



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:36 PM UTC

PDB ID : 1GTH / pdb_00001gth
Title : DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG,
TERNARY COMPLEX WITH NADPH AND 5-IODOURACIL
Authors : Dobritsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2002-01-15
Resolution : 2.25 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

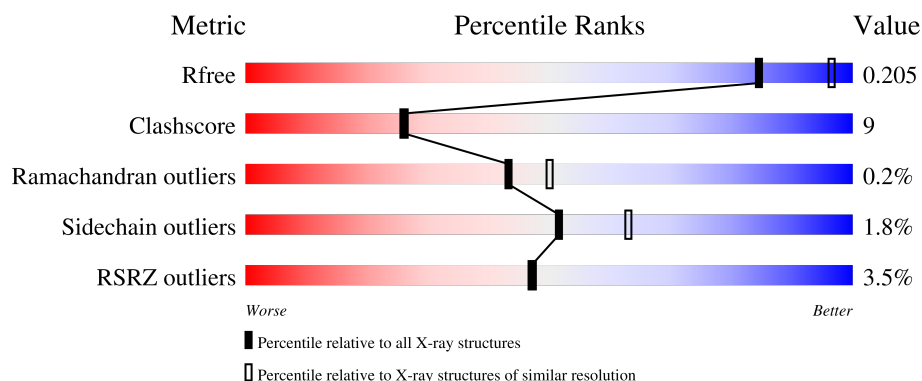
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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% 82% 16% ..
1	B	1025	3% 81% 17% ..
1	C	1025	3% 80% 18% ..
1	D	1025	4% 80% 18% ..

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	C	1027	-	-	X	-
2	SF4	D	1027	-	-	X	-
6	IDH	B	1034	-	-	X	-
7	IUR	C	1034	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 34762 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.

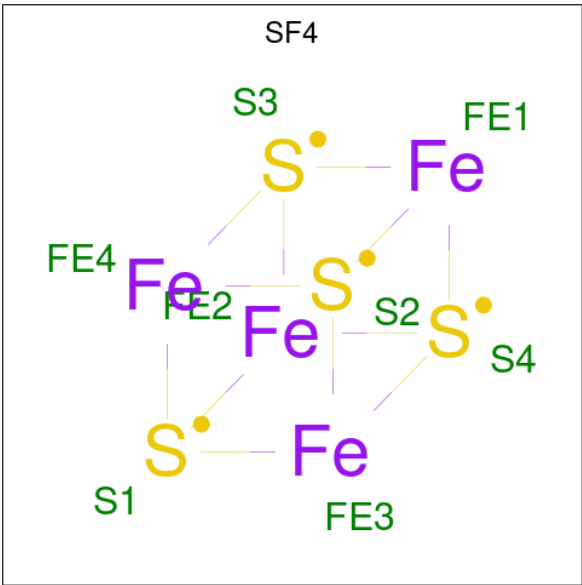
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0	0
			7770	4927	1317	1470	56			
1	B	1012	Total	C	N	O	S	0	0	0
			7719	4892	1309	1462	56			
1	C	1015	Total	C	N	O	S	0	0	0
			7740	4905	1313	1466	56			
1	D	1019	Total	C	N	O	S	0	0	0
			7770	4927	1317	1470	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).



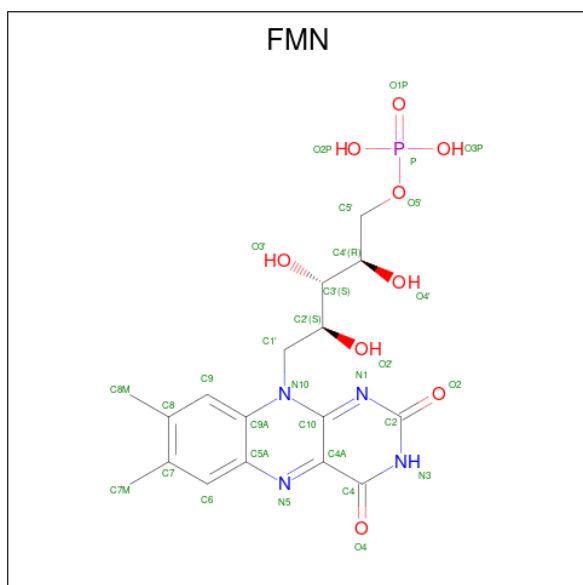
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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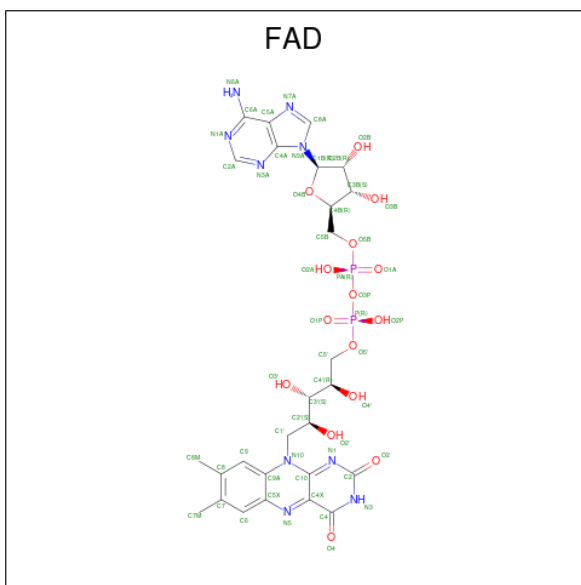
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

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



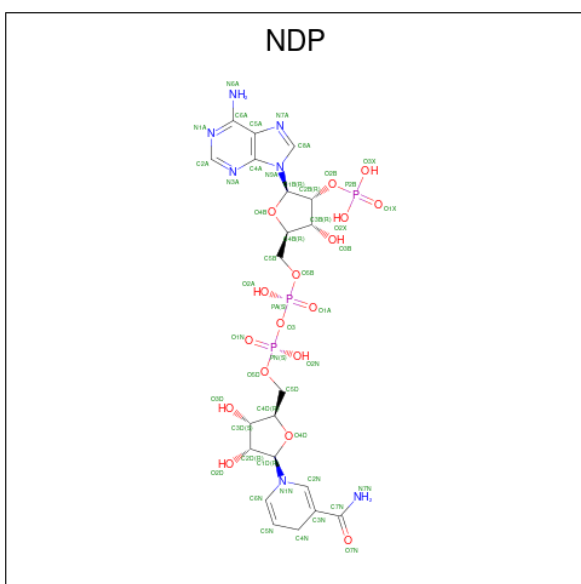
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



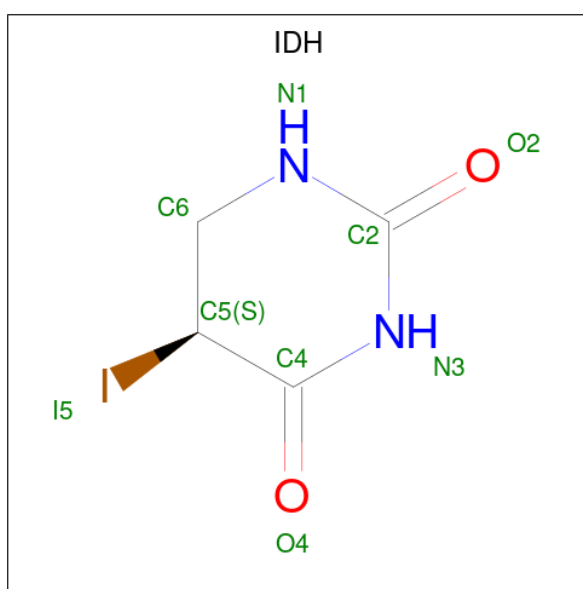
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

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



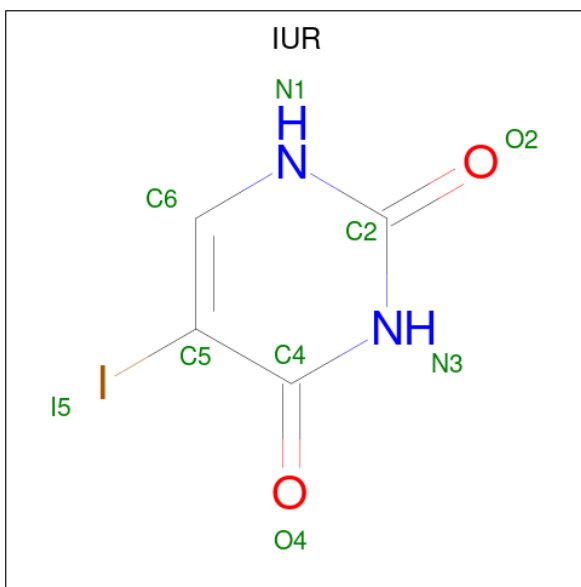
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is (5S)-5-iododihydro-2,4(1H,3H)-pyrimidin-2-one (CCD ID: IDH) (formula: $C_4H_5IN_2O_2$).



