASN:HB2	7:A:2120:HOH:O	2.03	0.57
4:B:1031:FAD:H1'1	5:B:1032:NDP:H3D	1.86	0.57
1:C:722:ARG:O	1:C:726:GLU:HG3	2.05	0.57
1:A:363:PHE:HE1	1:A:389:PRO:HB3	1.70	0.57
1:C:582:ILE:CD1	7:C:2719:HOH:O	2.53	0.57
1:A:745:LYS:HD2	7:A:2801:HOH:O	2.05	0.57
1:C:780:THR:HG22	1:D:762:TYR:CE2	2.39	0.56
1:C:861:LYS:HE3	7:C:2922:HOH:O	2.05	0.56
1:A:870:GLU:OE1	1:A:889:ILE:HG23	2.05	0.56
1:A:877:PRO:HD2	1:A:882:TYR:CG	2.40	0.56
1:B:877:PRO:HD2	1:B:882:TYR:CG	2.41	0.56
1:C:783:ARG:HD3	7:C:2852:HOH:O	2.05	0.56
1:A:371:ARG:HG2	1:A:371:ARG:NH1	2.20	0.56
1:C:246:GLU:HG3	1:C:909:ARG:HG2	1.87	0.56
1:A:828:GLN:HG2	7:A:2853:HOH:O	2.06	0.56
1:B:326:SER:HB3	7:B:2437:HOH:O	2.05	0.56
1:C:386:GLU:OE1	1:D:368:VAL:HG22	2.06	0.56
1:D:167:ASN:ND2	1:D:910:LYS:O	2.38	0.56
1:D:367:PHE:HZ	1:D:387:PHE:HB2	1.70	0.56
1:A:1014:LYS:HB3	7:A:3032:HOH:O	2.06	0.56
1:B:505:LYS:HE2	7:B:2602:HOH:O	2.06	0.56
1:C:367:PHE:CZ	1:D:367:PHE:CZ	2.94	0.56
1:A:775:LEU:O	1:A:779:THR:HG23	2.06	0.55
1:A:143:TYR:O	1:B:861:LYS:HE2	2.06	0.55
1:A:779:THR:HG22	1:A:808:SER:HB3	1.88	0.55
1:A:845:GLU:HG3	1:A:912:PHE:CD1	2.42	0.55
1:B:415:GLU:O	1:B:416:THR:OG1	2.20	0.55
1:C:978:HIS:HE1	1:D:84:ASP:OD2	1.88	0.55
1:C:993:LEU:HD23	1:C:993:LEU:C	2.32	0.55
1:B:783:ARG:HD3	7:B:2825:HOH:O	2.05	0.55
7:C:2879:HOH:O	1:D:22:THR:HG21	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:PRO:HG2	7:A:2379:HOH:O	2.06	0.55
1:C:172:ARG:HG3	7:C:2303:HOH:O	2.06	0.55
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.87	0.55
1:A:646:ASN:HD22	1:A:649:ASP:CG	2.14	0.55
1:A:870:GLU:OE2	1:A:896:ARG:NH2	2.28	0.55
1:A:1014:LYS:HE3	7:A:2976:HOH:O	2.07	0.55
1:A:780:THR:HG22	1:B:762:TYR:CZ	2.42	0.55
1:A:340:ALA:HB3	7:A:3050:HOH:O	2.06	0.55
1:B:413:GLN:HG3	1:B:417:GLY:O	2.06	0.55
1:C:845:GLU:HG3	1:C:912:PHE:CE1	2.42	0.55
1:A:379:LEU:O	1:A:383:GLU:HG3	2.07	0.54
1:B:131:PRO:HB2	1:B:373:VAL:HG11	1.89	0.54
1:B:582:ILE:HG13	7:B:2701:HOH:O	2.05	0.54
1:B:12:ILE:O	1:B:15:ILE:HG22	2.07	0.54
1:C:682:LEU:HD23	7:C:2777:HOH:O	2.06	0.54
1:C:410:ARG:HH22	1:D:429:LEU:HD13	1.73	0.54
1:D:193:LEU:N	1:D:193:LEU:HD22	2.22	0.54
1:D:582:ILE:HG13	7:D:2737:HOH:O	2.06	0.54
1:C:900:GLN:HG2	1:C:901:ASN:N	2.22	0.54
1:D:877:PRO:HD2	1:D:882:TYR:CG	2.43	0.54
1:C:897:LEU:C	1:C:899:GLU:H	2.15	0.54
1:D:574:LYS:HG3	1:D:614:SER:HB2	1.90	0.54
1:D:934:THR:OG1	1:D:937:GLU:HG3	2.07	0.54
1:C:582:ILE:HD11	1:D:1019:LEU:CD1	2.36	0.54
1:A:263:GLU:O	1:A:264:ASN:HB2	2.08	0.54
1:B:261:LEU:HD21	1:B:451:LEU:HD21	1.90	0.54
1:C:691:VAL:HG21	1:C:720:ILE:HG23	1.90	0.54
1:B:908:GLU:O	1:B:909:ARG:C	2.52	0.53
1:B:1011:TYR:HE2	1:B:1013:PRO:HG3	1.73	0.53
1:A:367:PHE:CE1	1:B:367:PHE:CZ	2.96	0.53
1:C:27:ALA:O	1:D:497:LYS:HE2	2.09	0.53
1:D:911:PRO:HG2	7:D:2390:HOH:O	2.07	0.53
1:C:474:PRO:HG2	7:C:2277:HOH:O	2.07	0.53
1:C:582:ILE:HG13	1:D:1019:LEU:HD21	1.90	0.53
7:C:3092:HOH:O	1:D:35:LYS:HE3	2.08	0.53
1:D:793:THR:HG21	3:D:1030:FMN:O3'	2.09	0.53
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.91	0.53
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.91	0.53
1:D:115:MET:HE2	1:D:828:GLN:HE22	1.73	0.53
1:C:780:THR:HG22	1:D:762:TYR:OH	2.09	0.53
1:B:877:PRO:CG	1:B:977:THR:HB	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PRO:HB2	1:C:373:VAL:HG11	1.91	0.53
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.89	0.53
1:B:572:LEU:HD13	1:B:638:ILE:HB	1.90	0.53
1:B:691:VAL:HG21	1:B:720:ILE:HG23	1.90	0.53
1:C:331:ILE:HG23	1:C:433:VAL:HG21	1.91	0.53
1:B:896:ARG:HG2	1:B:896:ARG:NH1	2.21	0.53
7:A:2937:HOH:O	1:D:941:ILE:HD11	2.08	0.52
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.90	0.52
1:A:848:GLY:HA3	7:A:2866:HOH:O	2.09	0.52
1:C:143:TYR:O	1:D:861:LYS:HE2	2.09	0.52
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.91	0.52
1:C:12:ILE:O	1:C:15:ILE:HG22	2.10	0.52
1:C:793:THR:HG21	7:C:2871:HOH:O	2.10	0.52
1:D:54:LYS:NZ	1:D:895:MET:HG3	2.24	0.52
5:D:1032:NDP:O2N	5:D:1032:NDP:H4D	2.09	0.52
1:B:877:PRO:HG2	1:B:977:THR:HB	1.92	0.52
1:D:1011:TYR:CZ	1:D:1013:PRO:HG3	2.44	0.52
1:B:861:LYS:HE3	7:B:2040:HOH:O	2.09	0.52
1:C:497:LYS:HE2	1:D:27:ALA:O	2.10	0.52
1:D:53:GLU:HG3	1:D:887:LYS:HB3	1.92	0.52
1:D:219:LYS:HG3	1:D:260:SER:OG	2.08	0.52
1:B:779:THR:HG22	1:B:808:SER:HB3	1.92	0.52
1:B:1008:THR:HG23	7:B:3014:HOH:O	2.08	0.52
1:D:375:GLU:H	1:D:375:GLU:CD	2.18	0.52
1:A:859:HIS:HA	1:A:865:VAL:HG23	1.90	0.52
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.91	0.52
1:B:692:ARG:O	1:B:696:ARG:HD3	2.10	0.51
1:D:552:ALA:HB3	1:D:553:PRO:HD3	1.92	0.51
1:A:497:LYS:HE2	1:B:27:ALA:O	2.10	0.51
1:B:870:GLU:N	1:B:870:GLU:OE1	2.43	0.51
1:B:845:GLU:HG3	1:B:912:PHE:CE1	2.46	0.51
1:C:181:LYS:HD2	7:C:2272:HOH:O	2.10	0.51
1:A:235:ARG:NH2	4:A:1031:FAD:O4	2.34	0.51
1:A:307:LYS:HE3	7:A:2516:HOH:O	2.11	0.51
1:A:375:GLU:H	1:A:375:GLU:CD	2.19	0.51
1:A:410:ARG:NH2	1:B:391:LEU:HD21	2.25	0.51
1:B:219:LYS:HG3	1:B:260:SER:OG	2.09	0.51
1:B:1017:LEU:HB3	7:B:3030:HOH:O	2.10	0.51
1:C:877:PRO:HG2	1:C:977:THR:HB	1.93	0.51
1:B:608:LEU:HB2	1:B:742:MET:HE2	1.93	0.51
1:C:7:LYS:HE3	7:D:2753:HOH:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:900:GLN:HG2	1:C:901:ASN:H	1.76	0.51
1:D:892:GLU:HG3	7:D:2958:HOH:O	2.10	0.51
1:A:793:THR:HG21	7:A:2773:HOH:O	2.11	0.51
1:B:577:SER:HB2	7:B:2667:HOH:O	2.11	0.51
1:A:934:THR:OG1	1:A:937:GLU:HG3	2.09	0.51
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.46	0.50
1:A:1015:ARG:C	1:A:1017:LEU:N	2.54	0.50
1:A:896:ARG:NH2	7:A:2921:HOH:O	2.43	0.50
1:C:82:CYS:O	1:C:98:LYS:HD2	2.11	0.50
1:C:373:VAL:HG12	1:D:47:LYS:HD3	1.94	0.50
1:A:870:GLU:HG3	7:A:2902:HOH:O	2.11	0.50
1:A:945:VAL:HG13	1:A:1007:ARG:HG2	1.94	0.50
1:B:363:PHE:CE2	1:B:389:PRO:HB3	2.47	0.50
1:B:574:LYS:CG	1:B:614:SER:HB2	2.41	0.50
1:C:487:ASN:ND2	1:D:35:LYS:HZ1	2.00	0.50
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.94	0.50
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.46	0.50
1:B:696:ARG:O	1:B:700:GLN:HG3	2.11	0.50
1:A:100:PHE:CD1	1:A:100:PHE:C	2.90	0.50
1:A:845:GLU:CD	1:A:845:GLU:H	2.20	0.50
1:A:1015:ARG:O	1:A:1017:LEU:N	2.39	0.50
1:D:263:GLU:O	1:D:264:ASN:HB3	2.12	0.50
1:A:582:ILE:HG13	7:A:2702:HOH:O	2.11	0.49
1:C:410:ARG:NH2	1:D:429:LEU:HD13	2.27	0.49
1:C:552:ALA:HB3	1:C:553:PRO:HD3	1.94	0.49
1:A:20:PRO:HG2	1:A:961:MET:SD	2.52	0.49
1:C:953:CYS:HB3	7:C:3015:HOH:O	2.10	0.49
1:B:845:GLU:CD	1:B:845:GLU:H	2.21	0.49
1:C:430:LYS:HE3	7:D:2564:HOH:O	2.11	0.49
1:D:793:THR:OG1	1:D:814:GLN:HB2	2.12	0.49
1:A:937:GLU:OE1	1:D:1012:GLU:OE2	2.31	0.49
1:B:621:TRP:O	1:B:625:VAL:HG23	2.12	0.49
1:B:720:ILE:HG21	7:B:2758:HOH:O	2.12	0.49
1:C:371:ARG:HD3	5:C:1032:NDP:O1A	2.12	0.49
1:B:629:LYS:HE2	1:B:629:LYS:HA	1.95	0.49
1:A:1015:ARG:CZ	1:B:582:ILE:HD11	2.42	0.49
1:B:295:GLN:HG3	7:B:2415:HOH:O	2.13	0.49
1:C:841:LYS:O	1:C:916:LYS:HE2	2.12	0.49
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.95	0.49
1:C:39:LYS:HG3	7:C:2074:HOH:O	2.11	0.49
1:C:410:ARG:NH1	1:D:427:VAL:HG13	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:LYS:CG	1:C:614:SER:HB2	2.42	0.49
1:A:932:LEU:HD11	1:B:741:LEU:HD11	1.94	0.49
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.48	0.49
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.95	0.49
1:D:688:PRO:HG3	1:D:720:ILE:HD13	1.94	0.49
1:A:844:GLU:O	1:A:847:GLN:HG3	2.13	0.48
1:B:699:ARG:HA	1:B:699:ARG:NE	2.27	0.48
1:B:783:ARG:NH1	7:B:2825:HOH:O	2.36	0.48
1:C:414:ASP:C	1:C:416:THR:H	2.21	0.48
1:C:978:HIS:HD2	7:D:2242:HOH:O	1.95	0.48
1:A:193:LEU:HD22	1:A:193:LEU:N	2.27	0.48
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.13	0.48
1:B:1009:THR:HG21	7:B:2994:HOH:O	2.12	0.48
1:C:47:LYS:HD3	1:D:373:VAL:HG12	1.95	0.48
1:C:243:PHE:CD1	1:C:909:ARG:NH1	2.81	0.48
1:D:173:ASN:HB3	1:D:176:LEU:HD12	1.95	0.48
1:D:413:GLN:HG3	1:D:419:TRP:CD2	2.49	0.48
1:D:651:MET:HG2	1:D:701:ALA:HB2	1.95	0.48
1:A:864:PRO:HG3	7:A:2449:HOH:O	2.13	0.48
1:A:993:LEU:C	1:A:993:LEU:HD23	2.38	0.48
1:B:363:PHE:HE2	1:B:389:PRO:HB3	1.78	0.48
1:B:678:ARG:C	1:B:680:MET:N	2.71	0.48
1:C:909:ARG:HD2	7:C:2360:HOH:O	2.12	0.48
1:C:116:ILE:HD13	1:C:156:GLN:HG3	1.95	0.48
1:C:427:VAL:CG1	1:D:410:ARG:CZ	2.89	0.48
1:C:1017:LEU:O	1:C:1018:PRO:C	2.56	0.48
1:D:82:CYS:O	1:D:98:LYS:HD2	2.12	0.48
1:A:786:PRO:C	1:D:942:GLU:HG2	2.39	0.48
1:B:458:ARG:HG2	1:B:459:TRP:CZ3	2.49	0.48
1:A:574:LYS:CG	1:A:614:SER:HB2	2.43	0.48
1:B:1007:ARG:HD3	1:B:1009:THR:O	2.13	0.48
1:C:416:THR:HG22	1:C:416:THR:O	2.12	0.48
1:C:758:LYS:HD3	7:C:2837:HOH:O	2.14	0.48
1:A:866:PRO:HG3	7:A:2127:HOH:O	2.14	0.48
1:B:1011:TYR:CE2	1:B:1013:PRO:HG3	2.48	0.48
1:C:418:LYS:HD2	7:C:2549:HOH:O	2.12	0.48
1:B:172:ARG:HG3	7:B:2294:HOH:O	2.13	0.48
1:B:775:LEU:O	1:B:779:THR:HG23	2.14	0.48
1:D:577:SER:HB2	7:D:2703:HOH:O	2.14	0.48
1:A:877:PRO:CG	1:A:977:THR:HB	2.45	0.47
1:B:100:PHE:CD1	1:B:100:PHE:C	2.92	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ASN:ND2	7:B:2590:HOH:O	2.47	0.47
1:B:1009:THR:HB	7:B:2996:HOH:O	2.13	0.47
1:B:1014:LYS:HG3	7:B:3023:HOH:O	2.13	0.47
1:C:673:HIS:O	1:C:674:GLY:O	2.32	0.47
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.95	0.47
1:A:518:LYS:O	1:A:520:GLU:HG3	2.15	0.47
1:B:1017:LEU:O	1:B:1018:PRO:C	2.57	0.47
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.97	0.47
1:C:877:PRO:CG	1:C:977:THR:HB	2.45	0.47
1:C:692:ARG:O	1:C:696:ARG:HG3	2.15	0.47
1:D:468:THR:HA	1:D:502:TYR:CD2	2.49	0.47
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.45	0.47
1:A:132:THR:HB	1:A:137:VAL:HG23	1.97	0.47
1:A:300:ASP:O	1:A:402:ARG:NH1	2.47	0.47
1:A:410:ARG:HG3	1:A:425:GLN:HB3	1.97	0.47
1:A:582:ILE:HG13	7:A:2673:HOH:O	2.13	0.47
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.97	0.47
1:A:922:LYS:HE3	1:D:937:GLU:OE1	2.14	0.47
1:C:779:THR:HG22	1:C:808:SER:HB3	1.96	0.47
1:D:115:MET:CE	1:D:828:GLN:NE2	2.78	0.47
1:A:868:ILE:CD1	1:A:870:GLU:HB2	2.45	0.47
1:D:97:ILE:HD11	2:D:1026:SF4:S4	2.54	0.47
1:C:407:GLN:NE2	7:C:2543:HOH:O	2.48	0.47
7:C:2721:HOH:O	1:D:1014:LYS:HD3	2.15	0.47
1:D:1017:LEU:HD22	1:D:1018:PRO:HD2	1.97	0.47
1:B:193:LEU:N	1:B:193:LEU:HD22	2.30	0.47
1:C:363:PHE:HE2	1:C:389:PRO:HB3	1.80	0.47
1:D:12:ILE:O	1:D:15:ILE:HG22	2.15	0.47
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.96	0.46
1:A:49:CYS:SG	1:A:51:HIS:CE1	3.08	0.46
1:A:572:LEU:HD13	1:A:638:ILE:HB	1.95	0.46
1:D:22:THR:HA	7:D:2056:HOH:O	2.15	0.46
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.50	0.46
1:B:173:ASN:HB3	1:B:176:LEU:HG	1.97	0.46
1:C:375:GLU:CD	1:C:375:GLU:H	2.23	0.46
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.15	0.46
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.97	0.46
1:C:146:GLU:HG2	1:D:67:LEU:HD23	1.98	0.46
1:C:909:ARG:O	1:C:911:PRO:HD3	2.14	0.46
1:A:82:CYS:O	1:A:98:LYS:HD2	2.15	0.46
1:A:699:ARG:NH2	1:A:730:ASP:OD2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:THR:HG22	1:B:762:TYR:OH	2.16	0.46
1:B:828:GLN:HG2	7:B:2848:HOH:O	2.14	0.46
1:C:518:LYS:O	1:C:520:GLU:HG3	2.15	0.46
1:C:191:ALA:O	1:C:279:ALA:HA	2.16	0.46
1:C:897:LEU:C	1:C:899:GLU:N	2.74	0.46
1:B:1007:ARG:NH1	7:B:2993:HOH:O	2.44	0.46
1:C:688:PRO:HG3	1:C:720:ILE:HD13	1.98	0.46
1:A:582:ILE:HD12	1:B:1019:LEU:HD22	1.97	0.46
1:C:1019:LEU:HD21	1:D:582:ILE:HD13	1.98	0.46
1:D:20:PRO:HG2	1:D:961:MET:SD	2.56	0.46
1:D:410:ARG:HG2	1:D:411:THR:N	2.30	0.46
1:D:574:LYS:CG	1:D:614:SER:HB2	2.45	0.46
1:D:680:MET:CE	1:D:688:PRO:HD3	2.43	0.46
1:D:859:HIS:HA	1:D:865:VAL:HG13	1.97	0.46
1:D:993:LEU:C	1:D:993:LEU:HD23	2.41	0.46
1:A:175:CYS:HB3	7:A:2277:HOH:O	2.16	0.46
1:A:241:VAL:O	1:A:245:ILE:HG12	2.17	0.46
1:A:608:LEU:HB2	1:A:742:MET:HE2	1.98	0.46
1:C:2:ALA:HB1	1:C:3:PRO:HD2	1.96	0.46
1:C:582:ILE:HD11	1:D:1019:LEU:HD13	1.98	0.46
1:C:845:GLU:H	1:C:845:GLU:CD	2.23	0.46
1:D:248:MET:HE1	1:D:255:ILE:HD11	1.98	0.46
1:D:374:PRO:HG3	7:D:2231:HOH:O	2.16	0.46
1:D:868:ILE:HG22	1:D:870:GLU:H	1.80	0.46
1:A:870:GLU:HB3	1:A:889:ILE:CG2	2.46	0.45
1:C:582:ILE:HD11	1:D:1019:LEU:HD11	1.97	0.45
1:D:884:GLU:HB3	7:D:2112:HOH:O	2.16	0.45
1:B:82:CYS:O	1:B:98:LYS:HD2	2.16	0.45
1:B:191:ALA:O	1:B:279:ALA:HA	2.17	0.45
1:B:1014:LYS:HE3	7:B:3027:HOH:O	2.16	0.45
1:B:335:VAL:HG22	1:B:433:VAL:HB	1.97	0.45
1:B:711:THR:HG22	7:B:2774:HOH:O	2.15	0.45
1:D:367:PHE:CZ	1:D:387:PHE:CB	3.00	0.45
1:B:169:PRO:HD3	1:B:911:PRO:HB3	1.97	0.45
1:B:943:GLN:HG3	1:B:1011:TYR:CB	2.47	0.45
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.97	0.45
1:A:56:GLU:OE2	1:A:898:LYS:NZ	2.48	0.45
1:A:877:PRO:HG2	1:A:977:THR:HB	1.97	0.45
1:B:681:GLY:HA3	1:B:686:GLN:OE1	2.16	0.45
1:D:572:LEU:HD13	1:D:638:ILE:HB	1.98	0.45
1:C:616:LYS:HD3	1:C:620:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:ILE:CD1	1:A:893:GLU:HB2	2.46	0.45
1:D:263:GLU:O	1:D:264:ASN:CB	2.65	0.45
1:D:896:ARG:HD2	7:D:2960:HOH:O	2.15	0.45
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.16	0.45
1:A:413:GLN:HG3	1:A:419:TRP:CE2	2.52	0.45
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.99	0.45
1:B:49:CYS:SG	1:B:51:HIS:CE1	3.10	0.45
1:B:574:LYS:HG3	1:B:614:SER:HB2	1.98	0.45
1:B:870:GLU:O	1:B:889:ILE:HD13	2.17	0.45
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.99	0.45
1:D:100:PHE:CD1	1:D:100:PHE:C	2.95	0.45
1:D:451:LEU:O	1:D:454:ILE:HG12	2.17	0.45
4:A:1031:FAD:H1'1	5:A:1032:NDP:H3D	1.98	0.45
7:A:2197:HOH:O	1:B:22:THR:HG22	2.17	0.45
1:D:335:VAL:HG22	1:D:433:VAL:HB	1.99	0.45
1:B:346:ASP:OD2	4:B:1031:FAD:H6	2.17	0.44
1:C:100:PHE:CD1	1:C:100:PHE:C	2.95	0.44
1:D:367:PHE:HZ	1:D:387:PHE:CB	2.29	0.44
1:D:371:ARG:HH21	5:D:1032:NDP:H5N	1.82	0.44
1:A:261:LEU:HD21	1:A:451:LEU:HD21	1.99	0.44
1:A:786:PRO:CB	1:D:942:GLU:HA	2.47	0.44
1:B:696:ARG:NH2	7:B:2765:HOH:O	2.51	0.44
5:B:1032:NDP:H4D	5:B:1032:NDP:O2N	2.17	0.44
1:C:53:GLU:O	1:C:55:LEU:HG	2.17	0.44
1:D:131:PRO:HB2	1:D:373:VAL:HG11	2.00	0.44
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.52	0.44
1:C:367:PHE:CE1	1:D:367:PHE:CZ	3.05	0.44
7:C:2174:HOH:O	1:D:29:HIS:HB2	2.17	0.44
1:A:191:ALA:O	1:A:279:ALA:HA	2.17	0.44
1:D:608:LEU:HB2	1:D:742:MET:HE2	2.00	0.44
1:B:845:GLU:HG3	1:B:912:PHE:CG	2.52	0.44
1:D:83:ALA:O	1:D:84:ASP:C	2.61	0.44
1:A:1008:THR:HG23	7:A:3024:HOH:O	2.16	0.44
1:B:993:LEU:C	1:B:993:LEU:HD23	2.42	0.44
1:C:574:LYS:HG3	1:C:614:SER:HB2	2.00	0.44
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	2.00	0.44
1:D:116:ILE:HD13	1:D:156:GLN:HG3	1.99	0.44
1:D:414:ASP:C	1:D:416:THR:H	2.25	0.44
1:C:311:PRO:O	1:C:315:LYS:HG3	2.18	0.44
1:D:346:ASP:OD2	4:D:1031:FAD:H6	2.18	0.44
1:D:485:MET:O	1:D:487:ASN:OD1	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:CG2	7:B:2053:HOH:O	2.66	0.44
1:B:54:LYS:HD3	7:B:2050:HOH:O	2.18	0.44
1:D:870:GLU:OE1	1:D:870:GLU:N	2.45	0.43
1:A:97:ILE:HD11	2:A:1026:SF4:S4	2.58	0.43
1:A:784:ALA:C	1:A:786:PRO:HD3	2.44	0.43
1:B:39:LYS:HG3	7:B:2079:HOH:O	2.18	0.43
1:B:394:ARG:NH2	1:B:423:GLU:OE2	2.51	0.43
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.47	0.43
1:C:673:HIS:ND1	1:C:673:HIS:C	2.76	0.43
1:C:893:GLU:OE1	1:C:896:ARG:NH2	2.44	0.43
1:D:412:GLU:O	1:D:419:TRP:HA	2.18	0.43
1:A:248:MET:HE1	1:A:255:ILE:HD11	1.99	0.43
1:B:116:ILE:HD13	1:B:156:GLN:HG3	1.99	0.43
1:B:896:ARG:NH1	1:B:896:ARG:CG	2.80	0.43
1:D:54:LYS:NZ	1:D:895:MET:CG	2.81	0.43
1:D:57:ASN:HB2	7:D:2119:HOH:O	2.18	0.43
1:A:870:GLU:HB3	1:A:889:ILE:HG23	2.00	0.43
1:B:167:ASN:HD22	1:B:911:PRO:HA	1.83	0.43
1:A:368:VAL:HG23	1:B:386:GLU:OE1	2.17	0.43
1:A:776:ARG:HB2	1:B:740:GLY:HA2	2.00	0.43
1:B:20:PRO:HG2	1:B:961:MET:SD	2.58	0.43
1:B:181:LYS:HD2	7:B:2263:HOH:O	2.19	0.43
1:D:629:LYS:CE	1:D:629:LYS:HA	2.49	0.43
1:D:877:PRO:CG	1:D:977:THR:HB	2.49	0.43
1:A:613:ILE:HD13	1:A:642:MET:HE2	1.99	0.43
1:A:870:GLU:O	1:A:874:LYS:CD	2.65	0.43
1:C:22:THR:HG22	7:D:2204:HOH:O	2.18	0.43
1:C:859:HIS:HE1	7:C:3051:HOH:O	2.02	0.43
1:C:1017:LEU:HD22	1:C:1018:PRO:HD2	2.00	0.43
7:C:2820:HOH:O	1:D:775:LEU:HD12	2.18	0.43
1:A:667:LEU:HD21	1:A:698:VAL:HG21	2.00	0.43
1:A:929:LEU:HB2	1:D:941:ILE:CD1	2.48	0.43
1:B:150:ILE:HB	2:B:1027:SF4:S4	2.59	0.43
1:B:868:ILE:HG22	1:B:870:GLU:H	1.84	0.43
1:C:193:LEU:N	1:C:193:LEU:HD22	2.34	0.43
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.59	0.43
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.49	0.43
1:B:140:CYS:HA	2:B:1027:SF4:S3	2.58	0.43
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.85	0.43
1:C:369:ASN:ND2	1:D:50:PHE:CD1	2.87	0.43
1:C:1019:LEU:HD11	1:D:582:ILE:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:PRO:HG2	1:C:961:MET:SD	2.59	0.43
1:D:97:ILE:HA	1:D:100:PHE:CD2	2.54	0.43
1:D:680:MET:HE3	7:D:2806:HOH:O	2.18	0.43
1:A:621:TRP:O	1:A:625:VAL:HG23	2.19	0.43
1:B:375:GLU:CD	1:B:375:GLU:H	2.26	0.43
1:B:379:LEU:O	1:B:383:GLU:HG3	2.19	0.43
1:B:892:GLU:HG3	7:B:2908:HOH:O	2.19	0.43
1:C:759:ARG:HH21	1:D:933:GLY:HA3	1.84	0.43
1:D:264:ASN:ND2	7:D:2411:HOH:O	2.51	0.43
1:D:487:ASN:HB3	5:D:1032:NDP:C2N	2.48	0.43
1:D:621:TRP:O	1:D:625:VAL:HG23	2.19	0.43
1:A:263:GLU:O	1:A:264:ASN:CB	2.67	0.42
1:A:570:PHE:HB3	1:A:636:ILE:HB	2.01	0.42
1:A:574:LYS:HG3	1:A:614:SER:HB2	2.01	0.42
1:C:608:LEU:HB2	1:C:742:MET:HE2	2.01	0.42
1:C:871:LEU:HD12	1:C:871:LEU:HA	1.90	0.42
1:A:83:ALA:O	1:A:84:ASP:C	2.62	0.42
1:B:173:ASN:HB3	1:B:176:LEU:CD1	2.49	0.42
1:C:83:ALA:O	1:C:84:ASP:C	2.62	0.42
1:C:845:GLU:HG3	1:C:912:PHE:CG	2.54	0.42
1:C:990:THR:O	1:C:990:THR:CG2	2.68	0.42
1:A:427:VAL:CG1	1:B:410:ARG:CZ	2.92	0.42
1:A:582:ILE:CD1	1:B:1019:LEU:HD22	2.49	0.42
1:B:394:ARG:NH1	1:B:409:VAL:HG21	2.34	0.42
1:C:248:MET:HE1	1:C:255:ILE:HD11	2.01	0.42
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.19	0.42
1:C:2:ALA:HB1	1:C:3:PRO:CD	2.50	0.42
1:C:427:VAL:CG1	1:D:410:ARG:NH1	2.80	0.42
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.55	0.42
1:C:783:ARG:NH1	7:C:2852:HOH:O	2.50	0.42
1:D:870:GLU:O	1:D:874:LYS:HG3	2.19	0.42
1:D:877:PRO:HG2	1:D:977:THR:HB	2.00	0.42
1:A:760:THR:HG23	1:B:932:LEU:HD23	2.01	0.42
1:D:167:ASN:ND2	1:D:911:PRO:HA	2.34	0.42
1:D:375:GLU:CD	1:D:375:GLU:N	2.78	0.42
1:B:371:ARG:HG2	1:B:371:ARG:HH11	1.85	0.42
1:C:859:HIS:HA	1:C:865:VAL:HG23	2.02	0.42
1:D:868:ILE:HG22	1:D:870:GLU:OE1	2.19	0.42
1:A:519:PRO:HB3	1:B:28:LEU:HD22	2.00	0.42
1:B:989:CYS:O	1:B:990:THR:HB	2.20	0.42
1:C:328:LEU:O	1:C:329:PRO:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ARG:HG3	1:C:409:VAL:HG13	2.01	0.42
1:D:916:LYS:HB2	1:D:917:PRO:HD2	2.01	0.42
1:A:335:VAL:HG22	1:A:433:VAL:HB	2.02	0.42
1:A:868:ILE:HG12	1:A:870:GLU:HB2	2.00	0.42
1:C:825:THR:HA	7:C:2879:HOH:O	2.19	0.42
1:C:132:THR:HB	1:C:137:VAL:HG23	2.01	0.42
1:C:771:ARG:N	1:C:772:PRO:CD	2.83	0.42
1:C:989:CYS:O	1:C:990:THR:HB	2.20	0.42
1:D:50:PHE:O	1:D:384:LYS:HD2	2.20	0.42
1:B:56:GLU:OE2	1:B:898:LYS:NZ	2.53	0.42
1:B:173:ASN:HB3	1:B:176:LEU:HD12	2.02	0.42
1:B:734:ALA:HA	1:B:735:THR:HA	1.69	0.42
1:B:899:GLU:HB2	7:B:2913:HOH:O	2.18	0.42
1:C:760:THR:CG2	1:D:932:LEU:HD23	2.50	0.42
1:A:132:THR:HB	1:A:137:VAL:CG2	2.50	0.41
1:B:872:MET:HE1	7:B:2959:HOH:O	2.20	0.41
1:C:173:ASN:OD1	1:C:173:ASN:N	2.49	0.41
1:D:367:PHE:HE1	1:D:389:PRO:HD3	1.85	0.41
1:A:54:LYS:NZ	1:A:895:MET:CG	2.82	0.41
1:B:83:ALA:O	1:B:84:ASP:C	2.62	0.41
1:C:29:HIS:HB2	7:D:2191:HOH:O	2.20	0.41
1:A:52:CYS:O	1:A:53:GLU:C	2.63	0.41
1:A:172:ARG:HG3	7:A:2312:HOH:O	2.20	0.41
1:A:646:ASN:ND2	1:A:649:ASP:CG	2.78	0.41
1:A:783:ARG:NE	7:A:2825:HOH:O	2.52	0.41
1:A:898:LYS:HD2	7:A:2120:HOH:O	2.19	0.41
1:C:140:CYS:HA	2:C:1027:SF4:S3	2.60	0.41
1:C:487:ASN:ND2	1:D:35:LYS:HZ3	2.17	0.41
1:D:669:LEU:HD13	1:D:691:VAL:HG22	2.02	0.41
1:D:734:ALA:HA	1:D:735:THR:HA	1.66	0.41
1:B:57:ASN:ND2	1:B:898:LYS:HB2	2.35	0.41
1:B:410:ARG:HG2	1:B:411:THR:N	2.34	0.41
1:A:410:ARG:HB2	1:A:422:ASP:HB2	2.03	0.41
1:D:191:ALA:HB2	1:D:276:TYR:CD2	2.56	0.41
1:A:549:ALA:HB2	1:A:814:GLN:HB3	2.03	0.41
1:A:771:ARG:N	1:A:772:PRO:CD	2.84	0.41
1:B:629:LYS:HA	1:B:629:LYS:CE	2.50	0.41
1:C:261:LEU:HD21	1:C:451:LEU:HD21	2.02	0.41
1:C:629:LYS:HA	1:C:629:LYS:HE2	2.03	0.41
1:C:892:GLU:HG3	7:C:2950:HOH:O	2.19	0.41
1:D:150:ILE:HB	2:D:1027:SF4:S4	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD22	1:B:519:PRO:HB3	2.03	0.41
1:C:42:LYS:HE3	1:C:44:ASN:O	2.20	0.41
1:A:394:ARG:HG3	1:A:409:VAL:HG13	2.02	0.41
1:A:582:ILE:HD11	1:B:1015:ARG:NE	2.36	0.41
1:B:458:ARG:NE	1:B:459:TRP:CZ3	2.88	0.41
1:B:671:ALA:HA	1:B:672:PRO:HD3	1.88	0.41
1:C:716:ASP:OD2	1:C:719:SER:HB3	2.21	0.41
1:A:35:LYS:NZ	1:B:487:ASN:ND2	2.69	0.41
1:A:601:GLY:HA3	1:A:602:PRO:HD2	1.97	0.41
1:B:53:GLU:HB2	7:B:2907:HOH:O	2.20	0.41
1:C:392:SER:HA	1:C:393:PRO:HD3	1.93	0.41
1:C:415:GLU:HA	1:C:415:GLU:OE1	2.21	0.41
1:D:191:ALA:O	1:D:279:ALA:HA	2.21	0.41
1:B:934:THR:OG1	1:B:937:GLU:HG3	2.21	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.02	0.41
1:C:35:LYS:HE2	7:D:2627:HOH:O	2.19	0.41
1:C:621:TRP:O	1:C:625:VAL:HG23	2.21	0.41
1:D:54:LYS:HZ1	1:D:895:MET:HG3	1.85	0.41
1:D:413:GLN:HG3	1:D:419:TRP:CE2	2.55	0.41
1:D:680:MET:HE2	1:D:688:PRO:HD2	1.97	0.41
1:A:54:LYS:HZ1	1:A:895:MET:CG	2.34	0.40
7:A:2757:HOH:O	1:B:722:ARG:HD2	2.20	0.40
1:C:1007:ARG:NE	1:C:1011:TYR:HB2	2.35	0.40
1:D:413:GLN:HA	1:D:418:LYS:O	2.20	0.40
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.62	0.40
1:A:929:LEU:HB2	1:D:941:ILE:HD12	2.02	0.40
1:B:863:LYS:HA	1:B:864:PRO:HD3	1.95	0.40
1:C:779:THR:O	1:C:783:ARG:HG3	2.21	0.40
1:C:898:LYS:O	1:C:898:LYS:HG2	2.21	0.40
1:D:54:LYS:HE2	7:D:2118:HOH:O	2.21	0.40
1:D:363:PHE:HE2	1:D:389:PRO:HB3	1.86	0.40
1:A:734:ALA:HA	1:A:735:THR:HA	1.67	0.40
1:C:865:VAL:HA	1:C:866:PRO:HD3	1.94	0.40
1:A:192:LEU:C	1:A:193:LEU:HD22	2.47	0.40
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.56	0.40
1:C:519:PRO:HB3	1:D:28:LEU:HD22	2.04	0.40
1:D:616:LYS:HD3	1:D:620:TYR:CE1	2.56	0.40
1:D:911:PRO:HG3	7:D:2122:HOH:O	2.21	0.40
1:B:962:THR:O	1:B:966:SER:HB2	2.22	0.40
5:B:1032:NDP:H8A	7:B:2546:HOH:O	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ASP:OD1	1:D:395:LYS:NZ[1_656]	2.18	0.02