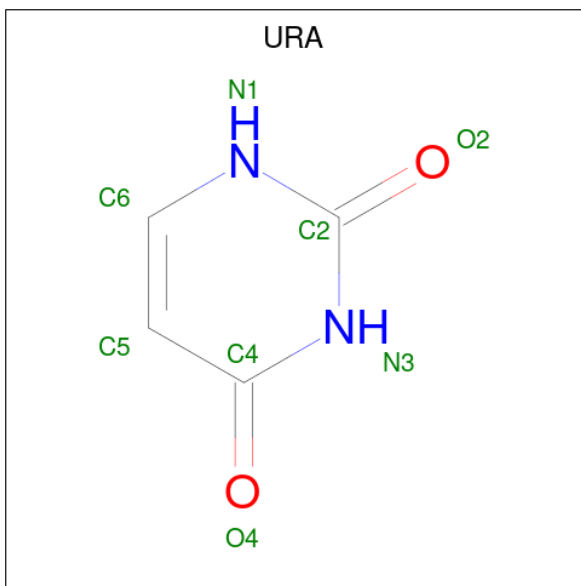
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O		0	0
			8	4	2	2			
6	B	1	Total	C	I	N	O	0	0
			9	4	1	2	2		

- Molecule 7 is 5-iodouracil (CCD ID: IUR) (formula: $C_4H_3IN_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	I	N	O	
			9	4	1	2	2	
							0	0

- Molecule 8 is URACIL (CCD ID: URA) (formula: $C_4H_4N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O		
			8	4	2	2		
							0	0

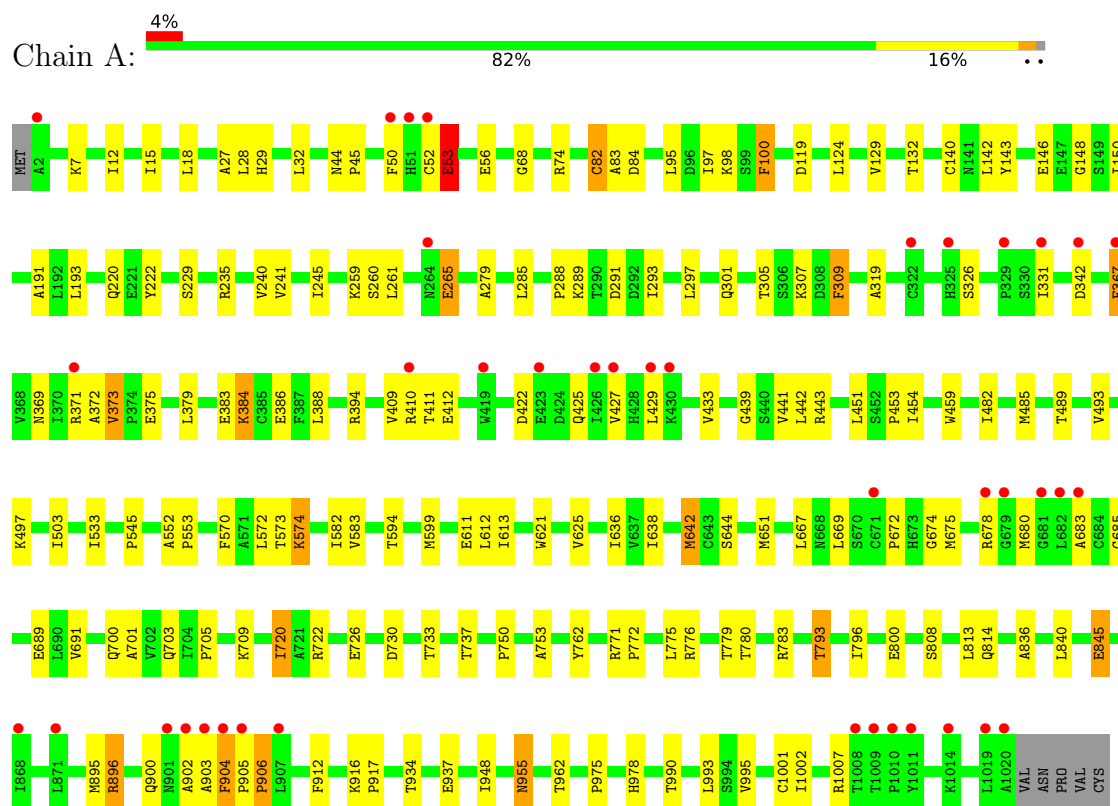
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	839	Total 839	O 839	0	0
9	B	869	Total 869	O 869	0	0
9	C	701	Total 701	O 701	0	0
9	D	664	Total 664	O 664	0	0

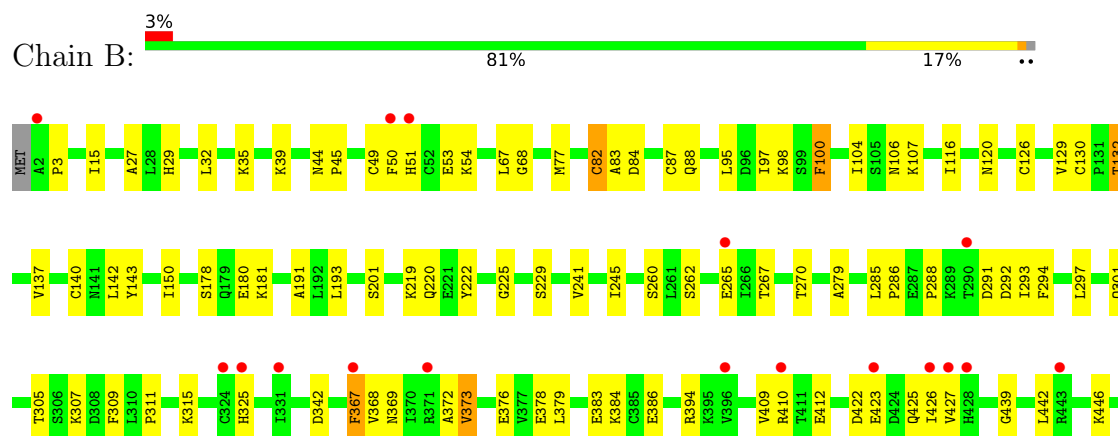
3 Residue-property plots [i](#)

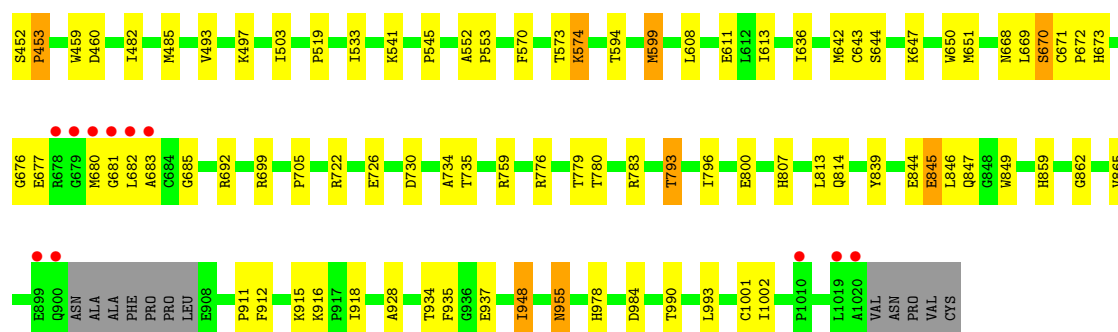
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

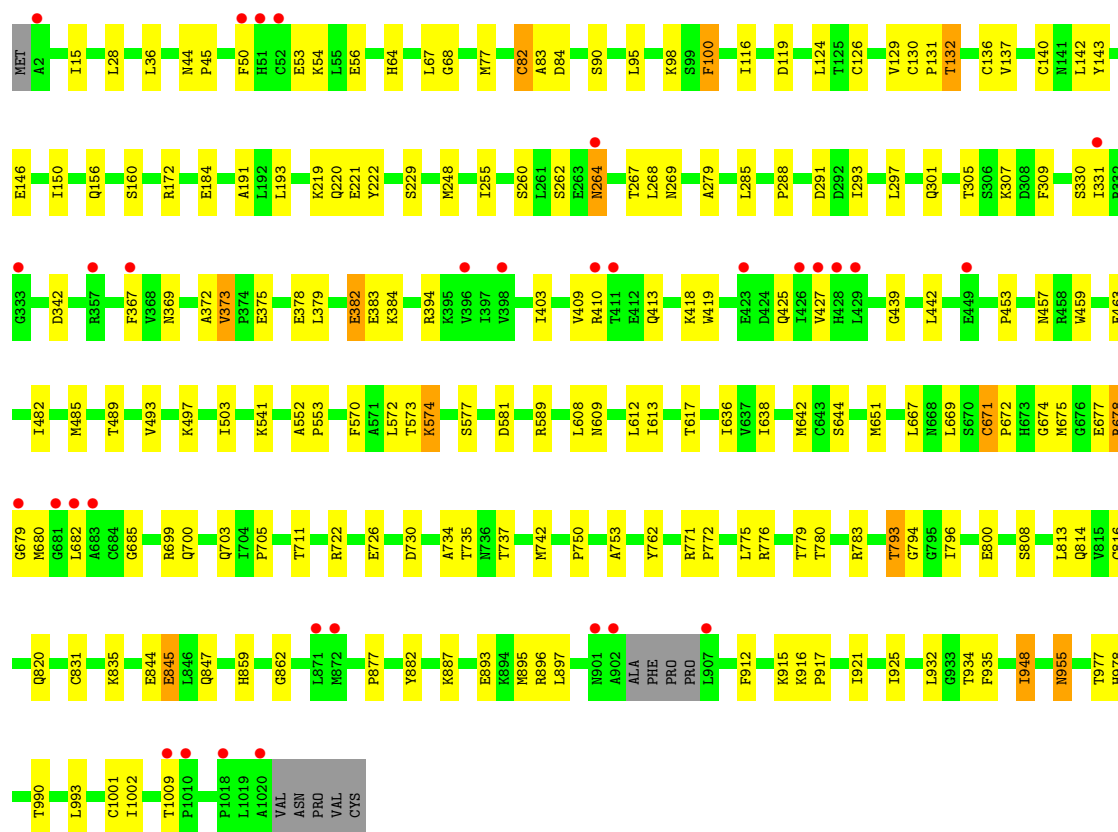
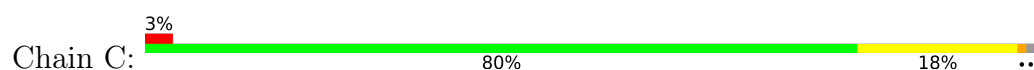


• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

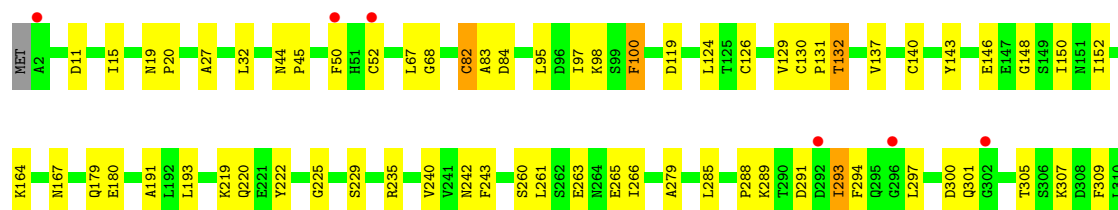
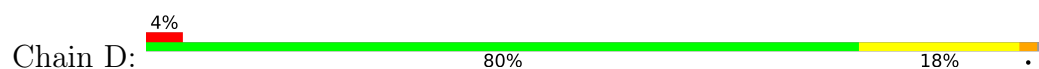


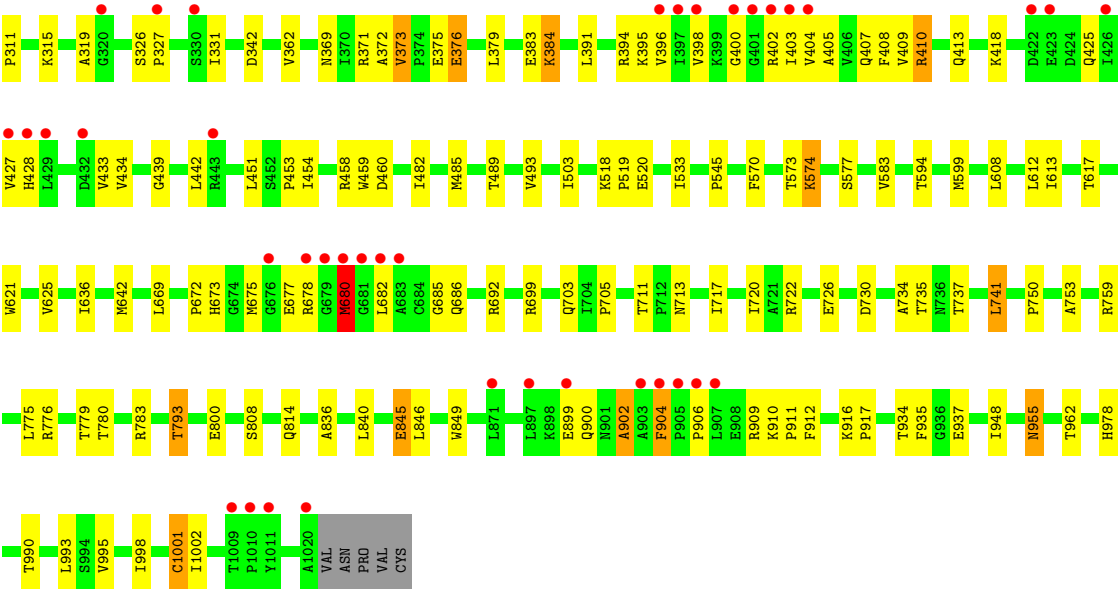


• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE



• 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	82.21Å 159.69Å 167.59Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	25.00 – 2.25 25.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.25) 98.2 (25.00-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.26Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.209 0.175 , 0.205	Depositor DCC
R_{free} test set	3984 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	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	34762	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: FAD, SF4, URA, FMN, IDH, NDP, IUR

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	0.40	1/7932 (0.0%)	0.89	23/10751 (0.2%)
1	B	0.41	0/7877	0.90	20/10672 (0.2%)
1	C	0.38	0/7898	0.89	20/10701 (0.2%)
1	D	0.39	0/7932	0.89	22/10751 (0.2%)
All	All	0.39	1/31639 (0.0%)	0.89	85/42875 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	642	MET	SD-CE	-5.14	1.66	1.79