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	1014/1025 (99%)	972 (96%)	34 (3%)	8 (1%)	16	11
1	B	1017/1025 (99%)	966 (95%)	39 (4%)	12 (1%)	10	6
1	C	1017/1025 (99%)	973 (96%)	37 (4%)	7 (1%)	18	14
1	D	1017/1025 (99%)	974 (96%)	36 (4%)	7 (1%)	18	14
All	All	4065/4100 (99%)	3885 (96%)	146 (4%)	34 (1%)	16	11

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	678	ARG
1	A	903	ALA
1	A	904	PHE
1	A	908	GLU
1	B	416	THR
1	B	675	MET
1	B	678	ARG
1	B	901	ASN
1	B	902	ALA
1	B	903	ALA
1	C	678	ARG
1	D	415	GLU
1	D	906	PRO
1	D	908	GLU
1	B	677	GLU
1	B	679	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3	PRO
1	C	674	GLY
1	C	680	MET
1	C	1018	PRO
1	D	676	GLY
1	A	907	LEU
1	B	909	ARG
1	B	1018	PRO
1	C	898	LYS
1	D	3	PRO
1	D	1018	PRO
1	A	3	PRO
1	A	906	PRO
1	C	415	GLU
1	B	3	PRO
1	D	53	GLU
1	B	905	PRO
1	A	794	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/853 (99%)	835 (99%)	10 (1%)	63	70
1	B	847/853 (99%)	840 (99%)	7 (1%)	73	80
1	C	847/853 (99%)	833 (98%)	14 (2%)	53	60
1	D	847/853 (99%)	843 (100%)	4 (0%)	81	87
All	All	3386/3412 (99%)	3351 (99%)	35 (1%)	68	75

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PHE
1	A	363	PHE
1	A	368	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	453	PRO
1	A	482	ILE
1	A	793	THR
1	A	845	GLU
1	A	900	GLN
1	A	906	PRO
1	A	955	ASN
1	B	100	PHE
1	B	167	ASN
1	B	453	PRO
1	B	680	MET
1	B	793	THR
1	B	845	GLU
1	B	906	PRO
1	C	100	PHE
1	C	173	ASN
1	C	326	SER
1	C	331	ILE
1	C	368	VAL
1	C	402	ARG
1	C	453	PRO
1	C	758	LYS
1	C	793	THR
1	C	845	GLU
1	C	916	LYS
1	C	950	GLU
1	C	1017	LEU
1	C	1018	PRO
1	D	39	LYS
1	D	100	PHE
1	D	453	PRO
1	D	950	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	57	ASN
1	A	242	ASN
1	A	295	GLN
1	A	299	GLN
1	A	407	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	494	ASN
1	A	623	GLN
1	A	828	GLN
1	A	859	HIS
1	A	972	GLN
1	B	51	HIS
1	B	57	ASN
1	B	167	ASN
1	B	299	GLN
1	B	413	GLN
1	B	487	ASN
1	B	494	ASN
1	B	623	GLN
1	B	828	GLN
1	B	847	GLN
1	B	930	GLN
1	C	295	GLN
1	C	299	GLN
1	C	407	GLN
1	C	487	ASN
1	C	623	GLN
1	C	828	GLN
1	C	859	HIS
1	C	878	ASN
1	C	930	GLN
1	C	978	HIS
1	D	51	HIS
1	D	299	GLN
1	D	623	GLN
1	D	878	ASN
1	D	930	GLN
1	D	972	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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	1027	-	0,12,12	-	-	-		
2	SF4	C	1027	-	0,12,12	-	-	-		
3	FMN	C	1030	-	33,33,33	1.93	8 (24%)	48,50,50	1.85	11 (22%)
5	NDP	A	1032	-	51,52,52	1.89	11 (21%)	71,80,80	2.51	15 (21%)
5	NDP	B	1032	-	51,52,52	1.91	11 (21%)	71,80,80	2.50	15 (21%)
6	URF	C	1033	-	9,9,9	2.33	4 (44%)	12,12,12	2.25	4 (33%)
3	FMN	D	1030	-	33,33,33	1.89	8 (24%)	48,50,50	1.84	10 (20%)
5	NDP	D	1032	-	51,52,52	2.01	15 (29%)	71,80,80	1.89	18 (25%)
2	SF4	A	1029	-	0,12,12	-	-	-		
2	SF4	D	1028	1	0,12,12	-	-	-		
2	SF4	C	1026	-	0,12,12	-	-	-		
5	NDP	C	1032	-	51,52,52	2.59	16 (31%)	71,80,80	1.91	20 (28%)
2	SF4	D	1026	-	0,12,12	-	-	-		
2	SF4	A	1027	-	0,12,12	-	-	-		
6	URF	A	1033	-	9,9,9	2.24	4 (44%)	12,12,12	2.26	4 (33%)
2	SF4	B	1026	-	0,12,12	-	-	-		
2	SF4	B	1029	-	0,12,12	-	-	-		
4	FAD	B	1031	-	58,58,58	2.41	23 (39%)	85,89,89	1.64	10 (11%)
2	SF4	A	1028	-	0,12,12	-	-	-		
2	SF4	D	1029	1	0,12,12	-	-	-		
6	URF	B	1033	-	9,9,9	2.28	5 (55%)	12,12,12	2.26	4 (33%)
2	SF4	B	1028	-	0,12,12	-	-	-		
2	SF4	A	1026	-	0,12,12	-	-	-		
3	FMN	A	1030	-	33,33,33	1.91	8 (24%)	48,50,50	1.87	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	A	1031	-	58,58,58	2.38	26 (44%)	85,89,89	1.68	10 (11%)
3	FMN	B	1030	-	33,33,33	1.92	8 (24%)	48,50,50	1.86	12 (25%)
4	FAD	D	1031	-	58,58,58	2.41	24 (41%)	85,89,89	1.63	8 (9%)
2	SF4	C	1028	-	0,12,12	-	-	-	-	-
6	URF	D	1033	-	9,9,9	2.27	4 (44%)	12,12,12	2.22	4 (33%)
2	SF4	C	1029	-	0,12,12	-	-	-	-	-
2	SF4	D	1027	1	0,12,12	-	-	-	-	-
4	FAD	C	1031	-	58,58,58	2.39	27 (46%)	85,89,89	1.66	10 (11%)

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	1027	-	-	-	0/6/5/5
2	SF4	C	1027	-	-	-	0/6/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
5	NDP	B	1032	-	3/3/14/17	13/34/77/77	0/5/5/5
5	NDP	A	1032	-	3/3/14/17	14/34/77/77	0/5/5/5
6	URF	C	1033	-	-	-	0/1/1/1
5	NDP	D	1032	-	3/3/14/17	10/34/77/77	0/5/5/5
2	SF4	A	1029	-	-	-	0/6/5/5
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	C	1026	-	-	-	0/6/5/5
5	NDP	C	1032	-	3/3/14/17	7/34/77/77	0/5/5/5
2	SF4	D	1026	-	-	-	0/6/5/5
2	SF4	A	1027	-	-	-	0/6/5/5
6	URF	A	1033	-	-	-	0/1/1/1
2	SF4	B	1026	-	-	-	0/6/5/5
2	SF4	B	1029	-	-	-	0/6/5/5
4	FAD	B	1031	-	-	3/34/50/50	0/6/6/6
2	SF4	A	1028	-	-	-	0/6/5/5
2	SF4	D	1029	1	-	-	0/6/5/5
6	URF	B	1033	-	-	-	0/1/1/1
2	SF4	B	1028	-	-	-	0/6/5/5
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1026	-	-	-	0/6/5/5
4	FAD	A	1031	-	-	3/34/50/50	0/6/6/6
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	D	1031	-	-	3/34/50/50	0/6/6/6
2	SF4	C	1029	-	-	-	0/6/5/5
2	SF4	C	1028	-	-	-	0/6/5/5
6	URF	D	1033	-	-	-	0/1/1/1
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1027	1	-	-	0/6/5/5
4	FAD	C	1031	-	-	3/34/50/50	0/6/6/6

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1032	NDP	PN-O3	11.59	1.72	1.59
4	B	1031	FAD	PA-O3P	9.28	1.69	1.59
4	D	1031	FAD	PA-O3P	9.17	1.69	1.59
4	C	1031	FAD	PA-O3P	9.04	1.69	1.59
4	A	1031	FAD	PA-O3P	8.64	1.68	1.59
4	A	1031	FAD	P-O3P	-7.27	1.51	1.59
4	D	1031	FAD	P-O3P	-6.84	1.52	1.59
4	B	1031	FAD	P-O3P	-6.79	1.52	1.59
4	C	1031	FAD	P-O3P	-6.73	1.52	1.59
5	D	1032	NDP	C4N-C3N	-6.32	1.38	1.50
5	C	1032	NDP	PA-O3	5.81	1.65	1.59
5	B	1032	NDP	C4N-C3N	-5.46	1.39	1.50
5	B	1032	NDP	C4N-C5N	-5.36	1.35	1.49
5	A	1032	NDP	C4N-C3N	-5.32	1.39	1.50
5	A	1032	NDP	C4N-C5N	-5.12	1.35	1.49
5	A	1032	NDP	C5B-C4B	-5.02	1.36	1.51
5	B	1032	NDP	C5B-C4B	-4.91	1.36	1.51
5	D	1032	NDP	PA-O3	-4.52	1.54	1.59
3	A	1030	FMN	C4A-N5	4.49	1.40	1.30
3	B	1030	FMN	C4A-N5	4.48	1.40	1.30
3	B	1030	FMN	C7M-C7	4.39	1.59	1.51
3	C	1030	FMN	C4A-N5	4.36	1.40	1.30
5	B	1032	NDP	C2N-C3N	4.35	1.47	1.35
3	D	1030	FMN	C4A-N5	4.35	1.40	1.30
4	B	1031	FAD	PA-O2A	-4.20	1.35	1.55
4	D	1031	FAD	PA-O2A	-4.17	1.36	1.55
5	A	1032	NDP	C2N-C3N	4.10	1.46	1.35
3	C	1030	FMN	C7M-C7	4.08	1.58	1.51
3	A	1030	FMN	C7M-C7	4.05	1.58	1.51
5	C	1032	NDP	C4N-C3N	-4.04	1.42	1.50
4	C	1031	FAD	PA-O2A	-4.03	1.36	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1030	FMN	C7M-C7	4.03	1.58	1.51
6	C	1033	URF	C2-N1	4.01	1.41	1.36
4	A	1031	FAD	PA-O2A	-4.01	1.36	1.55
5	C	1032	NDP	C2D-C3D	-3.99	1.42	1.53
6	B	1033	URF	C2-N1	3.99	1.41	1.36
5	C	1032	NDP	PN-O5D	3.98	1.75	1.59
5	D	1032	NDP	C2N-C3N	3.92	1.46	1.35
6	A	1033	URF	C2-N1	3.91	1.41	1.36
6	D	1033	URF	C2-N1	3.89	1.41	1.36
4	D	1031	FAD	C5'-C4'	3.89	1.57	1.51
5	D	1032	NDP	C4N-C5N	-3.88	1.38	1.49
3	B	1030	FMN	C1'-N10	-3.69	1.38	1.47
3	C	1030	FMN	C1'-N10	-3.68	1.38	1.47
5	D	1032	NDP	C5B-C4B	-3.65	1.40	1.51
6	D	1033	URF	C6-N1	3.65	1.42	1.36
4	B	1031	FAD	C5'-C4'	3.63	1.56	1.51
6	C	1033	URF	C6-N1	3.61	1.42	1.36
5	C	1032	NDP	C4N-C5N	-3.61	1.39	1.49
5	C	1032	NDP	O2D-C2D	3.56	1.51	1.43
6	B	1033	URF	C6-N1	3.55	1.42	1.36
3	D	1030	FMN	C1'-N10	-3.54	1.39	1.47
3	A	1030	FMN	C1'-N10	-3.53	1.39	1.47
4	A	1031	FAD	C9A-N10	3.45	1.47	1.41
4	C	1031	FAD	C9A-N10	3.44	1.47	1.41
5	D	1032	NDP	C2D-C1D	3.44	1.64	1.53
4	B	1031	FAD	C9A-N10	3.43	1.47	1.41
4	D	1031	FAD	P-O2P	-3.43	1.39	1.55
4	A	1031	FAD	P-O2P	-3.42	1.39	1.55
3	C	1030	FMN	C9A-C5A	3.40	1.46	1.41
4	C	1031	FAD	C4X-N5	3.39	1.38	1.30
3	C	1030	FMN	C4'-C3'	3.38	1.59	1.53
4	B	1031	FAD	C4X-N5	3.37	1.38	1.30
3	A	1030	FMN	C4'-C3'	3.35	1.59	1.53
6	A	1033	URF	C6-N1	3.34	1.41	1.36
4	C	1031	FAD	P-O2P	-3.32	1.40	1.55
3	D	1030	FMN	C4'-C3'	3.31	1.59	1.53
3	A	1030	FMN	C9A-C5A	3.28	1.46	1.41
4	D	1031	FAD	C9A-N10	3.27	1.46	1.41
4	D	1031	FAD	C4X-N5	3.26	1.37	1.30
4	C	1031	FAD	C5'-C4'	3.25	1.56	1.51
4	B	1031	FAD	P-O2P	-3.25	1.40	1.55
5	A	1032	NDP	C1D-N1N	3.23	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1032	NDP	C2D-C1D	3.22	1.63	1.53
4	A	1031	FAD	C5'-C4'	3.20	1.56	1.51
5	C	1032	NDP	C2N-C3N	3.17	1.43	1.35
5	D	1032	NDP	O4D-C1D	3.16	1.49	1.42
4	A	1031	FAD	C4X-N5	3.13	1.37	1.30
3	B	1030	FMN	C9A-C5A	3.11	1.46	1.41
5	C	1032	NDP	C8A-N9A	3.11	1.42	1.37
5	B	1032	NDP	C2D-C1D	3.10	1.63	1.53
3	B	1030	FMN	C9A-N10	3.10	1.46	1.41
4	D	1031	FAD	C9A-C5X	3.09	1.46	1.41
3	C	1030	FMN	C1'-C2'	3.08	1.56	1.52
4	C	1031	FAD	C9A-C5X	3.02	1.46	1.41
3	A	1030	FMN	C1'-C2'	3.02	1.56	1.52
4	B	1031	FAD	C9A-C5X	3.02	1.46	1.41
3	D	1030	FMN	C1'-C2'	3.02	1.56	1.52
3	D	1030	FMN	C9A-C5A	3.00	1.46	1.41
4	C	1031	FAD	C8-C7	2.99	1.48	1.40
3	B	1030	FMN	C4'-C3'	2.97	1.58	1.53
4	A	1031	FAD	C8-C7	2.97	1.48	1.40
5	A	1032	NDP	C5D-C4D	2.96	1.60	1.51
5	D	1032	NDP	C6N-N1N	2.96	1.44	1.37
6	C	1033	URF	C6-C5	2.95	1.36	1.33
5	D	1032	NDP	O5D-C5D	2.94	1.55	1.44
4	A	1031	FAD	C9A-C5X	2.93	1.45	1.41
3	D	1030	FMN	C9A-N10	2.92	1.46	1.41
4	D	1031	FAD	C8-C7	2.91	1.48	1.40
3	C	1030	FMN	C9A-N10	2.91	1.46	1.41
5	C	1032	NDP	PA-O5B	2.88	1.70	1.59
3	A	1030	FMN	C9A-N10	2.87	1.46	1.41
3	B	1030	FMN	C1'-C2'	2.87	1.56	1.52
4	B	1031	FAD	O5'-C5'	2.85	1.55	1.44
4	B	1031	FAD	C8-C7	2.80	1.47	1.40
5	B	1032	NDP	C5D-C4D	2.78	1.59	1.51
5	D	1032	NDP	C6N-C5N	2.76	1.41	1.33
5	B	1032	NDP	C8A-N9A	2.74	1.42	1.37
5	C	1032	NDP	C2D-C1D	2.73	1.62	1.53
4	B	1031	FAD	C6-C5X	2.73	1.44	1.40
4	D	1031	FAD	C1'-C2'	2.70	1.56	1.52
4	A	1031	FAD	O5'-C5'	2.69	1.54	1.44
5	B	1032	NDP	C1D-N1N	2.67	1.53	1.46
4	D	1031	FAD	C4A-N3A	2.64	1.39	1.34
4	C	1031	FAD	O5'-C5'	2.64	1.54	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1031	FAD	C6-C5X	2.63	1.44	1.40
5	A	1032	NDP	C8A-N9A	2.63	1.42	1.37
4	C	1031	FAD	C5A-C4A	2.63	1.43	1.39
5	C	1032	NDP	C5B-C4B	-2.63	1.43	1.51
4	A	1031	FAD	C1'-C2'	2.62	1.56	1.52
4	B	1031	FAD	C5A-C6A	2.62	1.48	1.41
4	D	1031	FAD	O5'-C5'	2.62	1.54	1.44
6	A	1033	URF	C6-C5	2.59	1.36	1.33
4	B	1031	FAD	C5A-C4A	2.58	1.43	1.39
6	D	1033	URF	C6-C5	2.56	1.36	1.33
4	D	1031	FAD	C5A-C6A	2.53	1.48	1.41
4	A	1031	FAD	C4A-N3A	2.53	1.39	1.34
4	C	1031	FAD	C6-C5X	2.52	1.43	1.40
4	C	1031	FAD	C1'-C2'	2.51	1.56	1.52
4	B	1031	FAD	O4B-C4B	2.51	1.50	1.45
4	A	1031	FAD	C9-C9A	2.49	1.43	1.39
4	C	1031	FAD	C4A-N3A	2.49	1.39	1.34
4	D	1031	FAD	C2A-N1A	2.48	1.38	1.33
5	A	1032	NDP	P2B-O2B	-2.48	1.55	1.59
5	D	1032	NDP	C2B-C1B	-2.48	1.47	1.53
4	C	1031	FAD	O4B-C4B	2.47	1.50	1.45
4	D	1031	FAD	C10-N1	2.46	1.38	1.33
4	A	1031	FAD	C5A-C6A	2.46	1.47	1.41
6	A	1033	URF	F5-C5	-2.45	1.30	1.35
4	A	1031	FAD	O4B-C4B	2.45	1.50	1.45
6	B	1033	URF	C6-C5	2.45	1.35	1.33
4	D	1031	FAD	O4B-C4B	2.44	1.50	1.45
4	B	1031	FAD	C2A-N1A	2.44	1.38	1.33
4	C	1031	FAD	C9-C9A	2.44	1.43	1.39
4	C	1031	FAD	C10-N1	2.43	1.38	1.33
4	C	1031	FAD	C5A-C6A	2.42	1.47	1.41
5	D	1032	NDP	O3D-C3D	-2.39	1.37	1.43
5	C	1032	NDP	O4B-C1B	2.38	1.47	1.42
4	A	1031	FAD	C5A-C4A	2.37	1.43	1.39
4	A	1031	FAD	C10-N1	2.37	1.38	1.33
3	B	1030	FMN	C10-N1	2.36	1.38	1.33
6	B	1033	URF	F5-C5	-2.35	1.30	1.35
5	B	1032	NDP	PA-O2A	-2.35	1.44	1.55
4	B	1031	FAD	C4A-N3A	2.34	1.38	1.34
4	B	1031	FAD	C10-N1	2.34	1.37	1.33
5	D	1032	NDP	C8A-N9A	2.32	1.41	1.37
4	C	1031	FAD	C2A-N1A	2.30	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1031	FAD	P-O5'	-2.29	1.50	1.59
6	D	1033	URF	F5-C5	-2.29	1.31	1.35
4	A	1031	FAD	C5B-C4B	2.29	1.58	1.51
3	D	1030	FMN	C10-N1	2.29	1.37	1.33
4	D	1031	FAD	C5B-C4B	2.29	1.58	1.51
4	C	1031	FAD	P-O5'	-2.29	1.50	1.59
4	A	1031	FAD	P-O5'	-2.28	1.50	1.59
4	D	1031	FAD	C6-C5X	2.28	1.43	1.40
4	C	1031	FAD	C9-C8	2.27	1.42	1.39
4	B	1031	FAD	C9-C9A	2.27	1.43	1.39
4	D	1031	FAD	C5A-C4A	2.26	1.43	1.39
4	D	1031	FAD	C9-C8	2.25	1.42	1.39
4	D	1031	FAD	C9-C9A	2.24	1.43	1.39
3	C	1030	FMN	C10-N1	2.24	1.37	1.33
3	A	1030	FMN	C10-N1	2.23	1.37	1.33
4	D	1031	FAD	C2-N3	2.21	1.43	1.39
5	A	1032	NDP	C4A-N3A	2.21	1.38	1.34
4	C	1031	FAD	C5B-C4B	2.20	1.58	1.51
5	D	1032	NDP	C1D-N1N	2.20	1.52	1.46
5	B	1032	NDP	C4A-N3A	2.20	1.38	1.34
5	C	1032	NDP	C4A-N3A	2.19	1.38	1.34
4	B	1031	FAD	C2-N3	2.18	1.43	1.39
4	C	1031	FAD	C2-N3	2.18	1.43	1.39
4	A	1031	FAD	C2A-N1A	2.18	1.37	1.33
4	B	1031	FAD	O4B-C1B	2.17	1.47	1.42
4	D	1031	FAD	P-O5'	-2.16	1.50	1.59
5	D	1032	NDP	C4A-N3A	2.15	1.38	1.34
4	C	1031	FAD	C3B-C4B	2.15	1.58	1.53
4	B	1031	FAD	C5B-C4B	2.14	1.58	1.51
4	C	1031	FAD	O4B-C1B	2.14	1.46	1.42
6	C	1033	URF	F5-C5	-2.13	1.31	1.35
4	C	1031	FAD	C4-N3	2.12	1.42	1.38
4	B	1031	FAD	C9-C8	2.08	1.42	1.39
4	A	1031	FAD	C9-C8	2.07	1.42	1.39
6	B	1033	URF	C4-C5	2.06	1.46	1.44
5	C	1032	NDP	C3B-C2B	-2.05	1.48	1.53
4	A	1031	FAD	C2-N3	2.05	1.43	1.39
4	D	1031	FAD	C4-N3	2.05	1.42	1.38
5	A	1032	NDP	C2B-C1B	-2.04	1.48	1.53
4	A	1031	FAD	C4-N3	2.04	1.42	1.38
5	C	1032	NDP	C6N-N1N	2.02	1.42	1.37
5	B	1032	NDP	C6N-N1N	2.02	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1031	FAD	C3B-C4B	2.01	1.58	1.53
4	C	1031	FAD	PA-O5B	-2.01	1.51	1.59
4	A	1031	FAD	O4B-C1B	2.00	1.46	1.42

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1032	NDP	O2N-PN-O3	-11.83	75.29	107.27
5	B	1032	NDP	O2N-PN-O3	-11.74	75.54	107.27
5	A	1032	NDP	O3-PN-O1N	-9.51	82.11	110.70
5	B	1032	NDP	O3-PN-O1N	-9.34	82.62	110.70
4	A	1031	FAD	O3P-PA-O1A	-8.82	84.16	110.70
4	D	1031	FAD	O3P-PA-O1A	-8.57	84.93	110.70
4	C	1031	FAD	O3P-PA-O1A	-8.55	84.99	110.70
4	B	1031	FAD	O3P-PA-O1A	-8.35	85.59	110.70
5	C	1032	NDP	C1D-N1N-C2N	-7.66	108.52	121.14
4	C	1031	FAD	O2A-PA-O3P	-7.10	88.07	107.27
5	D	1032	NDP	O5D-PN-O1N	-7.04	81.04	108.94
4	B	1031	FAD	O2A-PA-O3P	-6.98	88.40	107.27
4	A	1031	FAD	O2A-PA-O3P	-6.94	88.51	107.27
4	D	1031	FAD	O2A-PA-O3P	-6.89	88.64	107.27
5	B	1032	NDP	O2N-PN-O5D	-6.53	77.97	107.57
5	A	1032	NDP	O2N-PN-O5D	-6.36	78.73	107.57
5	B	1032	NDP	O5D-PN-O1N	-5.16	88.50	108.94
5	A	1032	NDP	O5D-PN-O1N	-5.09	88.76	108.94
5	D	1032	NDP	C1D-N1N-C2N	-5.00	112.91	121.14
5	B	1032	NDP	C3N-C2N-N1N	-4.85	116.08	123.20
3	C	1030	FMN	C10-N1-C2	4.80	127.25	116.85
3	A	1030	FMN	C10-N1-C2	4.73	127.10	116.85
3	D	1030	FMN	C10-N1-C2	4.73	127.09	116.85
5	B	1032	NDP	O2N-PN-O1N	4.73	134.43	112.44
5	A	1032	NDP	O2N-PN-O1N	4.69	134.28	112.44
3	B	1030	FMN	C10-N1-C2	4.61	126.82	116.85
6	B	1033	URF	F5-C5-C4	4.61	120.50	116.47
6	C	1033	URF	F5-C5-C4	4.56	120.46	116.47
6	A	1033	URF	F5-C5-C4	4.53	120.44	116.47
6	D	1033	URF	F5-C5-C4	4.44	120.36	116.47
5	A	1032	NDP	C3N-C2N-N1N	-4.16	117.09	123.20
3	C	1030	FMN	C4A-C10-N1	-4.09	114.56	124.59
3	B	1030	FMN	C4-C4A-C10	4.08	123.93	116.93
3	A	1030	FMN	C4A-C10-N1	-4.07	114.61	124.59
3	A	1030	FMN	C4-C4A-C10	4.02	123.83	116.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1030	FMN	C4A-C10-N1	-4.02	114.73	124.59
3	B	1030	FMN	C4A-C10-N1	-4.01	114.76	124.59
3	A	1030	FMN	O4'-C4'-C3'	3.97	118.54	109.25
3	C	1030	FMN	O4'-C4'-C3'	3.97	118.54	109.25
3	D	1030	FMN	O3'-C3'-C2'	-3.95	99.95	108.93
3	D	1030	FMN	O4'-C4'-C3'	3.88	118.34	109.25
3	B	1030	FMN	O4'-C4'-C3'	3.88	118.33	109.25
3	D	1030	FMN	C4-C4A-C10	3.88	123.59	116.93
3	C	1030	FMN	C4-C4A-C10	3.87	123.57	116.93
5	C	1032	NDP	C6N-N1N-C2N	3.83	123.42	119.32
3	A	1030	FMN	O3'-C3'-C2'	-3.81	100.27	108.93
3	B	1030	FMN	O3'-C3'-C2'	-3.77	100.36	108.93
5	D	1032	NDP	O2N-PN-O1N	3.74	129.85	112.44
4	B	1031	FAD	O2A-PA-O1A	3.70	129.68	112.44
4	D	1031	FAD	O2A-PA-O1A	3.69	129.62	112.44
3	C	1030	FMN	O3'-C3'-C2'	-3.64	100.67	108.93
4	A	1031	FAD	O2A-PA-O1A	3.64	129.36	112.44
4	C	1031	FAD	O2A-PA-O1A	3.61	129.25	112.44
5	C	1032	NDP	C3N-C2N-N1N	-3.52	118.04	123.20
6	C	1033	URF	C5-C6-N1	3.45	122.38	119.49
6	A	1033	URF	C5-C6-N1	3.43	122.36	119.49
5	C	1032	NDP	O3-PN-O1N	-3.34	100.65	110.70
6	D	1033	URF	C5-C6-N1	3.33	122.28	119.49
6	B	1033	URF	C5-C6-N1	3.29	122.24	119.49
3	C	1030	FMN	C5'-C4'-C3'	-3.24	106.10	112.22
6	B	1033	URF	C6-C5-C4	-3.23	119.33	122.11
3	A	1030	FMN	C5'-C4'-C3'	-3.22	106.14	112.22
6	D	1033	URF	C6-C5-C4	-3.22	119.34	122.11
6	D	1033	URF	C5-C4-N3	3.16	115.53	112.64
3	B	1030	FMN	C5'-C4'-C3'	-3.16	106.26	112.22
5	D	1032	NDP	O2N-PN-O5D	-3.16	93.26	107.57
6	C	1033	URF	C6-C5-C4	-3.15	119.40	122.11
6	A	1033	URF	C6-C5-C4	-3.15	119.40	122.11
5	D	1032	NDP	O4D-C1D-C2D	-3.15	99.89	106.62
5	D	1032	NDP	O7N-C7N-N7N	-3.11	115.93	122.89
5	D	1032	NDP	C3D-C2D-C1D	3.10	107.33	101.46
5	C	1032	NDP	C2B-C1B-N9A	-3.09	108.67	113.75
6	A	1033	URF	C5-C4-N3	3.05	115.43	112.64
3	D	1030	FMN	C5'-C4'-C3'	-3.03	106.51	112.22
4	C	1031	FAD	O4B-C1B-N9A	-3.01	102.31	108.09
6	C	1033	URF	C5-C4-N3	3.00	115.38	112.64
5	C	1032	NDP	O7N-C7N-N7N	-2.97	116.23	122.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1031	FAD	O4B-C1B-N9A	-2.94	102.44	108.09
6	B	1033	URF	C5-C4-N3	2.93	115.32	112.64
5	D	1032	NDP	O5D-C5D-C4D	-2.93	99.01	108.99
4	A	1031	FAD	O4B-C1B-N9A	-2.92	102.48	108.09
5	D	1032	NDP	C3N-C2N-N1N	-2.90	118.94	123.20
5	A	1032	NDP	O7N-C7N-N7N	-2.89	116.41	122.89
5	C	1032	NDP	C1D-N1N-C6N	2.84	126.77	120.77
4	D	1031	FAD	O4B-C1B-N9A	-2.79	102.73	108.09
5	B	1032	NDP	O7N-C7N-N7N	-2.77	116.68	122.89
5	C	1032	NDP	O2B-C2B-C3B	2.76	121.57	111.68
5	C	1032	NDP	O4B-C1B-N9A	2.72	113.32	108.09
3	A	1030	FMN	C4A-C10-N10	2.70	120.35	116.48
3	D	1030	FMN	C4A-C10-N10	2.65	120.27	116.48
3	B	1030	FMN	C4A-C10-N10	2.63	120.25	116.48
5	C	1032	NDP	O2N-PN-O5D	2.62	119.45	107.57
3	C	1030	FMN	C4A-C10-N10	2.62	120.23	116.48
5	D	1032	NDP	O4B-C1B-C2B	2.62	111.09	106.59
4	A	1031	FAD	C5'-C4'-C3'	-2.59	107.34	112.22
5	C	1032	NDP	C4B-O4B-C1B	-2.58	103.76	109.47
5	D	1032	NDP	C1D-N1N-C6N	2.57	126.21	120.77
3	B	1030	FMN	O3'-C3'-C4'	2.57	114.76	108.93
4	A	1031	FAD	C2A-N1A-C6A	2.56	122.94	118.73
4	C	1031	FAD	C5'-C4'-C3'	-2.55	107.40	112.22
3	A	1030	FMN	O3'-C3'-C4'	2.52	114.65	108.93
4	A	1031	FAD	C5X-C9A-N10	-2.51	115.70	117.97
4	C	1031	FAD	C2A-N1A-C6A	2.49	122.82	118.73
4	B	1031	FAD	C2A-N1A-C6A	2.48	122.81	118.73
5	D	1032	NDP	O2B-C2B-C3B	2.47	120.52	111.68
5	B	1032	NDP	O4D-C1D-C2D	-2.46	101.35	106.62
4	B	1031	FAD	C5'-C4'-C3'	-2.46	107.58	112.22
4	D	1031	FAD	C2A-N1A-C6A	2.46	122.76	118.73
3	D	1030	FMN	O3'-C3'-C4'	2.45	114.50	108.93
5	D	1032	NDP	O3-PA-O1A	-2.44	103.35	110.70
4	D	1031	FAD	C5'-C4'-C3'	-2.44	107.61	112.22
5	A	1032	NDP	O4B-C1B-N9A	2.42	112.74	108.09
4	C	1031	FAD	C5X-C9A-N10	-2.41	115.79	117.97
5	B	1032	NDP	C3D-C2D-C1D	2.40	106.01	101.46
5	D	1032	NDP	N3A-C2A-N1A	-2.39	124.97	128.58
5	D	1032	NDP	O3D-C3D-C4D	-2.37	104.27	111.08
5	D	1032	NDP	O2N-PN-O3	2.37	113.68	107.27
4	C	1031	FAD	C4-N3-C2	-2.36	121.46	125.64
4	D	1031	FAD	C5X-C9A-N10	-2.35	115.84	117.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1030	FMN	O3'-C3'-C4'	2.35	114.27	108.93
4	B	1031	FAD	C5X-C9A-N10	-2.35	115.84	117.97
4	A	1031	FAD	C4-N3-C2	-2.35	121.47	125.64
5	A	1032	NDP	O2B-C2B-C3B	2.33	120.03	111.68
4	B	1031	FAD	C4-N3-C2	-2.32	121.53	125.64
5	B	1032	NDP	O2B-C2B-C3B	2.31	119.96	111.68
5	B	1032	NDP	N3A-C2A-N1A	-2.28	125.13	128.58
3	C	1030	FMN	N10-C10-N1	2.27	125.20	118.51
3	B	1030	FMN	C4-C4A-N5	-2.25	115.10	118.21
5	A	1032	NDP	O5B-C5B-C4B	-2.25	101.34	108.99
5	C	1032	NDP	O5D-C5D-C4D	-2.24	101.36	108.99
5	C	1032	NDP	N3A-C2A-N1A	-2.23	125.20	128.58
5	A	1032	NDP	N9A-C8A-N7A	-2.23	110.77	113.94
4	D	1031	FAD	C4-N3-C2	-2.22	121.70	125.64
3	A	1030	FMN	N10-C10-N1	2.22	125.04	118.51
5	B	1032	NDP	O5B-C5B-C4B	-2.21	101.47	108.99
3	B	1030	FMN	N10-C10-N1	2.20	124.99	118.51
4	B	1031	FAD	C4'-C3'-C2'	-2.20	109.91	113.57
3	D	1030	FMN	N10-C10-N1	2.20	124.98	118.51
5	A	1032	NDP	O4B-C1B-C2B	2.19	110.36	106.59
5	C	1032	NDP	O4B-C1B-C2B	2.18	110.35	106.59
5	B	1032	NDP	O4B-C1B-N9A	2.16	112.24	108.09
5	A	1032	NDP	N3A-C2A-N1A	-2.16	125.31	128.58
5	C	1032	NDP	N9A-C8A-N7A	-2.16	110.87	113.94
5	C	1032	NDP	P2B-O2B-C2B	2.16	129.20	123.43
5	D	1032	NDP	N9A-C8A-N7A	-2.15	110.88	113.94
3	A	1030	FMN	C4-C4A-N5	-2.15	115.24	118.21
5	C	1032	NDP	O2N-PN-O1N	2.15	122.42	112.44
5	B	1032	NDP	N9A-C8A-N7A	-2.10	110.95	113.94
3	D	1030	FMN	N3-C2-N1	-2.10	115.03	119.50
5	A	1032	NDP	O4D-C1D-C2D	-2.09	102.14	106.62
4	C	1031	FAD	C10-N1-C2	2.09	121.36	116.85
4	C	1031	FAD	C4'-C3'-C2'	-2.08	110.11	113.57
4	A	1031	FAD	C10-N1-C2	2.08	121.34	116.85
5	B	1032	NDP	O4B-C1B-C2B	2.07	110.15	106.59
5	A	1032	NDP	C2B-C1B-N9A	-2.06	110.36	113.75
3	B	1030	FMN	C6-C5A-C9A	2.06	121.88	119.05
3	C	1030	FMN	N3-C2-N1	-2.05	115.14	119.50
5	C	1032	NDP	O2A-PA-O3	-2.05	101.73	107.27
3	C	1030	FMN	C4-C4A-N5	-2.05	115.38	118.21
3	A	1030	FMN	N3-C2-N1	-2.05	115.15	119.50
3	B	1030	FMN	N3-C2-N1	-2.04	115.16	119.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1031	FAD	C4'-C3'-C2'	-2.04	110.18	113.57
5	D	1032	NDP	C4B-O4B-C1B	-2.02	105.00	109.47
4	B	1031	FAD	C10-N1-C2	2.02	121.22	116.85
5	C	1032	NDP	C2D-C1D-N1N	-2.01	108.37	113.31
5	C	1032	NDP	C5D-C4D-C3D	-2.00	108.00	115.21

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1032	NDP	C4D
5	A	1032	NDP	C2D
5	A	1032	NDP	C3D
5	B	1032	NDP	C4D
5	B	1032	NDP	C2D
5	B	1032	NDP	C3D
5	C	1032	NDP	C4D
5	C	1032	NDP	C2D
5	C	1032	NDP	C3D
5	D	1032	NDP	C4D
5	D	1032	NDP	C2D
5	D	1032	NDP	C3D

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	C5B-O5B-PA-O1A
4	A	1031	FAD	PA-O3P-P-O5'
4	B	1031	FAD	C5B-O5B-PA-O1A
4	B	1031	FAD	PA-O3P-P-O5'
4	C	1031	FAD	C5B-O5B-PA-O1A
4	C	1031	FAD	PA-O3P-P-O5'
4	D	1031	FAD	C5B-O5B-PA-O1A
4	D	1031	FAD	PA-O3P-P-O5'
5	A	1032	NDP	C5D-O5D-PN-O1N
5	A	1032	NDP	C5D-O5D-PN-O2N
5	A	1032	NDP	C4D-C5D-O5D-PN
5	B	1032	NDP	C5D-O5D-PN-O1N
5	B	1032	NDP	C5D-O5D-PN-O2N
5	B	1032	NDP	C4D-C5D-O5D-PN
5	C	1032	NDP	C3B-C2B-O2B-P2B
5	D	1032	NDP	C5D-O5D-PN-O3
5	D	1032	NDP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	1032	NDP	C5D-O5D-PN-O2N
5	D	1032	NDP	C4D-C5D-O5D-PN
5	D	1032	NDP	O4D-C4D-C5D-O5D
5	D	1032	NDP	C3D-C4D-C5D-O5D
5	B	1032	NDP	O4D-C1D-N1N-C2N
5	C	1032	NDP	O4D-C1D-N1N-C2N
5	A	1032	NDP	C3B-C2B-O2B-P2B
5	A	1032	NDP	C2D-C1D-N1N-C2N
5	A	1032	NDP	C2D-C1D-N1N-C6N
5	A	1032	NDP	O4D-C1D-N1N-C2N
5	A	1032	NDP	C1B-C2B-O2B-P2B
5	B	1032	NDP	C1B-C2B-O2B-P2B
5	C	1032	NDP	C1B-C2B-O2B-P2B
5	D	1032	NDP	C1B-C2B-O2B-P2B
5	B	1032	NDP	C3B-C2B-O2B-P2B
5	D	1032	NDP	C3B-C2B-O2B-P2B
5	B	1032	NDP	C3D-C4D-C5D-O5D
5	A	1032	NDP	C3D-C4D-C5D-O5D
5	C	1032	NDP	PN-O3-PA-O5B
4	A	1031	FAD	C2B-C1B-N9A-C8A
4	B	1031	FAD	C2B-C1B-N9A-C8A
4	C	1031	FAD	C2B-C1B-N9A-C8A
4	D	1031	FAD	C2B-C1B-N9A-C8A
5	D	1032	NDP	O4D-C1D-N1N-C2N
3	B	1030	FMN	C4'-C5'-O5'-P
3	C	1030	FMN	C4'-C5'-O5'-P
3	D	1030	FMN	C4'-C5'-O5'-P
5	A	1032	NDP	C5D-O5D-PN-O3
5	B	1032	NDP	C5D-O5D-PN-O3
3	A	1030	FMN	C4'-C5'-O5'-P
5	C	1032	NDP	C4D-C5D-O5D-PN
5	B	1032	NDP	PN-O3-PA-O2A
5	B	1032	NDP	C2N-C3N-C7N-N7N
5	B	1032	NDP	C2D-C1D-N1N-C6N
5	A	1032	NDP	PN-O3-PA-O1A
5	D	1032	NDP	PA-O3-PN-O1N
5	B	1032	NDP	O4B-C4B-C5B-O5B
5	C	1032	NDP	O4D-C4D-C5D-O5D
5	A	1032	NDP	PN-O3-PA-O2A
5	A	1032	NDP	PA-O3-PN-O2N
5	B	1032	NDP	PA-O3-PN-O2N
5	C	1032	NDP	PN-O3-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1032	NDP	O4B-C4B-C5B-O5B