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	THR	N-CA-C	-8.23	98.04	110.14
1	D	305	THR	N-CA-C	-8.08	97.61	110.14
1	A	305	THR	N-CA-C	-7.92	97.86	110.14
1	A	574	LYS	N-CA-C	-7.90	99.60	110.35
1	C	305	THR	N-CA-C	-7.67	98.25	110.14
1	C	574	LYS	N-CA-C	-7.52	100.12	110.35
1	A	82	CYS	N-CA-C	7.51	120.56	110.35
1	B	574	LYS	N-CA-C	-7.44	100.23	110.35
1	D	574	LYS	N-CA-C	-7.42	100.26	110.35
1	B	285	LEU	CA-C-N	7.42	127.13	119.56
1	B	285	LEU	C-N-CA	7.42	127.13	119.56
1	D	955	ASN	N-CA-C	7.30	121.54	111.90
1	D	82	CYS	N-CA-C	7.23	119.90	110.43
1	C	955	ASN	N-CA-C	7.06	121.22	111.90
1	C	285	LEU	CA-C-N	7.06	126.74	119.82
1	C	285	LEU	C-N-CA	7.06	126.74	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	503	ILE	N-CA-C	-6.83	103.83	110.72
1	A	955	ASN	N-CA-C	6.81	120.96	112.24
1	B	82	CYS	N-CA-C	6.71	119.48	110.35
1	C	82	CYS	N-CA-C	6.68	119.18	110.43
1	B	955	ASN	N-CA-C	6.67	120.77	112.24
1	B	503	ILE	N-CA-C	-6.58	104.07	110.72
1	D	129	VAL	N-CA-C	6.53	120.55	113.43
1	C	68	GLY	N-CA-C	-6.51	102.30	112.58
1	B	129	VAL	N-CA-C	6.51	120.52	113.43
1	D	904	PHE	CA-C-N	6.42	127.00	120.38
1	D	904	PHE	C-N-CA	6.42	127.00	120.38
1	C	671	CYS	CA-C-N	6.38	126.07	119.56
1	C	671	CYS	C-N-CA	6.38	126.07	119.56
1	D	68	GLY	N-CA-C	-6.33	102.57	112.58
1	A	132	THR	N-CA-C	6.32	118.98	111.33
1	D	143	TYR	N-CA-C	-6.28	104.88	112.54
1	D	503	ILE	N-CA-C	-6.24	104.41	110.72
1	D	1001	CYS	N-CA-C	-6.23	104.57	111.36
1	A	1001	CYS	N-CA-C	-6.22	104.58	111.36
1	A	68	GLY	N-CA-C	-6.21	102.76	112.58
1	A	309	PHE	N-CA-C	6.21	117.92	111.03
1	D	132	THR	N-CA-C	6.21	118.84	111.33
1	B	132	THR	N-CA-C	6.20	118.83	111.33
1	C	129	VAL	N-CA-C	6.17	120.15	113.43
1	A	285	LEU	CA-C-N	6.08	125.78	119.82
1	A	285	LEU	C-N-CA	6.08	125.78	119.82
1	D	285	LEU	CA-C-N	5.99	125.67	119.56
1	D	285	LEU	C-N-CA	5.99	125.67	119.56
1	B	309	PHE	N-CA-C	5.93	117.62	111.03
1	C	143	TYR	N-CA-C	-5.92	104.96	111.82
1	C	1001	CYS	N-CA-C	-5.88	104.95	111.36
1	B	1001	CYS	N-CA-C	-5.82	105.01	111.36
1	B	68	GLY	N-CA-C	-5.79	103.43	112.58
1	C	132	THR	N-CA-C	5.78	119.14	111.75
1	A	503	ILE	N-CA-C	-5.76	104.90	110.72
1	D	229	SER	N-CA-C	5.75	119.55	112.54
1	B	143	TYR	N-CA-C	-5.74	105.53	112.54
1	A	143	TYR	N-CA-C	-5.73	105.55	112.54
1	A	573	THR	N-CA-C	-5.71	102.85	110.55
1	B	594	THR	N-CA-C	-5.60	105.76	112.59
1	A	384	LYS	N-CA-C	5.60	119.30	111.74
1	A	129	VAL	N-CA-C	5.58	119.51	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	GLY	N-CA-C	5.57	122.61	112.58
1	C	573	THR	N-CA-C	-5.54	103.07	110.55
1	B	573	THR	N-CA-C	-5.46	103.18	110.55
1	C	948	ILE	N-CA-C	5.43	116.12	108.36
1	D	594	THR	N-CA-C	-5.42	105.97	112.59
1	D	573	THR	N-CA-C	-5.40	103.26	110.55
1	D	235	ARG	N-CA-C	-5.34	106.70	113.43
1	A	904	PHE	CA-C-N	5.33	123.55	119.66
1	A	904	PHE	C-N-CA	5.33	123.55	119.66
1	D	680	MET	N-CA-C	5.33	117.57	109.63
1	B	229	SER	N-CA-C	5.30	119.46	112.89
1	A	229	SER	N-CA-C	5.29	119.44	112.89
1	D	384	LYS	N-CA-C	5.23	118.85	111.52
1	A	459	TRP	N-CA-C	-5.21	106.70	113.16
1	C	229	SER	N-CA-C	5.18	119.32	112.89
1	D	617	THR	N-CA-C	5.17	117.36	110.53
1	C	459	TRP	N-CA-C	-5.16	106.76	113.16
1	D	148	GLY	N-CA-C	5.15	121.58	112.83
1	C	384	LYS	N-CA-C	5.12	118.69	111.52
1	B	286	PRO	N-CA-C	5.12	120.49	113.84
1	C	617	THR	N-CA-C	5.11	117.28	110.53
1	B	948	ILE	N-CA-C	5.10	115.65	108.36
1	A	720	ILE	CB-CA-C	-5.08	105.20	112.22
1	B	670	SER	N-CA-C	5.08	120.21	112.54
1	A	594	THR	N-CA-C	-5.07	106.34	112.88
1	B	384	LYS	N-CA-C	5.01	118.51	111.74
1	A	235	ARG	N-CA-C	-5.00	107.12	113.43