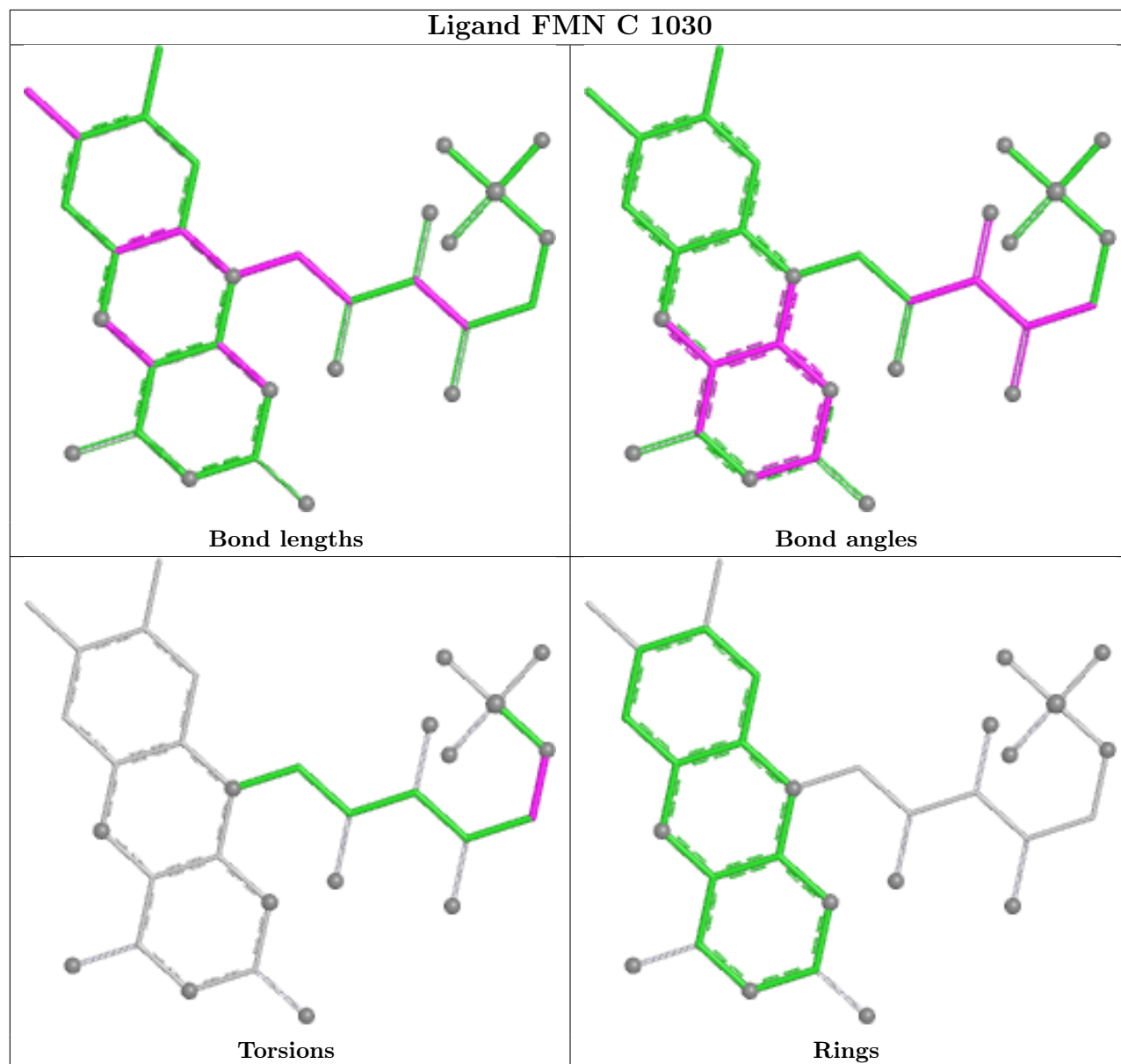
There are no ring outliers.

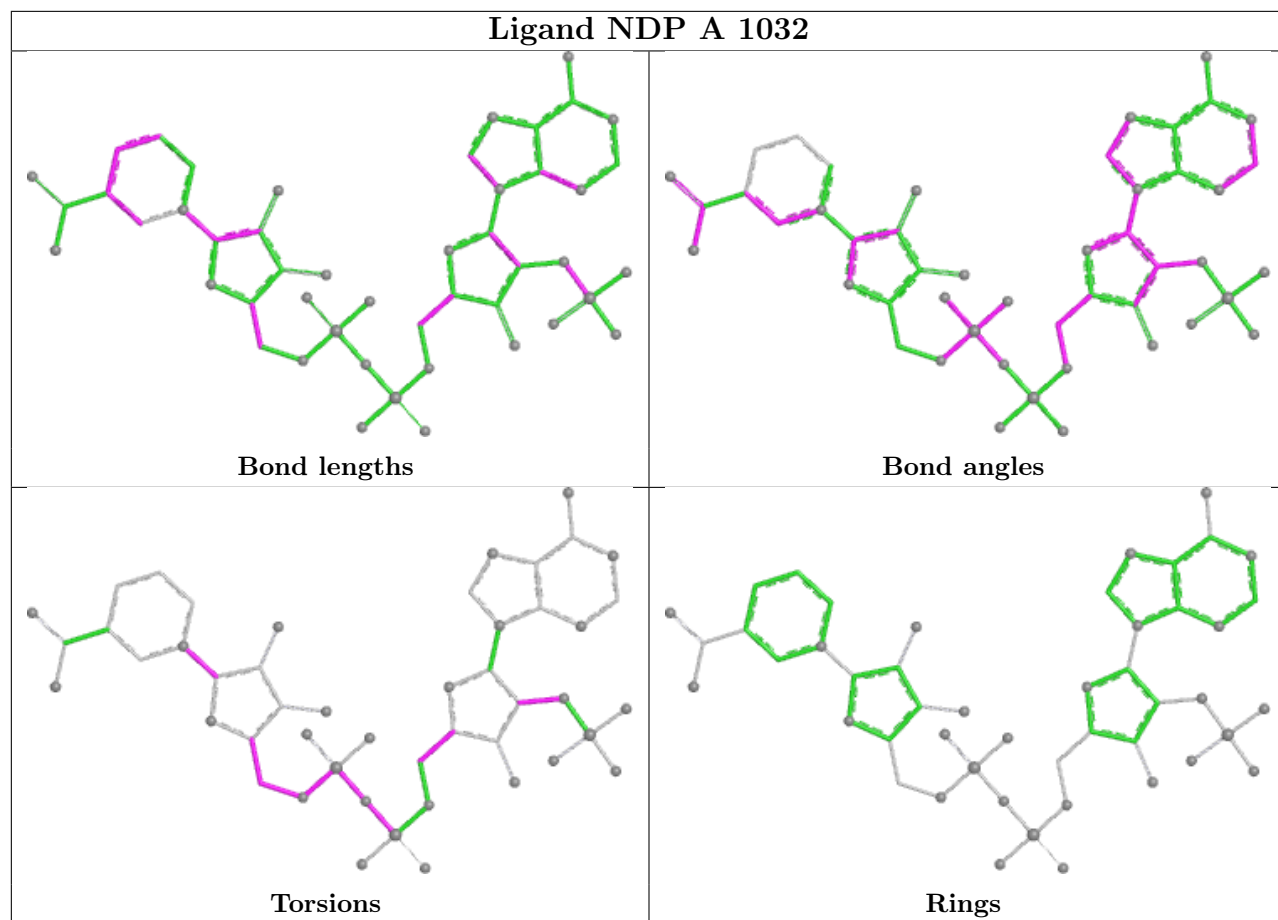
14 monomers are involved in 24 short contacts:

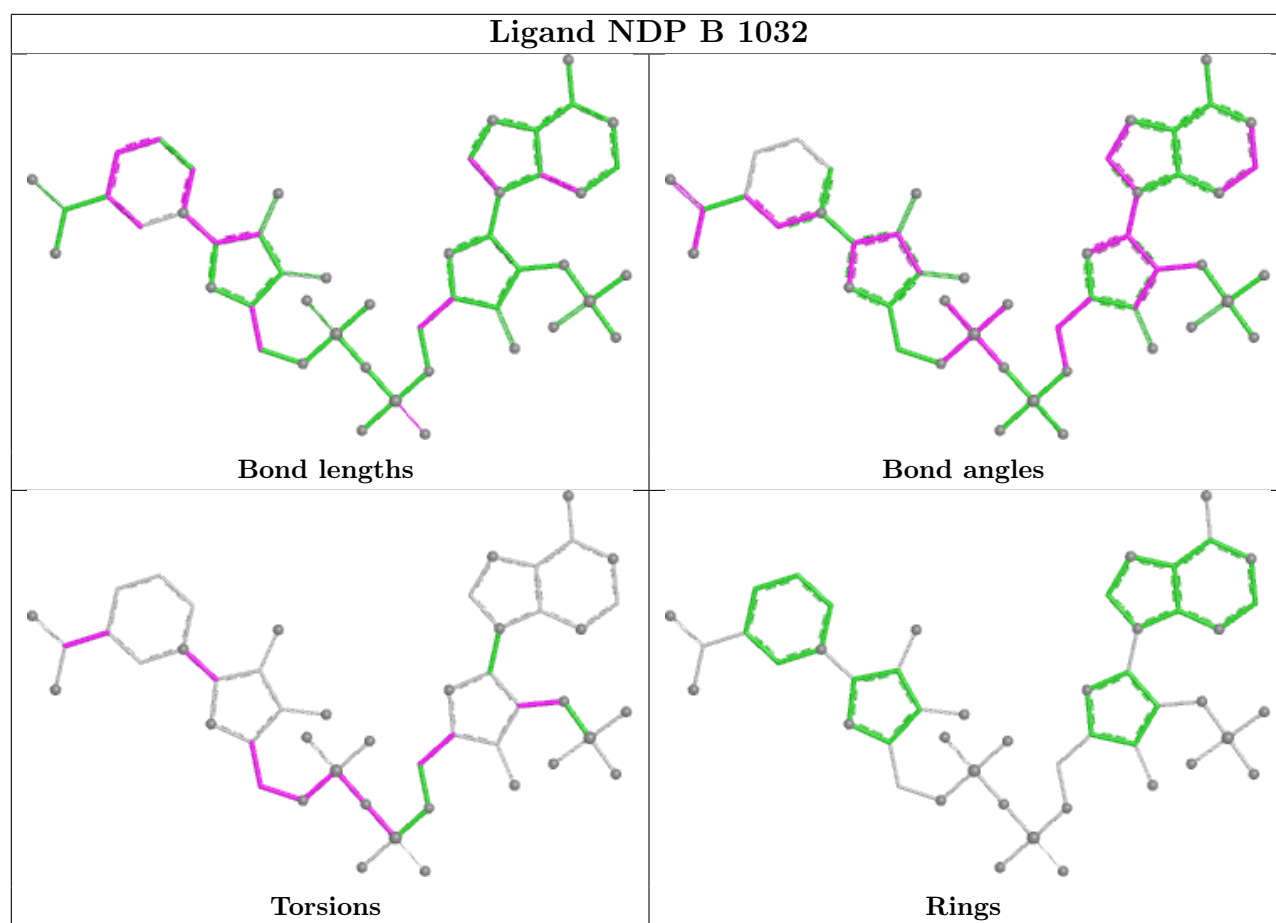
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1027	SF4	2	0
2	C	1027	SF4	1	0
5	A	1032	NDP	1	0
5	B	1032	NDP	3	0
3	D	1030	FMN	1	0
5	D	1032	NDP	7	0
5	C	1032	NDP	1	0
2	D	1026	SF4	1	0
2	A	1027	SF4	1	0
4	B	1031	FAD	2	0
2	A	1026	SF4	1	0
4	A	1031	FAD	2	0
4	D	1031	FAD	1	0
2	D	1027	SF4	2	0

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.