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	7770	0	7797	144	0
1	B	7719	0	7747	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7740	0	7769	175	0
1	D	7770	0	7798	204	0
2	A	32	0	0	2	0
2	B	32	0	0	2	0
2	C	32	0	0	2	0
2	D	32	0	0	3	0
3	A	31	0	19	0	0
3	B	31	0	19	1	0
3	C	31	0	19	1	0
3	D	31	0	19	0	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
4	C	53	0	31	0	0
4	D	53	0	31	1	0
5	A	48	0	26	6	0
5	B	48	0	26	5	0
5	C	48	0	26	6	0
5	D	48	0	26	5	0
6	A	8	0	4	1	0
6	B	9	0	5	4	0
7	C	9	0	3	4	0
8	D	8	0	3	0	0
9	A	839	0	0	17	0
9	B	869	0	0	21	0
9	C	701	0	0	15	0
9	D	664	0	0	22	0
All	All	34762	0	31430	593	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (593) 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:C:427:VAL:HG21	1:D:410:ARG:HH21	1.25	1.02
1:C:264:ASN:H	1:C:264:ASN:HD22	1.17	0.91
1:D:904:PHE:O	1:D:906:PRO:HD3	1.70	0.90
1:C:410:ARG:NH1	1:D:427:VAL:HG13	1.87	0.89
1:C:410:ARG:HH12	1:D:427:VAL:HG22	1.36	0.88
1:D:909:ARG:HG2	1:D:909:ARG:HH11	1.39	0.87
1:D:319:ALA:CB	1:D:904:PHE:HB2	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:GLY:HA2	9:B:2602:HOH:O	1.74	0.86
1:D:642:MET:HE1	1:D:675:MET:HG3	1.56	0.85
1:D:291:ASP:OD1	1:D:293:ILE:HG13	1.77	0.84
1:C:410:ARG:NH1	1:D:427:VAL:HG22	1.92	0.84
1:C:613:ILE:HG22	7:C:1034:IUR:I5	2.48	0.84
1:A:427:VAL:HG22	1:B:410:ARG:NH2	1.94	0.83
1:D:319:ALA:HB1	1:D:904:PHE:HB2	1.60	0.83
1:C:410:ARG:HH22	1:D:427:VAL:HG22	1.42	0.82
1:C:427:VAL:CG2	1:D:410:ARG:HH21	1.90	0.82
1:A:410:ARG:HH21	1:B:427:VAL:HG22	1.43	0.82
1:A:582:ILE:HD12	9:A:2256:HOH:O	1.77	0.82
1:C:642:MET:HE1	1:C:675:MET:HG3	1.61	0.82
1:B:669:LEU:HD23	9:B:2601:HOH:O	1.79	0.82
1:A:342:ASP:HB3	5:A:1032:NDP:H42N	1.63	0.81
1:B:859:HIS:HD2	1:B:862:GLY:H	1.28	0.81
1:C:410:ARG:NH2	1:D:427:VAL:HG22	1.96	0.81
1:D:776:ARG:O	1:D:780:THR:HG23	1.80	0.81
1:C:859:HIS:HD2	1:C:862:GLY:H	1.28	0.80
1:C:369:ASN:HA	1:D:50:PHE:HE2	1.46	0.79
1:D:682:LEU:HD13	9:D:2465:HOH:O	1.81	0.79
1:D:398:VAL:HG22	1:D:403:ILE:HA	1.66	0.77
1:D:398:VAL:HG13	1:D:402:ARG:O	1.85	0.77
1:D:410:ARG:HD3	1:D:425:GLN:OE1	1.85	0.77
1:A:427:VAL:HG22	1:B:410:ARG:HH21	1.50	0.77
1:A:642:MET:HE1	1:A:675:MET:HG3	1.67	0.77
1:B:39:LYS:HG3	9:B:2075:HOH:O	1.85	0.76
1:C:342:ASP:HB3	5:C:1032:NDP:H42N	1.65	0.76
1:B:54:LYS:HB3	9:B:2105:HOH:O	1.85	0.76
1:B:262:SER:HB3	1:B:265:GLU:OE1	1.85	0.76
1:C:410:ARG:HH12	1:D:427:VAL:CG2	1.98	0.75
1:A:50:PHE:CE2	1:B:369:ASN:HA	2.22	0.75
1:D:373:VAL:HG22	1:D:376:GLU:HB2	1.68	0.75
1:D:342:ASP:HB3	5:D:1032:NDP:H42N	1.69	0.75
1:A:642:MET:CE	1:A:675:MET:HE2	2.17	0.74
1:D:485:MET:HE3	9:D:2320:HOH:O	1.86	0.74
1:B:342:ASP:HB3	5:B:1032:NDP:H42N	1.70	0.73
1:B:644:SER:N	1:B:680:MET:HE2	2.04	0.73
1:C:613:ILE:CG2	7:C:1034:IUR:I5	3.07	0.73
1:D:301:GLN:O	1:D:403:ILE:HG22	1.88	0.73
1:B:671:CYS:SG	6:B:1034:IDH:I5	3.17	0.72
1:C:410:ARG:HE	1:D:410:ARG:NH2	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:711:THR:HG22	9:D:2454:HOH:O	1.89	0.72
1:A:441:VAL:HG21	1:A:443:ARG:HD2	1.70	0.72
1:A:369:ASN:HA	1:B:50:PHE:CE2	2.24	0.71
1:C:410:ARG:CZ	1:D:427:VAL:HG22	2.20	0.71
1:C:369:ASN:HA	1:D:50:PHE:CE2	2.26	0.71
1:C:762:TYR:CZ	1:D:780:THR:HG22	2.26	0.70
1:A:422:ASP:OD2	1:A:425:GLN:HG3	1.90	0.69
1:D:410:ARG:HH11	1:D:410:ARG:HG3	1.55	0.69
1:A:410:ARG:HH21	1:B:427:VAL:CG2	2.05	0.69
1:C:642:MET:HE3	1:C:675:MET:HE2	1.75	0.68
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.58	0.68
1:A:485:MET:HE1	1:B:32:LEU:HB2	1.74	0.68
1:C:644:SER:N	1:C:680:MET:HE2	2.09	0.68
1:C:410:ARG:NH2	1:D:410:ARG:NH1	2.41	0.68
1:C:642:MET:CE	1:C:675:MET:HE2	2.24	0.68
1:A:574:LYS:HE3	9:A:2520:HOH:O	1.93	0.67
1:C:410:ARG:HD2	1:C:425:GLN:OE1	1.95	0.67
1:A:410:ARG:CZ	1:B:410:ARG:NH2	2.58	0.67
1:C:820:GLN:O	1:D:962:THR:HG22	1.94	0.67
1:C:485:MET:HE1	1:D:32:LEU:HB2	1.77	0.66
1:D:395:LYS:HD2	1:D:407:GLN:OE1	1.95	0.66
1:C:672:PRO:HG2	1:C:737:THR:OG1	1.95	0.66
1:D:642:MET:HE3	1:D:675:MET:HE2	1.77	0.66
1:C:378:GLU:O	1:C:382:GLU:HG3	1.96	0.66
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.76	0.65
1:B:291:ASP:OD1	1:B:293:ILE:HG12	1.96	0.65
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.77	0.65
1:C:671:CYS:SG	7:C:1034:IUR:I5	3.23	0.65
1:D:180:GLU:CD	1:D:180:GLU:H	2.05	0.65
1:A:410:ARG:NH2	1:B:427:VAL:CG2	2.60	0.65
1:C:410:ARG:HH12	1:D:427:VAL:CB	2.09	0.65
1:D:720:ILE:CD1	9:D:2454:HOH:O	2.46	0.64
1:D:720:ILE:HD12	9:D:2454:HOH:O	1.97	0.64
1:A:369:ASN:HA	1:B:50:PHE:HE2	1.62	0.64
1:D:583:VAL:HG12	1:D:678:ARG:HH11	1.62	0.64
1:A:582:ILE:HA	9:A:2256:HOH:O	1.96	0.63
1:C:775:LEU:O	1:C:779:THR:HG23	1.98	0.63
1:A:896:ARG:HH21	1:A:900:GLN:HE22	1.45	0.63
1:B:410:ARG:HD2	1:B:425:GLN:OE1	1.98	0.63
1:C:581:ASP:CG	1:C:680:MET:HE1	2.23	0.63
1:D:319:ALA:HB2	1:D:904:PHE:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ARG:HH21	1:D:410:ARG:CZ	2.11	0.63
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.33	0.63
1:D:410:ARG:HH11	1:D:410:ARG:CG	2.12	0.63
1:B:682:LEU:HD12	9:B:2605:HOH:O	1.97	0.63
1:A:410:ARG:NH1	1:B:410:ARG:HH12	1.97	0.62
1:D:167:ASN:OD1	1:D:909:ARG:NH1	2.33	0.62
1:A:427:VAL:CG2	1:B:410:ARG:NH2	2.62	0.62
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.81	0.62
1:A:260:SER:HB3	1:A:265:GLU:OE1	2.00	0.61
1:D:52:CYS:HB3	1:D:384:LYS:HG2	1.82	0.61
1:D:909:ARG:HH11	1:D:909:ARG:CG	2.13	0.61
1:C:762:TYR:OH	1:D:780:THR:HG22	2.00	0.61
1:A:642:MET:HE1	1:A:675:MET:CG	2.30	0.60
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.82	0.60
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.82	0.60
1:D:722:ARG:O	1:D:726:GLU:HG3	2.01	0.60
1:C:932:LEU:HD21	1:D:741:LEU:HD11	1.83	0.60
1:A:934:THR:OG1	1:A:937:GLU:HG3	2.02	0.60
1:A:583:VAL:HG12	1:A:678:ARG:NH1	2.17	0.60
1:D:583:VAL:HG12	1:D:678:ARG:NH1	2.17	0.60
1:A:990:THR:HG22	1:A:990:THR:O	2.02	0.59
1:B:574:LYS:HE3	9:B:2549:HOH:O	2.00	0.59
1:B:409:VAL:HG22	1:B:422:ASP:O	2.02	0.59
1:B:422:ASP:OD2	1:B:425:GLN:HG3	2.02	0.59
1:D:682:LEU:HD11	1:D:686:GLN:NE2	2.18	0.59
1:A:651:MET:HE3	1:A:700:GLN:HG3	1.84	0.59
1:A:689:GLU:OE2	1:D:327:PRO:HG3	2.02	0.59
1:A:439:GLY:HA2	5:A:1032:NDP:O2N	2.02	0.59
1:A:32:LEU:HB2	1:B:485:MET:HE1	1.84	0.59
1:D:909:ARG:HG2	1:D:909:ARG:NH1	2.15	0.58
1:D:775:LEU:O	1:D:779:THR:HG23	2.03	0.58
3:B:1030:FMN:C4A	6:B:1034:IDH:H5	2.33	0.58
1:C:54:LYS:HB3	9:C:2079:HOH:O	2.03	0.58
1:C:410:ARG:HH12	1:D:427:VAL:HG13	1.66	0.58
1:A:793:THR:HB	1:A:814:GLN:HB2	1.85	0.58
1:C:172:ARG:HG3	9:C:2191:HOH:O	2.04	0.58
1:C:990:THR:O	1:C:990:THR:HG22	2.03	0.58
1:D:379:LEU:O	1:D:383:GLU:HG3	2.04	0.58
9:A:2140:HOH:O	1:B:29:HIS:HB2	2.04	0.58
1:C:439:GLY:HA2	5:C:1032:NDP:O2N	2.04	0.58
1:C:779:THR:HG22	1:C:808:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:GLU:O	1:B:673:HIS:HE1	1.87	0.58
1:A:410:ARG:NE	1:B:410:ARG:NH2	2.52	0.57
1:C:36:LEU:HB3	9:C:2064:HOH:O	2.03	0.57
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.85	0.57
1:D:82:CYS:O	1:D:98:LYS:HD2	2.05	0.57
1:B:439:GLY:HA2	5:B:1032:NDP:O2N	2.05	0.57
1:A:572:LEU:HD13	1:A:638:ILE:HB	1.86	0.57
1:C:269:ASN:HB2	9:C:2243:HOH:O	2.04	0.57
1:C:672:PRO:HA	1:C:682:LEU:HD22	1.86	0.57
1:C:146:GLU:HG2	1:D:67:LEU:HD23	1.84	0.57
1:A:443:ARG:NH1	9:A:2401:HOH:O	2.38	0.57
9:C:2507:HOH:O	1:D:775:LEU:HD12	2.03	0.57
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.86	0.57
1:B:379:LEU:O	1:B:383:GLU:HG3	2.04	0.57
1:C:410:ARG:NH1	1:D:427:VAL:CG1	2.65	0.57
1:D:779:THR:HG22	1:D:808:SER:HB3	1.85	0.57
1:A:29:HIS:HB2	9:B:2161:HOH:O	2.05	0.56
1:C:845:GLU:HG3	1:C:912:PHE:CE2	2.40	0.56
1:A:342:ASP:CB	5:A:1032:NDP:H42N	2.34	0.56
1:C:410:ARG:NH2	1:D:410:ARG:CZ	2.68	0.56
1:D:395:LYS:HB2	1:D:407:GLN:HB2	1.86	0.56
1:B:342:ASP:OD1	1:B:372:ALA:HB1	2.05	0.56
1:D:993:LEU:C	1:D:993:LEU:HD23	2.30	0.56
1:A:342:ASP:OD1	1:A:372:ALA:HB1	2.06	0.56
1:A:1007:ARG:HD3	9:A:2812:HOH:O	2.06	0.56
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.87	0.56
1:A:220:GLN:HG3	1:A:222:TYR:CZ	2.41	0.56
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.06	0.56
1:D:846:LEU:HD22	1:D:849:TRP:CE2	2.41	0.56
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.87	0.55
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.88	0.55
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.88	0.55
1:D:909:ARG:NH1	9:D:2572:HOH:O	2.39	0.55
1:C:877:PRO:HG3	1:C:977:THR:HB	1.89	0.55
1:D:642:MET:CE	1:D:675:MET:HE2	2.36	0.55
1:A:683:ALA:HB1	9:A:2567:HOH:O	2.06	0.55
1:A:642:MET:HE3	1:A:675:MET:HE2	1.88	0.55
1:D:678:ARG:HD3	9:D:2374:HOH:O	2.07	0.55
1:D:489:THR:O	1:D:493:VAL:HG23	2.06	0.55
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.89	0.55
1:D:439:GLY:HA2	5:D:1032:NDP:O2N	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ASN:H	1:C:264:ASN:ND2	1.97	0.54
1:D:916:LYS:HB2	1:D:917:PRO:HD2	1.89	0.54
1:C:410:ARG:HH12	1:D:427:VAL:CG1	2.20	0.54
1:D:669:LEU:O	1:D:685:GLY:HA3	2.07	0.54
1:A:896:ARG:NH2	1:A:900:GLN:HE22	2.05	0.54
1:B:409:VAL:HG21	1:B:423:GLU:HA	1.89	0.54
1:B:668:ASN:O	9:B:2601:HOH:O	2.18	0.54
1:B:613:ILE:HG22	6:B:1034:IDH:I5	2.77	0.54
1:C:291:ASP:OD1	1:C:293:ILE:HG12	2.08	0.54
1:C:722:ARG:O	1:C:726:GLU:HG3	2.06	0.54
1:D:613:ILE:HG21	1:D:642:MET:HE2	1.89	0.54
1:A:410:ARG:NH2	1:B:427:VAL:HG21	2.23	0.54
1:A:611:GLU:O	6:A:1033:IDH:H6C2	2.08	0.54
1:A:722:ARG:CZ	1:D:300:ASP:HB3	2.38	0.54
1:D:962:THR:HG21	1:D:995:VAL:HG11	1.90	0.54
1:B:132:THR:HB	1:B:137:VAL:HG23	1.90	0.53
1:B:990:THR:HG22	1:B:990:THR:O	2.08	0.53
1:C:342:ASP:OD1	1:C:372:ALA:HB1	2.08	0.53
1:C:613:ILE:HG21	1:C:642:MET:HE2	1.90	0.53
1:A:410:ARG:CZ	1:B:410:ARG:CZ	2.86	0.53
1:D:408:PHE:HB2	1:D:427:VAL:HB	1.91	0.53
1:D:759:ARG:HG2	1:D:759:ARG:HH11	1.73	0.53