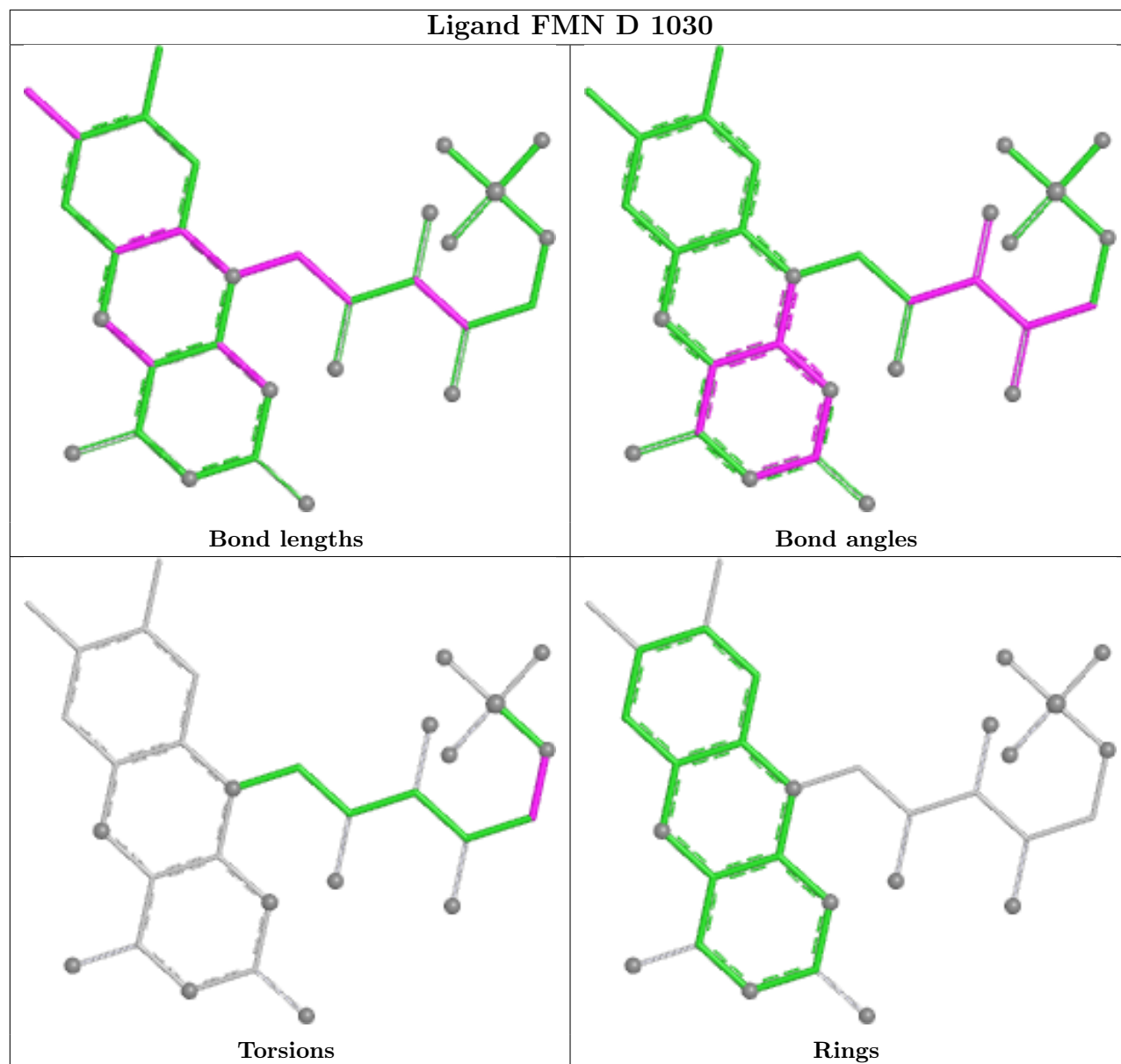
Ligand FMN C 1030

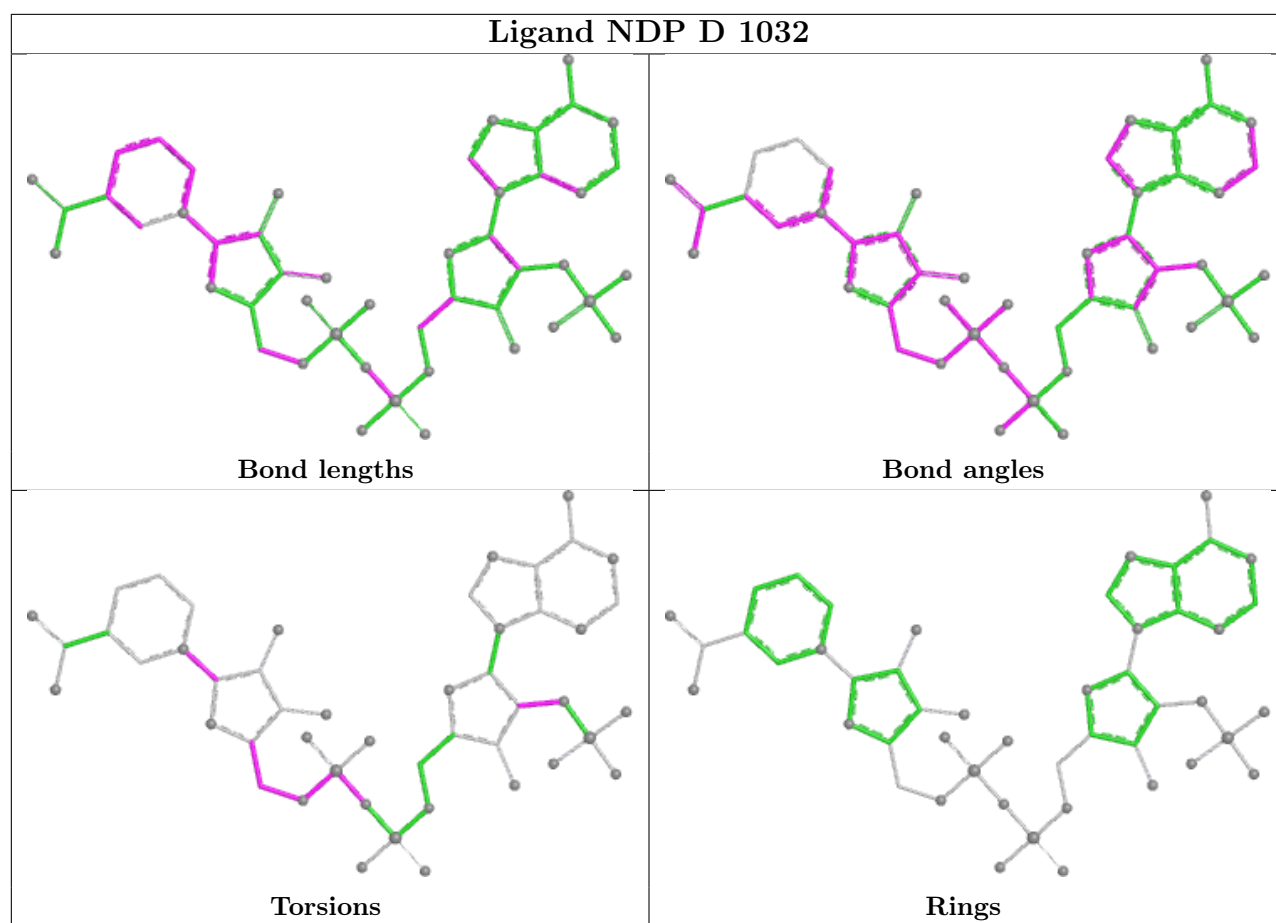


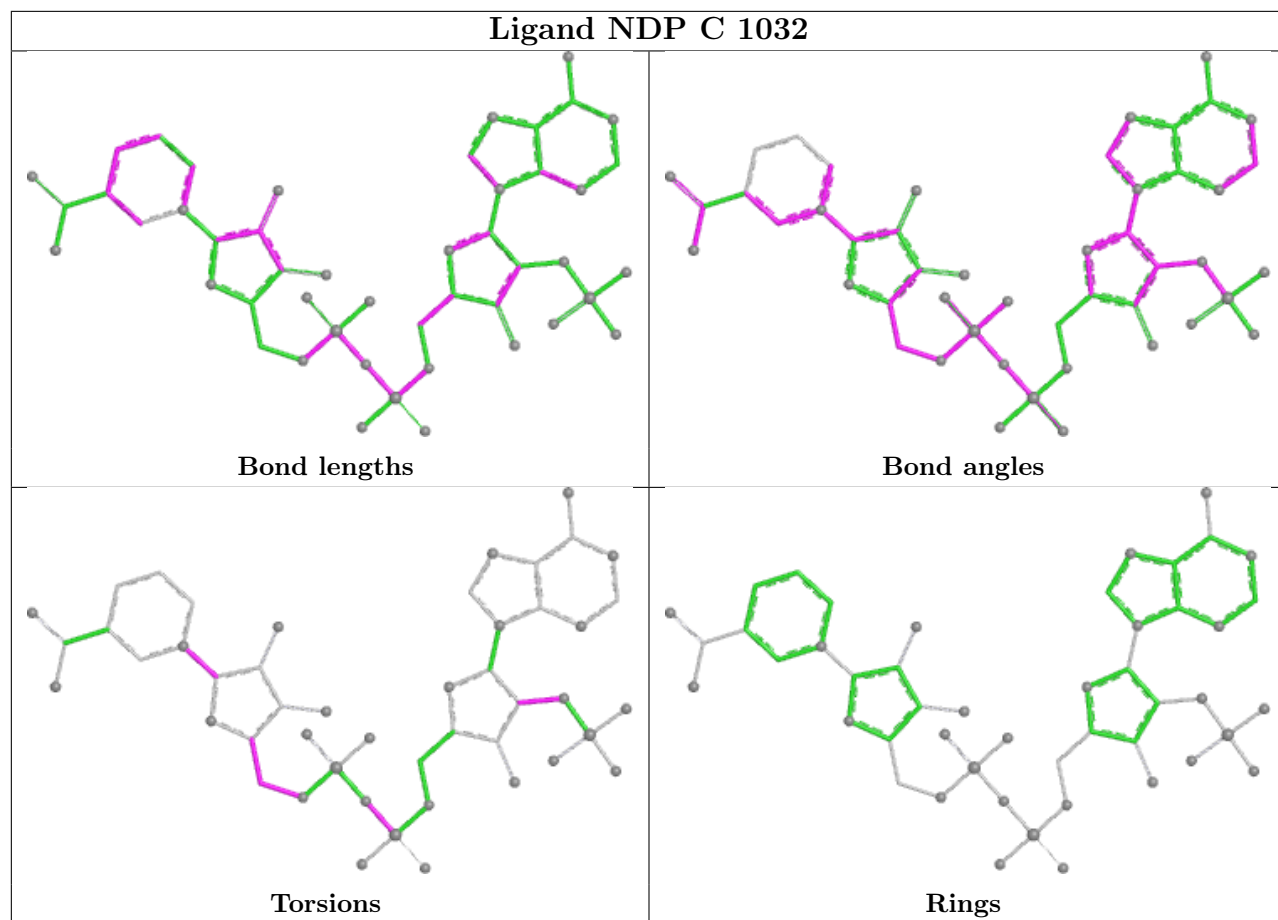


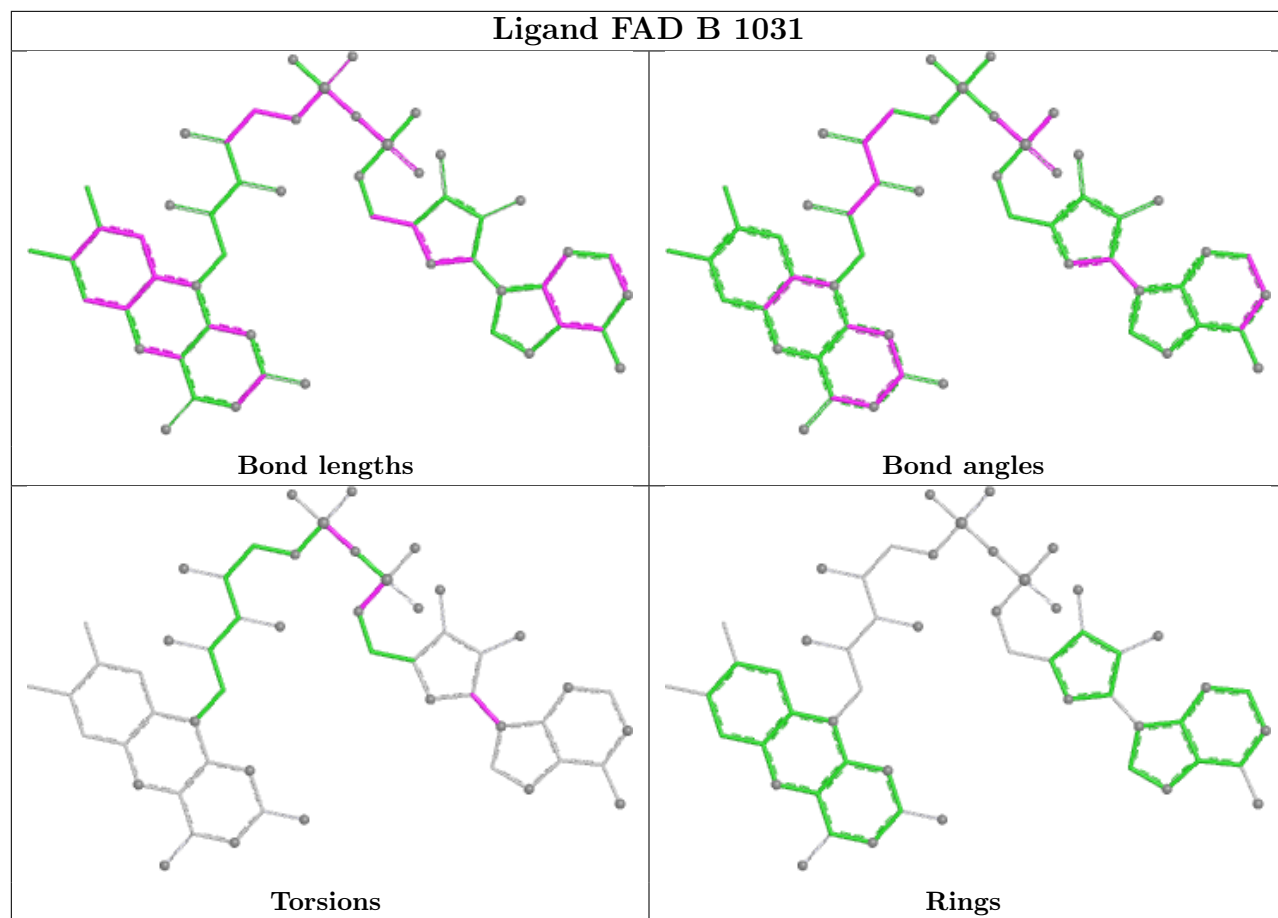


Ligand FMN D 1030

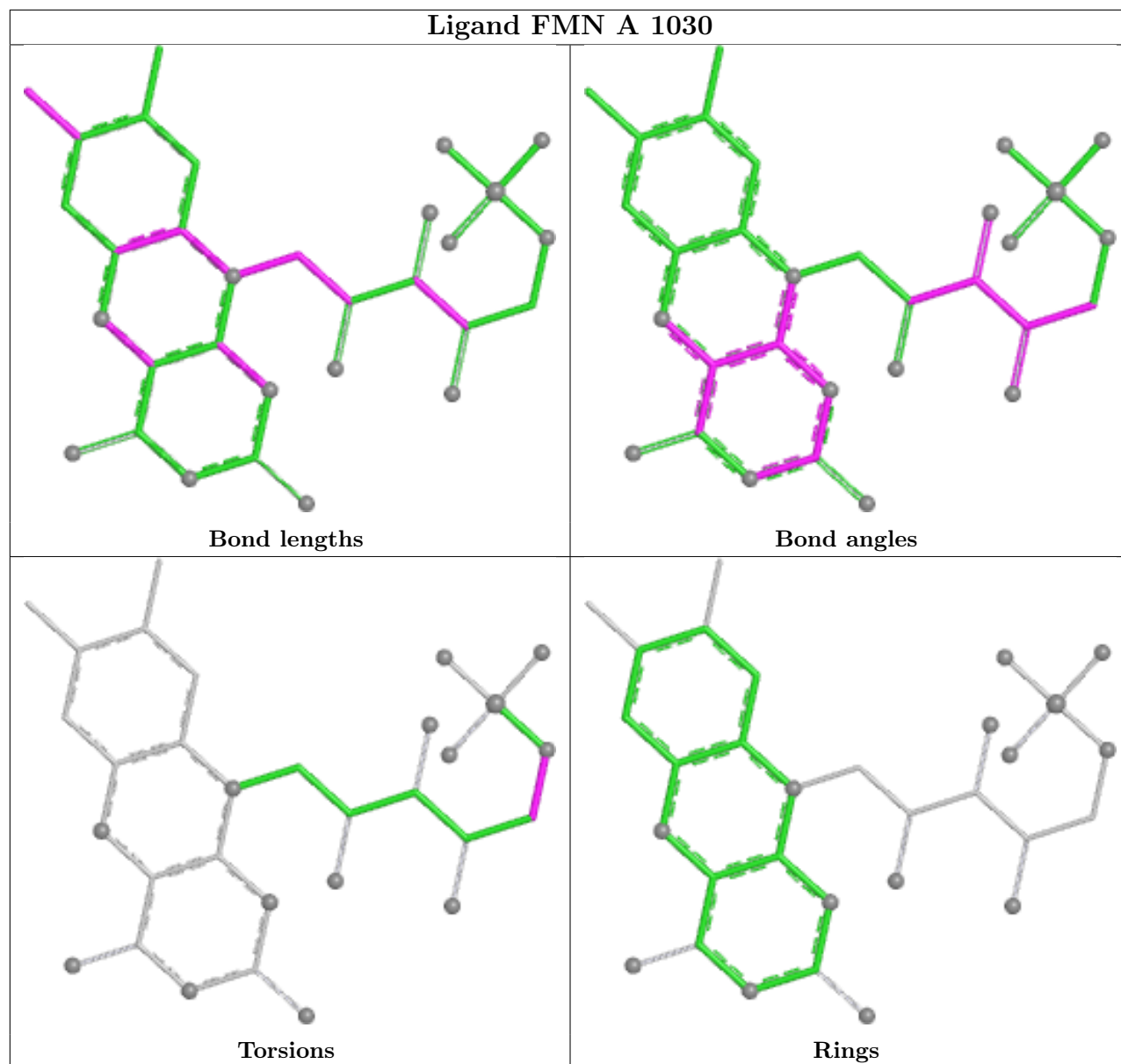


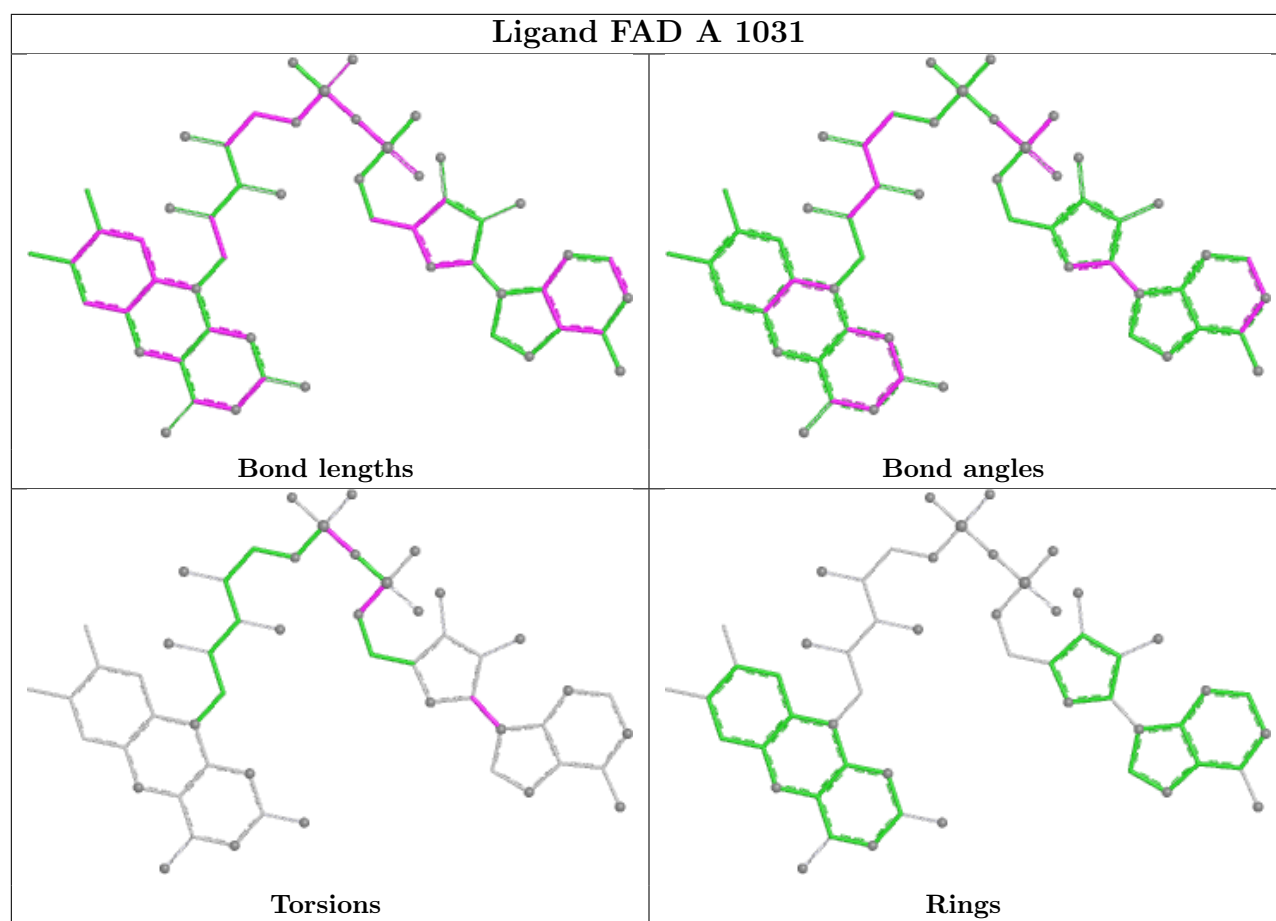




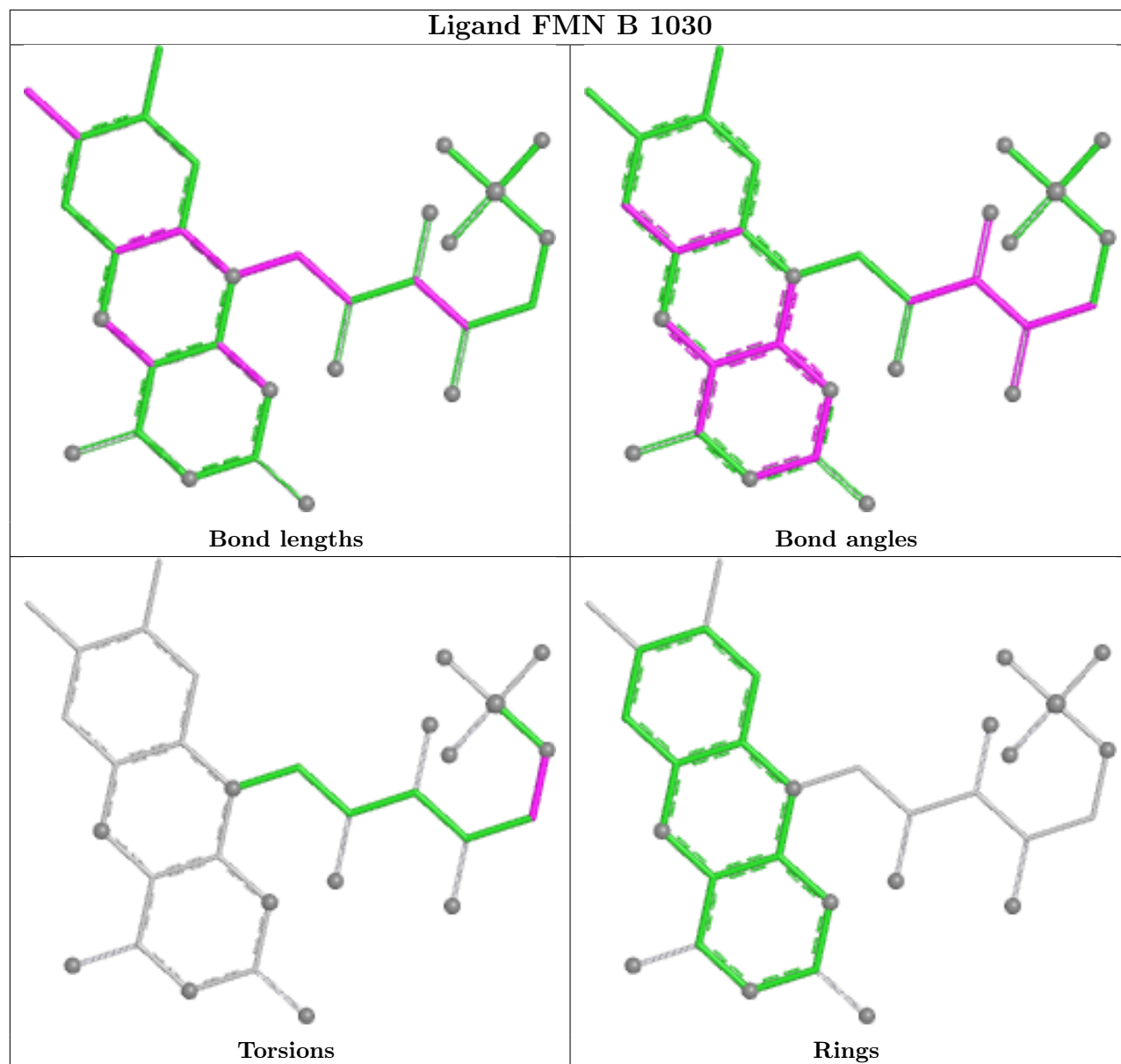


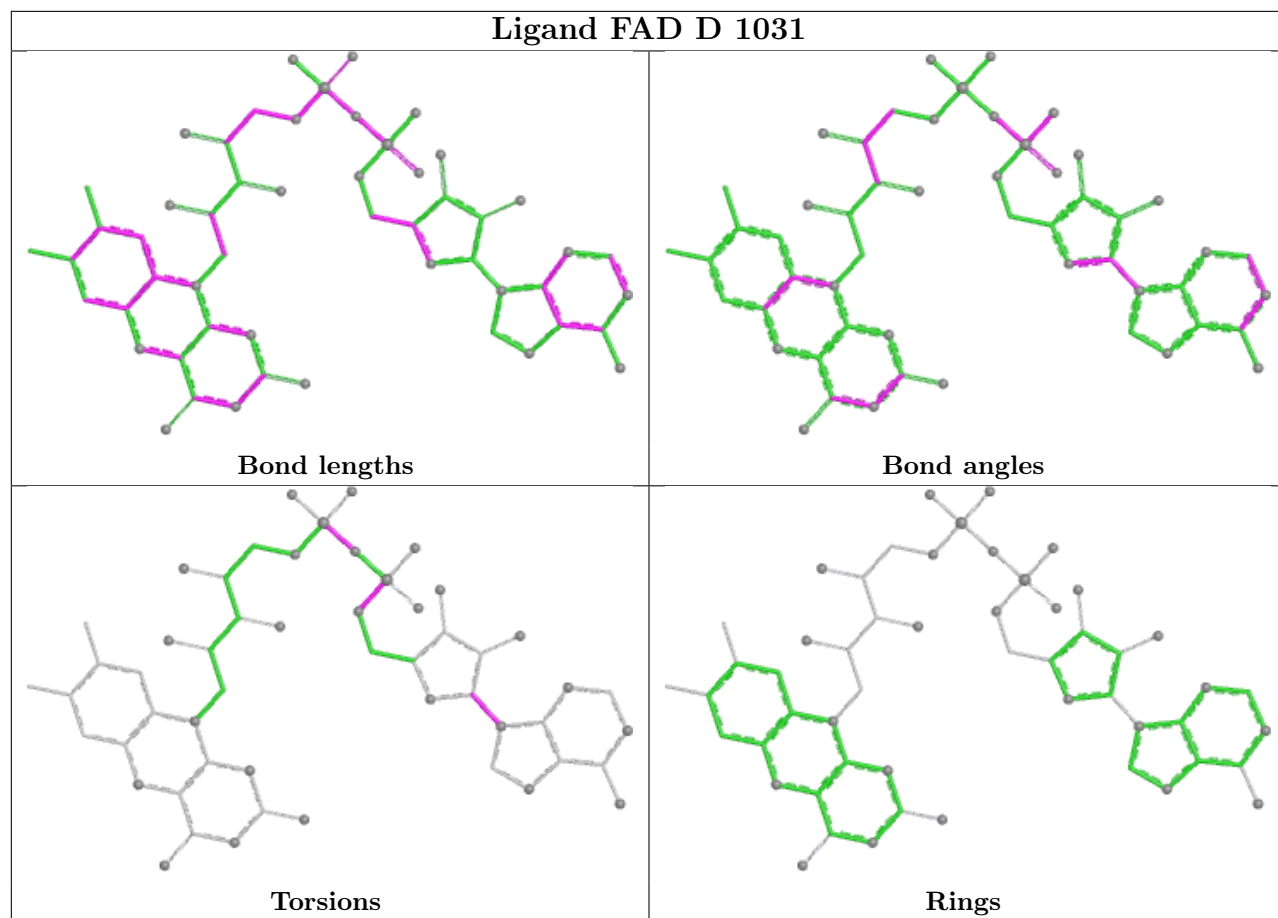
Ligand FMN A 1030

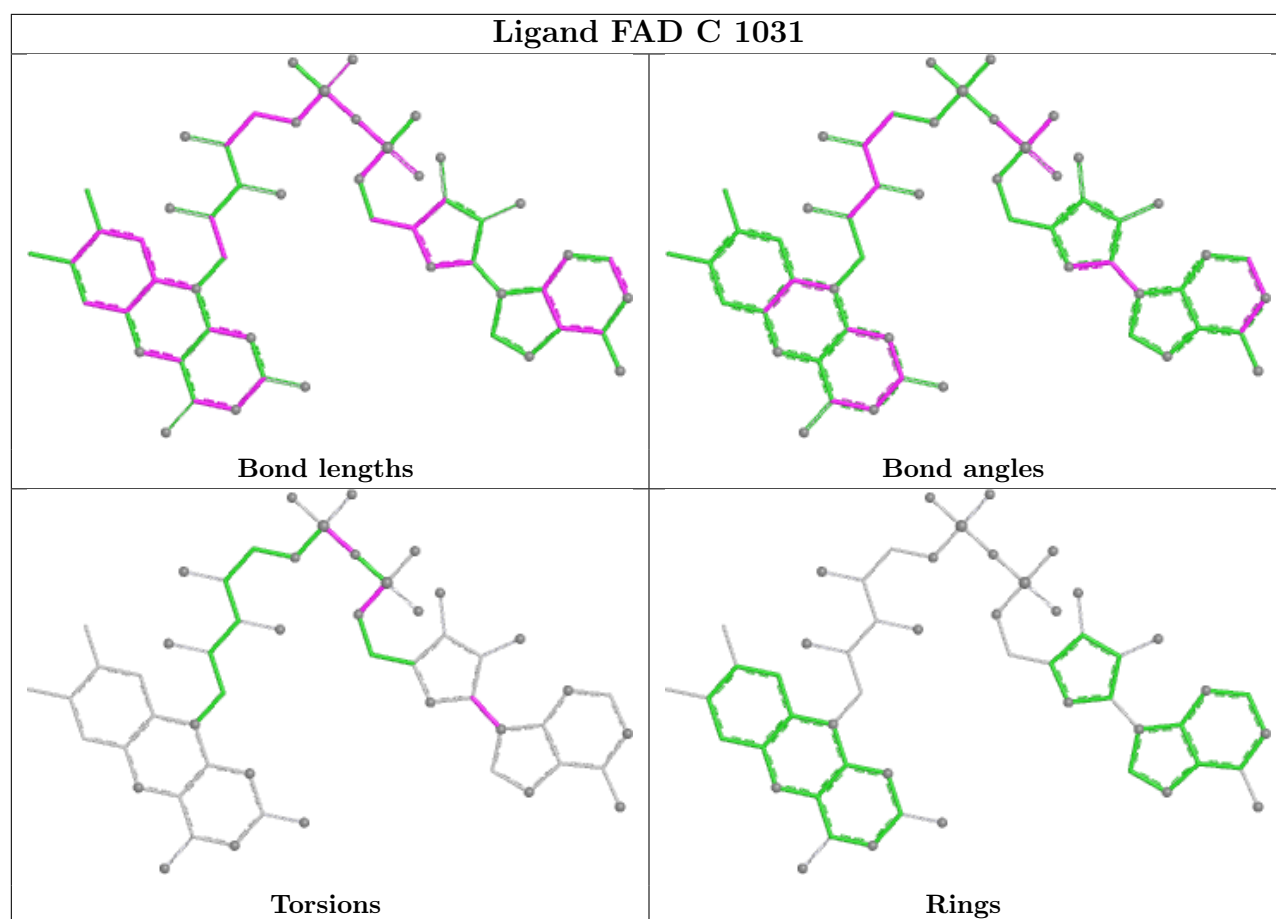




Ligand FMN B 1030







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	1000/1025 (97%)	-0.10	41 (4%)	41	40	7, 16, 39, 59	0
1	B	1006/1025 (98%)	-0.08	54 (5%)	31	30	9, 17, 41, 64	0
1	C	1013/1025 (98%)	-0.08	64 (6%)	26	24	8, 16, 41, 59	0
1	D	1005/1025 (98%)	-0.15	55 (5%)	30	29	8, 16, 40, 60	0
All	All	4024/4100 (98%)	-0.10	214 (5%)	32	31	7, 16, 40, 64	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	9.9
1	A	2	ALA	9.4
1	D	2	ALA	8.5
1	B	2	ALA	8.1
1	C	674	GLY	6.9
1	A	410	ARG	6.8
1	A	1017	LEU	6.3
1	C	53	GLU	6.3
1	D	52	CYS	5.7
1	D	50	PHE	5.6
1	C	1019	LEU	5.5
1	D	674	GLY	5.3
1	C	410	ARG	5.2
1	C	52	CYS	5.2
1	C	459	TRP	4.9
1	A	175	CYS	4.9
1	B	410	ARG	4.8
1	C	681	GLY	4.6
1	A	322	CYS	4.6
1	A	52	CYS	4.6
1	A	870	GLU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1010	PRO	4.5
1	D	410	ARG	4.4
1	D	51	HIS	4.4
1	D	679	GLY	4.4
1	B	679	GLY	4.4
1	B	680	MET	4.3
1	D	1020	ALA	4.2
1	D	459	TRP	4.1
1	B	52	CYS	4.1
1	C	873	GLY	4.1
1	D	868	ILE	4.0
1	C	173	ASN	4.0
1	A	674	GLY	4.0
1	B	1009	THR	4.0
1	B	1011	TYR	4.0
1	B	899	GLU	3.9
1	A	53	GLU	3.9
1	D	1010	PRO	3.9
1	C	51	HIS	3.8
1	C	904	PHE	3.8
1	D	22	THR	3.7
1	B	908	GLU	3.7
1	D	1011	TYR	3.7
1	A	50	PHE	3.7
1	A	325	HIS	3.7
1	C	324	CYS	3.7
1	A	367	PHE	3.7
1	B	459	TRP	3.6
1	C	415	GLU	3.6
1	C	367	PHE	3.6
1	B	1019	LEU	3.6
1	D	1019	LEU	3.6
1	A	681	GLY	3.6
1	C	420	ASN	3.6
1	D	414	ASP	3.5
1	D	264	ASN	3.5
1	B	175	CYS	3.5
1	B	51	HIS	3.5
1	A	459	TRP	3.4
1	B	678	ARG	3.4
1	D	175	CYS	3.4
1	D	898	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1011	TYR	3.4
1	C	898	LYS	3.4
1	A	324	CYS	3.4
1	A	1009	THR	3.4
1	D	415	GLU	3.4
1	D	173	ASN	3.3
1	B	415	GLU	3.3
1	D	909	ARG	3.3
1	C	323	ALA	3.3
1	A	682	LEU	3.3
1	D	1012	GLU	3.3
1	C	175	CYS	3.3
1	B	367	PHE	3.3
1	D	367	PHE	3.2
1	B	326	SER	3.2
1	B	416	THR	3.2
1	B	1018	PRO	3.2
1	C	419	TRP	3.2
1	B	1010	PRO	3.2
1	C	331	ILE	3.2
1	D	53	GLU	3.2
1	C	1018	PRO	3.2
1	C	426	ILE	3.1
1	A	22	THR	3.1
1	C	872	MET	3.0
1	C	326	SER	3.0
1	B	417	GLY	3.0
1	A	872	MET	3.0
1	C	179	GLN	3.0
1	C	902	ALA	3.0
1	B	173	ASN	3.0
1	C	869	ALA	2.9
1	C	682	LEU	2.9
1	C	424	ASP	2.9
1	D	873	GLY	2.9
1	B	324	CYS	2.8
1	D	871	LEU	2.8
1	A	868	ILE	2.8
1	B	426	ILE	2.8
1	C	907	LEU	2.8
1	C	870	GLU	2.8
1	B	681	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	173	ASN	2.7
1	A	51	HIS	2.7
1	B	859	HIS	2.7
1	C	325	HIS	2.7
1	D	680	MET	2.7
1	A	323	ALA	2.7
1	D	1009	THR	2.7
1	C	906	PRO	2.7
1	D	858	SER	2.7
1	B	413	GLN	2.7
1	C	1017	LEU	2.7
1	D	682	LEU	2.7
1	C	673	HIS	2.7
1	B	409	VAL	2.7
1	B	180	GLU	2.6
1	D	423	GLU	2.6
1	D	395	LYS	2.6
1	C	868	ILE	2.6
1	C	899	GLU	2.6
1	A	487	ASN	2.6
1	D	867	ARG	2.6
1	C	330	SER	2.6
1	B	896	ARG	2.5
1	C	984	ASP	2.5
1	B	424	ASP	2.5
1	D	911	PRO	2.5
1	D	1014	LYS	2.5
1	D	487	ASN	2.5
1	A	857	GLU	2.5
1	C	582	ILE	2.5
1	A	1012	GLU	2.4
1	B	53	GLU	2.4
1	B	1008	THR	2.4
1	C	905	PRO	2.4
1	C	1020	ALA	2.4
1	A	1014	LYS	2.4
1	B	682	LEU	2.4
1	A	984	ASP	2.4
1	A	402	ARG	2.4
1	B	696	ARG	2.4
1	C	1014	LYS	2.4
1	D	49	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	867	ARG	2.4
1	A	419	TRP	2.4
1	A	673	HIS	2.4
1	B	1017	LEU	2.3
1	C	900	GLN	2.3
1	D	828	GLN	2.3
1	C	329	PRO	2.3
1	D	857	GLU	2.3
1	C	264	ASN	2.3
1	C	487	ASN	2.3
1	D	418	LYS	2.3
1	B	323	ALA	2.3
1	B	868	ILE	2.3
1	C	368	VAL	2.3
1	A	896	ARG	2.3
1	A	11	ASP	2.3
1	B	414	ASP	2.3
1	D	872	MET	2.3
1	D	419	TRP	2.3
1	D	180	GLU	2.2
1	D	866	PRO	2.2
1	B	867	ARG	2.2
1	B	422	ASP	2.2
1	D	984	ASP	2.2
1	B	872	MET	2.2
1	B	419	TRP	2.2
1	B	911	PRO	2.2
1	D	1018	PRO	2.2
1	A	871	LEU	2.2
1	C	867	ARG	2.2
1	C	896	ARG	2.2
1	D	896	ARG	2.2
1	B	1014	LYS	2.2
1	D	54	LYS	2.2
1	C	320	GLY	2.2
1	C	1012	GLU	2.2
1	C	909	ARG	2.2
1	B	327	PRO	2.1
1	B	411	THR	2.2
1	C	1010	PRO	2.1
1	A	899	GLU	2.1
1	D	376	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	342	ASP	2.1
1	C	421	GLU	2.1
1	C	908	GLU	2.1
1	D	273	GLU	2.1
1	D	300	ASP	2.1
1	C	427	VAL	2.1
1	D	862	GLY	2.1
1	D	950	GLU	2.1
1	B	295	GLN	2.1
1	B	325	HIS	2.1
1	B	1020	ALA	2.1
1	D	1017	LEU	2.1
1	C	425	GLN	2.1
1	B	3	PRO	2.1
1	D	3	PRO	2.1
1	B	396	VAL	2.1
1	A	884	GLU	2.0
1	C	903	ALA	2.1
1	C	460	ASP	2.0
1	A	273	GLU	2.0
1	B	376	GLU	2.0
1	C	897	LEU	2.0
1	C	332	ARG	2.0
1	B	418	LYS	2.0
1	A	911	PRO	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 ⓘ

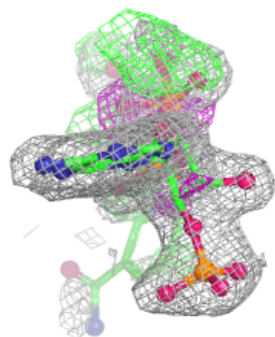
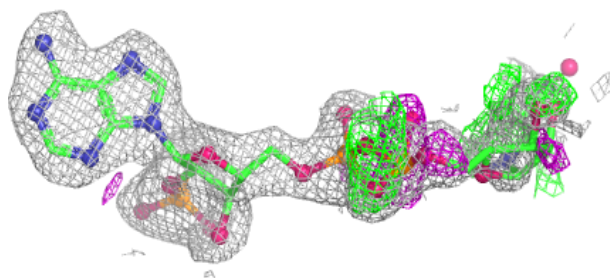
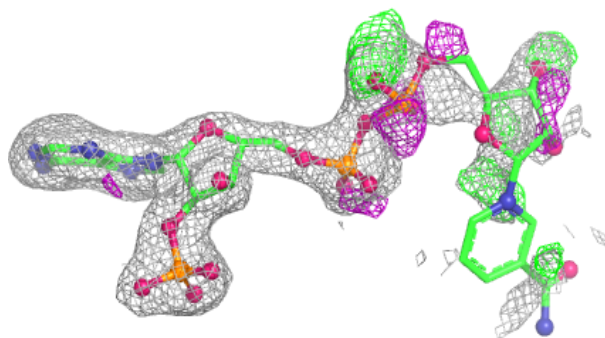
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NDP	A	1032	48/48	0.82	0.13	30,34,48,48	9
5	NDP	C	1032	48/48	0.84	0.15	30,33,50,52	9
5	NDP	D	1032	48/48	0.85	0.16	21,26,52,56	0
5	NDP	B	1032	48/48	0.89	0.12	19,24,42,46	0
6	URF	A	1033	9/9	0.92	0.08	22,23,24,26	0
6	URF	C	1033	9/9	0.93	0.08	19,20,22,23	0
6	URF	D	1033	9/9	0.93	0.07	17,19,20,25	0
6	URF	B	1033	9/9	0.94	0.08	19,20,21,23	0
2	SF4	D	1027	8/8	0.95	0.07	11,12,13,13	0
2	SF4	A	1026	8/8	0.95	0.07	14,14,15,15	0
2	SF4	A	1029	8/8	0.95	0.07	16,17,18,19	0
2	SF4	B	1026	8/8	0.95	0.07	13,14,15,16	0
2	SF4	B	1027	8/8	0.95	0.07	12,14,15,16	0
2	SF4	B	1028	8/8	0.95	0.07	15,16,17,17	0
2	SF4	C	1026	8/8	0.95	0.07	13,14,15,15	0
2	SF4	C	1027	8/8	0.95	0.07	11,13,14,15	0
2	SF4	C	1029	8/8	0.95	0.07	13,14,16,16	0
4	FAD	B	1031	53/53	0.96	0.06	8,13,15,15	0
2	SF4	A	1028	8/8	0.96	0.06	15,15,16,17	0
2	SF4	C	1028	8/8	0.96	0.06	13,14,15,15	0
2	SF4	B	1029	8/8	0.96	0.07	16,16,17,18	0
2	SF4	D	1026	8/8	0.96	0.06	13,13,14,14	0
2	SF4	A	1027	8/8	0.96	0.06	12,14,15,15	0
2	SF4	D	1028	8/8	0.96	0.06	15,16,16,17	0
2	SF4	D	1029	8/8	0.96	0.06	15,16,17,18	0
4	FAD	A	1031	53/53	0.96	0.06	9,12,14,14	0
3	FMN	A	1030	31/31	0.97	0.05	10,13,14,15	0
3	FMN	B	1030	31/31	0.97	0.05	10,14,15,16	0
4	FAD	C	1031	53/53	0.97	0.05	10,13,15,16	0
4	FAD	D	1031	53/53	0.97	0.06	9,12,14,15	0
3	FMN	C	1030	31/31	0.97	0.05	8,12,14,17	0
3	FMN	D	1030	31/31	0.97	0.06	10,12,13,14	0