1:A:56:GLU:OE2	1:A:895:MET:HE1	2.08	0.53
1:B:180:GLU:CD	1:B:180:GLU:H	2.17	0.53
1:C:845:GLU:HG3	1:C:912:PHE:CD2	2.43	0.53
1:B:95:LEU:HD21	1:B:116:ILE:HG23	1.91	0.53
1:D:288:PRO:HB3	1:D:307:LYS:HB2	1.91	0.53
1:A:394:ARG:HG3	1:A:409:VAL:HG13	1.90	0.53
1:B:669:LEU:O	1:B:685:GLY:HA3	2.09	0.53
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.39	0.53
1:C:672:PRO:HG3	9:C:2490:HOH:O	2.07	0.53
1:D:289:LYS:HD3	9:D:2664:HOH:O	2.09	0.53
1:D:95:LEU:HD23	1:D:119:ASP:HB2	1.90	0.53
1:A:410:ARG:CZ	1:B:410:ARG:HH22	2.22	0.53
1:B:342:ASP:CB	5:B:1032:NDP:H42N	2.37	0.53
1:B:722:ARG:O	1:B:726:GLU:HG3	2.09	0.53
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	1.91	0.53
1:A:82:CYS:O	1:A:98:LYS:HD2	2.09	0.52
1:B:844:GLU:O	1:B:847:GLN:HG3	2.08	0.52
1:A:644:SER:HA	1:A:680:MET:HG2	1.91	0.52
1:B:342:ASP:HB2	5:B:1032:NDP:C5N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ASP:CB	5:D:1032:NDP:H42N	2.38	0.52
9:A:2118:HOH:O	1:B:599:MET:HE1	2.09	0.52
1:B:650:TRP:HH2	9:B:2601:HOH:O	1.91	0.52
1:C:410:ARG:NE	1:D:410:ARG:NH2	2.56	0.52
1:D:458:ARG:NH1	9:D:2301:HOH:O	2.42	0.52
1:D:845:GLU:HG3	1:D:912:PHE:CD2	2.44	0.52
1:C:301:GLN:O	1:C:403:ILE:HG13	2.09	0.52
1:C:342:ASP:CB	5:C:1032:NDP:H42N	2.38	0.52
1:C:844:GLU:O	1:C:847:GLN:HG3	2.09	0.52
1:D:993:LEU:HD23	1:D:993:LEU:O	2.10	0.52
1:A:288:PRO:HB3	1:A:307:LYS:HB2	1.91	0.52
1:A:379:LEU:O	1:A:383:GLU:HG3	2.08	0.52
1:A:410:ARG:HG3	1:A:425:GLN:OE1	2.10	0.52
1:B:288:PRO:HB3	1:B:307:LYS:HB2	1.92	0.52
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.10	0.52
1:C:262:SER:HB3	1:C:264:ASN:ND2	2.25	0.52
1:A:388:LEU:CD1	1:A:429:LEU:HD21	2.39	0.52
1:A:53:GLU:HB2	9:A:2084:HOH:O	2.09	0.51
1:B:670:SER:HA	1:B:682:LEU:HD23	1.91	0.51
1:D:713:ASN:ND2	9:D:2465:HOH:O	2.36	0.51
1:B:409:VAL:CG2	1:B:422:ASP:O	2.58	0.51
1:B:672:PRO:HG2	1:B:673:HIS:CD2	2.46	0.51
1:C:267:THR:HG22	9:C:2321:HOH:O	2.11	0.51
1:C:410:ARG:HE	1:D:410:ARG:CZ	2.22	0.51
1:C:711:THR:HG22	9:C:2491:HOH:O	2.10	0.51
1:D:642:MET:HE1	1:D:675:MET:CG	2.33	0.51
1:A:845:GLU:HG3	1:A:912:PHE:CD2	2.45	0.51
1:C:394:ARG:HG3	1:C:409:VAL:HG13	1.92	0.51
1:C:613:ILE:HG23	7:C:1034:IUR:I5	2.80	0.51
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.93	0.51
1:C:916:LYS:HB2	1:C:917:PRO:HD2	1.92	0.51
1:D:394:ARG:HG3	1:D:409:VAL:CG1	2.39	0.51
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.91	0.51
1:C:77:MET:HE1	1:D:599:MET:HG2	1.92	0.51
1:C:221:GLU:HG2	9:C:2211:HOH:O	2.09	0.51
1:C:859:HIS:HD2	1:C:862:GLY:N	2.05	0.51
1:A:289:LYS:HA	9:A:2401:HOH:O	2.11	0.51
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.11	0.51
1:A:720:ILE:HG13	9:A:2568:HOH:O	2.11	0.51
1:D:682:LEU:O	1:D:686:GLN:HG3	2.10	0.51
1:D:717:ILE:HG13	1:D:720:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:O	1:B:497:LYS:HE2	2.11	0.50
1:C:95:LEU:HD23	1:C:119:ASP:HB2	1.92	0.50
1:A:613:ILE:HD13	1:A:642:MET:HE2	1.92	0.50
1:C:410:ARG:HH22	1:D:427:VAL:CG2	2.20	0.50
1:A:779:THR:HG22	1:A:808:SER:HB3	1.94	0.50
1:C:100:PHE:CD1	1:C:100:PHE:C	2.90	0.50
1:C:896:ARG:HG2	1:C:896:ARG:HH11	1.75	0.50
1:D:404:VAL:O	1:D:405:ALA:HB2	2.12	0.50
1:A:193:LEU:HD12	1:A:261:LEU:HB2	1.93	0.50
1:D:391:LEU:HD22	1:D:427:VAL:HG21	1.93	0.50
1:A:669:LEU:O	1:A:685:GLY:HA3	2.11	0.50
1:C:131:PRO:HB3	1:C:373:VAL:HG11	1.93	0.50
1:D:293:ILE:CG2	1:D:394:ARG:O	2.60	0.50
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.45	0.50
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.93	0.50
1:D:219:LYS:HG3	1:D:260:SER:OG	2.12	0.50
1:A:642:MET:HE1	1:A:675:MET:HE2	1.93	0.50
1:C:262:SER:HB3	1:C:264:ASN:HD21	1.77	0.50
1:C:669:LEU:O	1:C:685:GLY:HA3	2.11	0.50
1:A:410:ARG:NE	1:B:410:ARG:HH22	2.10	0.50
1:A:599:MET:HG2	1:B:77:MET:HE1	1.93	0.50
1:A:411:THR:O	1:A:412:GLU:HB3	2.11	0.49
1:A:95:LEU:HD23	1:A:119:ASP:HB2	1.93	0.49
1:C:267:THR:HG22	1:C:268:LEU:N	2.27	0.49
1:D:44:ASN:HB2	1:D:45:PRO:CD	2.42	0.49
1:D:909:ARG:NH1	1:D:909:ARG:CG	2.74	0.49
1:A:779:THR:O	1:A:783:ARG:HG3	2.11	0.49
1:B:95:LEU:HD11	1:B:120:ASN:HB2	1.93	0.49
1:A:52:CYS:HB2	1:A:384:LYS:HG2	1.95	0.49
1:B:267:THR:OG1	1:B:270:THR:HG23	2.12	0.49
1:C:410:ARG:CZ	1:D:410:ARG:NH1	2.75	0.49
1:C:642:MET:HE1	1:C:675:MET:CG	2.37	0.49
1:B:220:GLN:HG3	1:B:222:TYR:CZ	2.48	0.49
1:C:56:GLU:OE2	1:C:895:MET:HE1	2.13	0.49
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.43	0.49
1:A:74:ARG:CZ	1:B:599:MET:HE2	2.43	0.49
1:A:722:ARG:NH1	1:D:300:ASP:HB3	2.28	0.49
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.95	0.49
1:D:613:ILE:HD13	1:D:642:MET:HE2	1.93	0.49
1:A:497:LYS:HE2	1:B:27:ALA:O	2.13	0.49
1:C:288:PRO:HB3	1:C:307:LYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:TRP:O	1:B:460:ASP:HB2	2.13	0.49
1:D:735:THR:N	1:D:793:THR:HG23	2.28	0.49
1:A:902:ALA:O	1:A:903:ALA:C	2.55	0.48