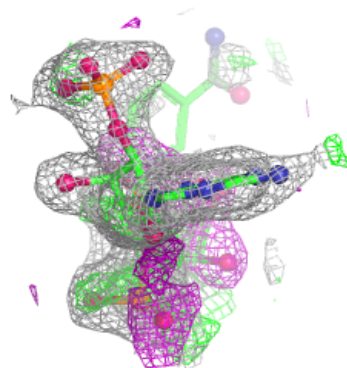
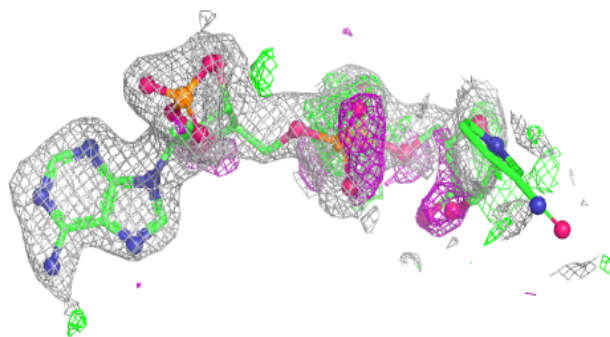
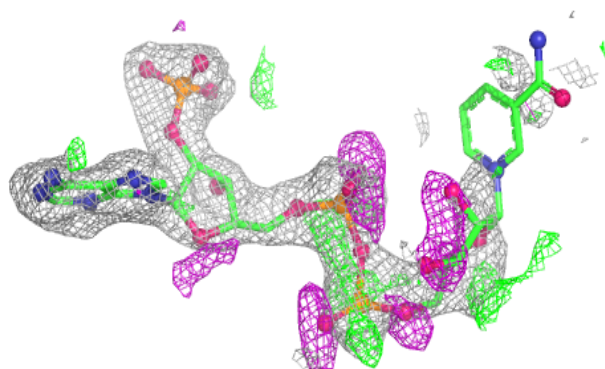
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP A 1032:

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

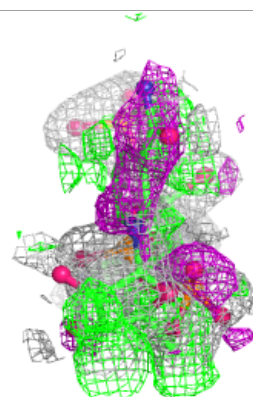
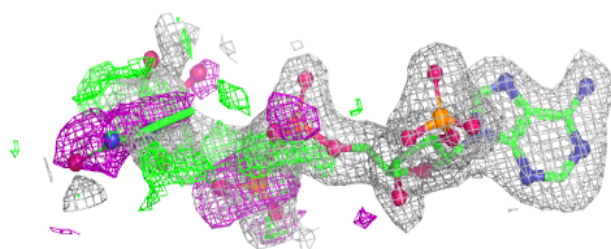
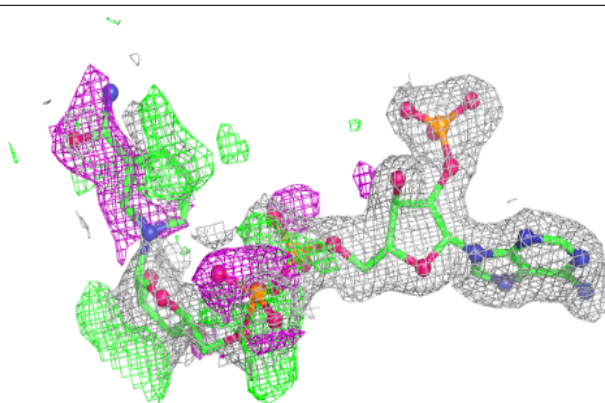
**Electron density around NDP C 1032:**

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

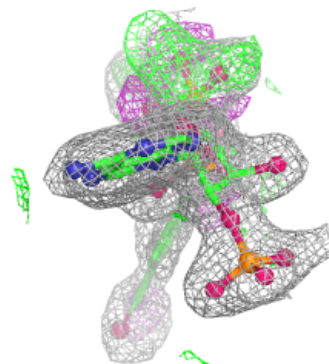
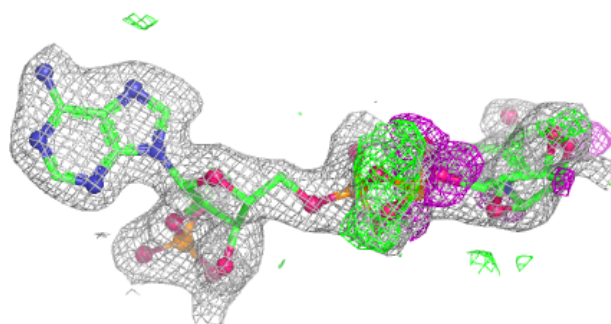
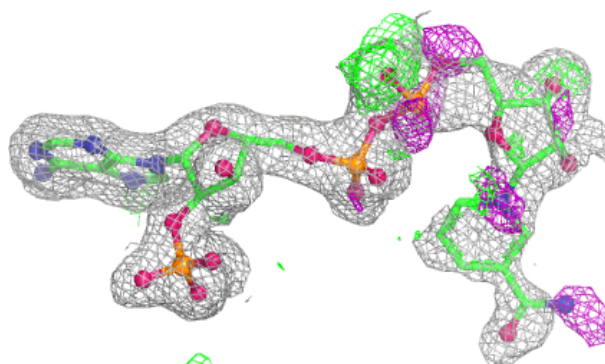


Electron density around NDP D 1032:

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

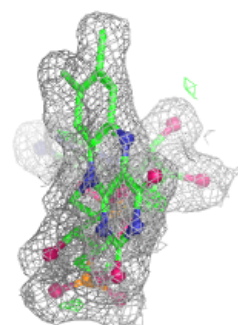
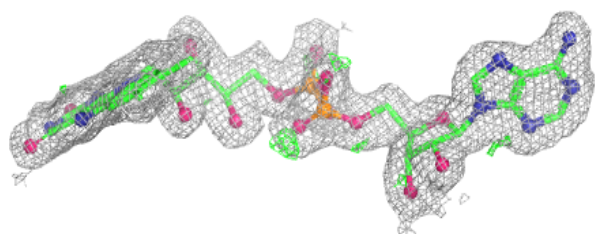
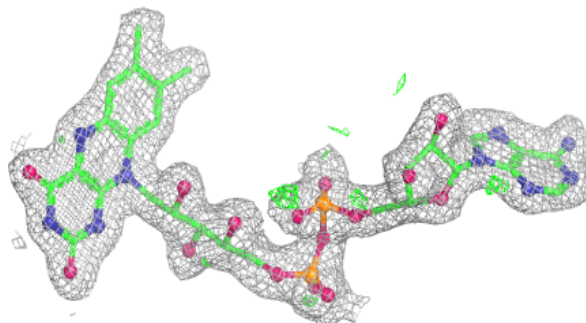
**Electron density around NDP B 1032:**

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

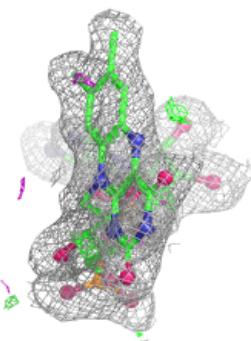
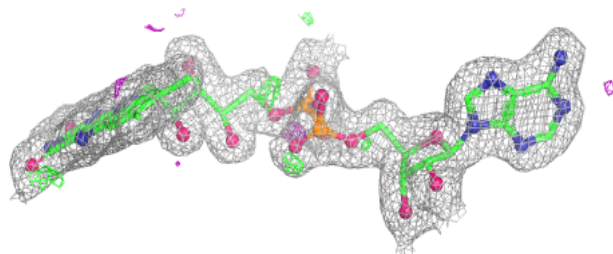
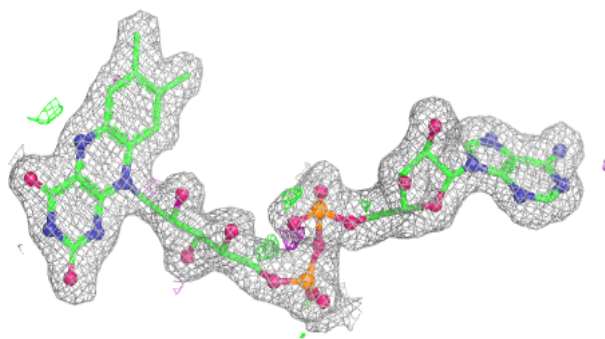


Electron density around FAD B 1031:

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

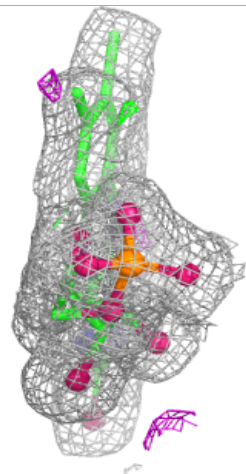
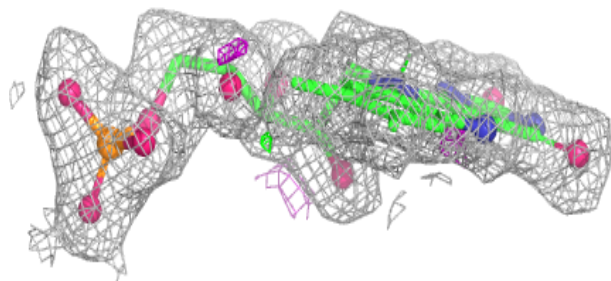
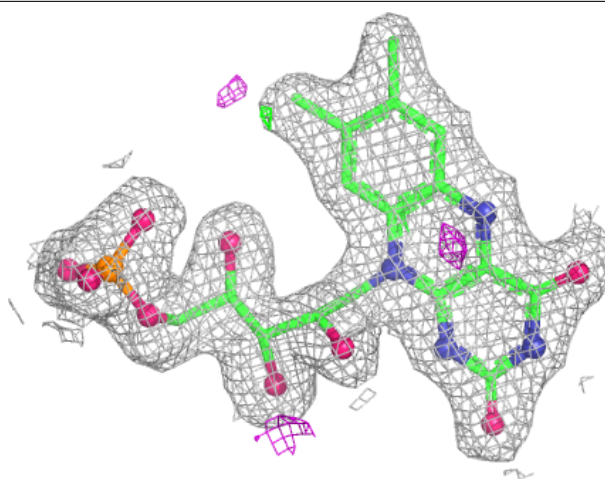
**Electron density around FAD A 1031:**

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



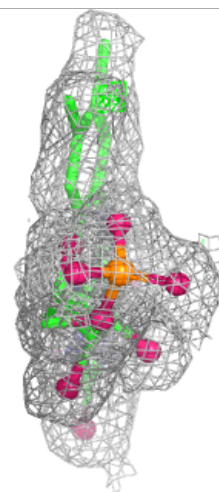
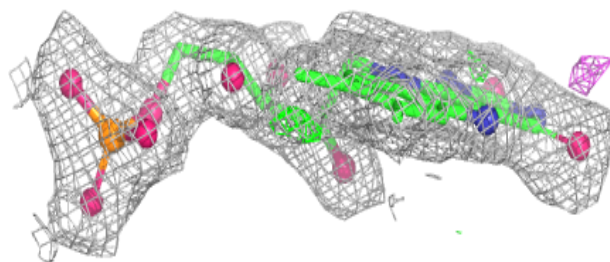
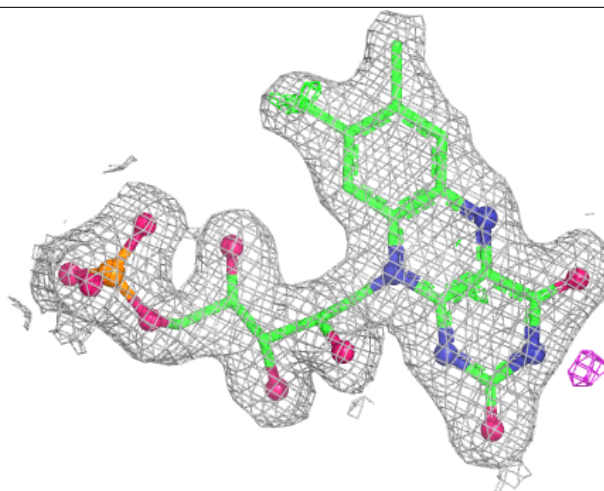
Electron density around FMN A 1030:

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



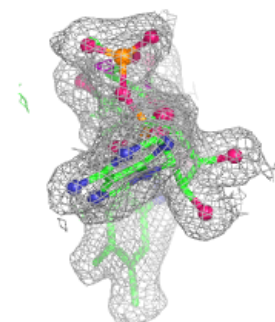
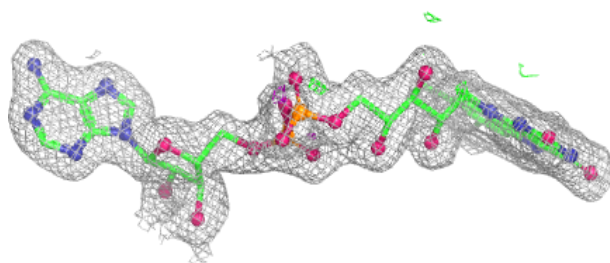
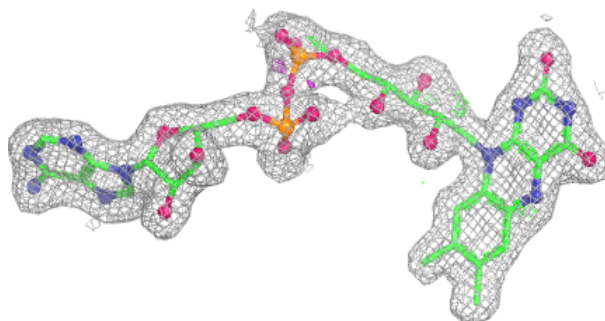
Electron density around FMN B 1030:

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

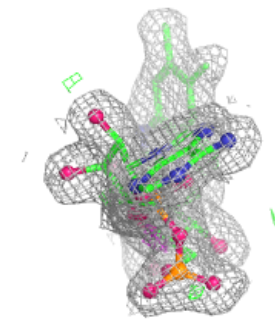
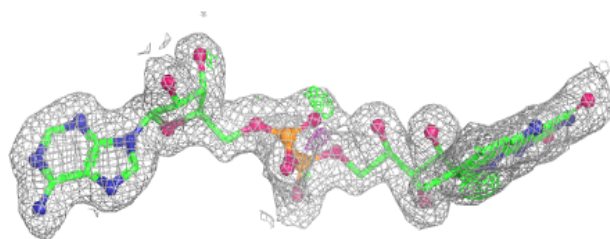
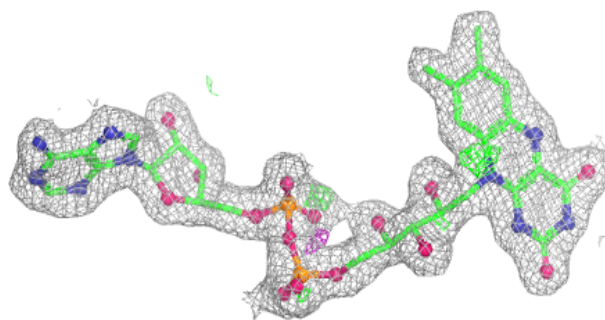


Electron density around FAD C 1031:

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

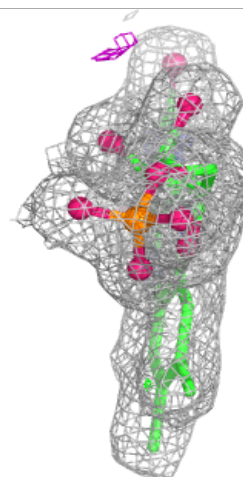
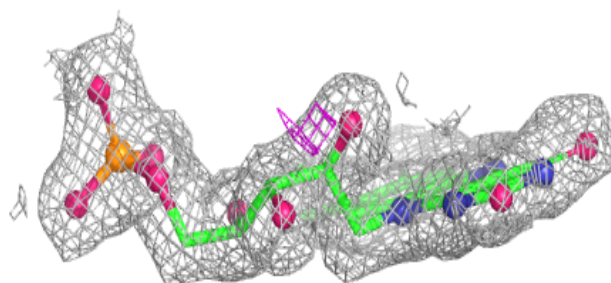
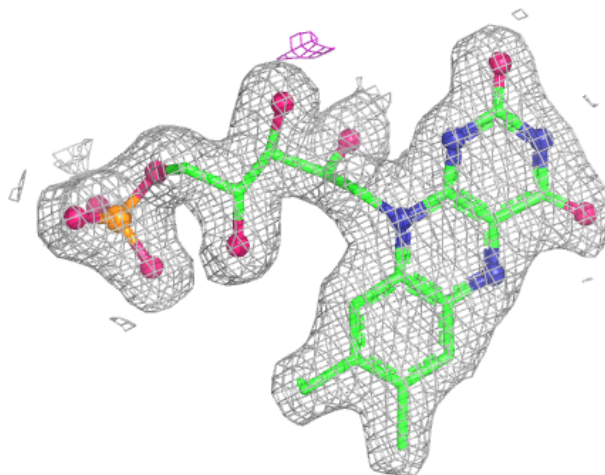
**Electron density around FAD D 1031:**

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



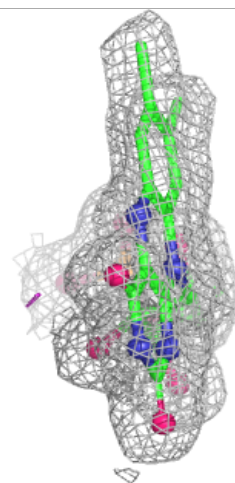
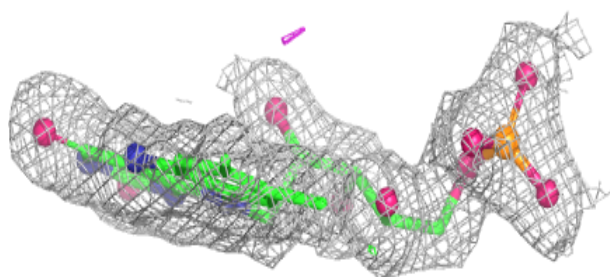
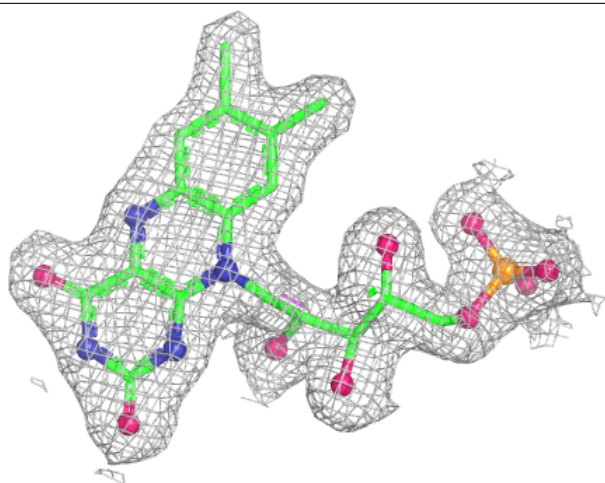
Electron density around FMN C 1030:

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



Electron density around FMN D 1030:

$2mF_o-DF_c$ (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.