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.95	0.48
1:D:342:ASP:OD1	1:D:372:ALA:HB1	2.13	0.48
1:B:82:CYS:O	1:B:98:LYS:HD2	2.13	0.48
1:C:53:GLU:CD	1:C:887:LYS:HB3	2.38	0.48
1:D:309:PHE:CE1	1:D:331:ILE:HD11	2.49	0.48
1:A:993:LEU:C	1:A:993:LEU:HD23	2.38	0.48
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.48	0.48
1:D:672:PRO:HG3	1:D:737:THR:OG1	2.13	0.48
1:B:676:GLY:HA2	1:B:680:MET:O	2.13	0.48
1:C:410:ARG:HH11	1:D:427:VAL:HG13	1.71	0.48
1:B:672:PRO:HA	1:B:682:LEU:CD1	2.43	0.48
1:B:699:ARG:HA	1:B:699:ARG:NE	2.28	0.48
1:A:410:ARG:CZ	1:B:410:ARG:NH1	2.76	0.48
1:D:672:PRO:HG2	1:D:673:HIS:ND1	2.28	0.48
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.14	0.48
1:B:132:THR:HB	1:B:137:VAL:CG2	2.44	0.48
1:B:779:THR:O	1:B:783:ARG:HG3	2.14	0.48
1:C:193:LEU:N	1:C:193:LEU:HD22	2.29	0.48
1:C:993:LEU:HD23	1:C:993:LEU:C	2.39	0.48
1:B:294:PHE:HA	1:B:297:LEU:HD12	1.96	0.47
1:C:379:LEU:O	1:C:383:GLU:HG3	2.14	0.47
1:B:178:SER:OG	1:B:181:LYS:HG3	2.14	0.47
1:B:734:ALA:HA	1:B:735:THR:HA	1.65	0.47
1:B:993:LEU:C	1:B:993:LEU:HD23	2.39	0.47
1:C:677:GLU:CD	1:D:934:THR:HB	2.39	0.47
1:C:877:PRO:HD2	1:C:882:TYR:CB	2.44	0.47
1:D:220:GLN:HG3	1:D:222:TYR:CZ	2.49	0.47
1:C:220:GLN:HG3	1:C:222:TYR:CZ	2.49	0.47
1:A:259:LYS:HE2	9:A:2287:HOH:O	2.13	0.47
1:A:386:GLU:OE1	1:B:367:PHE:HB2	2.14	0.47
1:B:325:HIS:HA	9:B:2363:HOH:O	2.14	0.47
1:C:126:CYS:HB3	1:C:130:CYS:SG	2.55	0.47
1:D:294:PHE:HA	1:D:297:LEU:HD12	1.97	0.47
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.45	0.47
1:D:293:ILE:HG21	1:D:394:ARG:O	2.15	0.47
1:D:990:THR:HG22	1:D:990:THR:O	2.14	0.47
1:A:319:ALA:CB	1:A:904:PHE:HB3	2.45	0.47
1:A:621:TRP:O	1:A:625:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.50	0.47
1:A:373:VAL:HG23	1:A:375:GLU:OE1	2.15	0.47
1:B:845:GLU:CD	1:B:845:GLU:H	2.21	0.47
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.95	0.47
1:C:497:LYS:HE2	1:D:27:ALA:O	2.15	0.47
1:D:396:VAL:HG13	1:D:403:ILE:CD1	2.45	0.47
1:D:750:PRO:O	1:D:753:ALA:HB2	2.14	0.47
1:B:845:GLU:HG3	1:B:912:PHE:CE2	2.50	0.47
1:C:410:ARG:NE	1:D:410:ARG:CZ	2.78	0.47
1:B:682:LEU:O	1:B:683:ALA:C	2.58	0.47
1:D:845:GLU:HG3	1:D:912:PHE:CE2	2.50	0.47
1:C:50:PHE:CE2	1:D:369:ASN:HA	2.50	0.47
1:C:734:ALA:HA	1:C:735:THR:HA	1.70	0.47
1:A:845:GLU:HG3	1:A:912:PHE:CE2	2.49	0.46
1:B:241:VAL:O	1:B:245:ILE:HG12	2.16	0.46
1:D:191:ALA:O	1:D:279:ALA:HA	2.16	0.46
1:D:307:LYS:HE3	9:D:2281:HOH:O	2.15	0.46
1:A:442:LEU:HD22	1:A:482:ILE:CD1	2.45	0.46
1:B:100:PHE:CD1	1:B:100:PHE:C	2.93	0.46
1:B:846:LEU:HD22	1:B:849:TRP:CE2	2.50	0.46
1:C:413:GLN:HG3	1:C:419:TRP:CE2	2.50	0.46
1:A:451:LEU:O	1:A:454:ILE:HG12	2.16	0.46
1:B:126:CYS:HB3	1:B:130:CYS:SG	2.55	0.46
1:C:896:ARG:HG2	1:C:896:ARG:NH1	2.30	0.46
1:D:131:PRO:HB3	1:D:373:VAL:HG11	1.97	0.46
1:D:793:THR:HB	1:D:814:GLN:HB2	1.97	0.46
1:A:326:SER:HB3	9:A:2345:HOH:O	2.15	0.46
1:B:839:TYR:HA	1:B:918:ILE:HD12	1.98	0.46
1:C:375:GLU:CD	1:C:375:GLU:H	2.23	0.46
1:D:900:GLN:C	1:D:902:ALA:H	2.23	0.46
1:C:64:HIS:HE1	1:C:382:GLU:OE2	1.98	0.46
1:D:371:ARG:HE	1:D:371:ARG:HB2	1.48	0.46
1:C:750:PRO:O	1:C:753:ALA:HB2	2.14	0.46
1:A:74:ARG:NH1	1:B:599:MET:HE2	2.31	0.46
1:A:775:LEU:HD12	9:B:2646:HOH:O	2.16	0.46
1:A:783:ARG:HD3	9:A:2623:HOH:O	2.15	0.46
1:B:533:ILE:O	1:B:545:PRO:HD3	2.16	0.46
1:B:642:MET:HE2	9:B:2602:HOH:O	2.15	0.46
1:B:915:LYS:HG3	9:B:2702:HOH:O	2.16	0.46
1:C:735:THR:N	1:C:793:THR:HG23	2.31	0.46
1:D:642:MET:HG2	1:D:680:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:CYS:O	1:C:98:LYS:HD2	2.16	0.46
1:C:644:SER:HA	1:C:679:GLY:O	2.16	0.46
1:A:331:ILE:HG23	1:A:433:VAL:HG21	1.98	0.46
1:A:191:ALA:O	1:A:279:ALA:HA	2.16	0.45
1:B:297:LEU:HA	1:B:301:GLN:OE1	2.15	0.45
1:C:219:LYS:HG3	1:C:260:SER:OG	2.17	0.45
1:D:899:GLU:OE1	1:D:899:GLU:HA	2.15	0.45
1:A:342:ASP:HB2	5:A:1032:NDP:C5N	2.46	0.45
1:B:140:CYS:HA	2:B:1027:SF4:S3	2.57	0.45
1:B:191:ALA:O	1:B:279:ALA:HA	2.16	0.45
1:B:613:ILE:CG2	6:B:1034:IDH:I5	3.35	0.45
1:C:934:THR:HB	1:D:677:GLU:OE2	2.15	0.45
1:D:132:THR:HB	1:D:137:VAL:HG23	1.98	0.45
1:C:776:ARG:O	1:C:780:THR:HG22	2.16	0.45
1:A:83:ALA:O	1:A:84:ASP:C	2.59	0.45
1:A:342:ASP:CB	5:A:1032:NDP:C5N	2.94	0.45
1:B:735:THR:N	1:B:793:THR:HG23	2.32	0.45
1:C:267:THR:HG22	1:C:269:ASN:H	1.80	0.45
1:A:12:ILE:O	1:A:15:ILE:HG22	2.16	0.45
1:B:570:PHE:HB3	1:B:636:ILE:HB	1.99	0.45
1:B:859:HIS:CD2	1:B:862:GLY:H	2.19	0.45
1:C:53:GLU:HG2	1:C:54:LYS:N	2.32	0.45
1:D:917:PRO:HA	9:D:2577:HOH:O	2.17	0.45
1:D:362:VAL:HG11	1:D:408:PHE:CE2	2.52	0.45
1:D:342:ASP:HB2	5:D:1032:NDP:C5N	2.47	0.45
9:A:2431:HOH:O	1:B:35:LYS:HE2	2.17	0.45
1:C:457:ASN:HB3	1:C:463:GLU:OE1	2.17	0.45
1:C:820:GLN:O	1:D:962:THR:CG2	2.64	0.45
1:A:100:PHE:CD1	1:A:100:PHE:C	2.95	0.45
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.99	0.45
1:B:845:GLU:HG3	1:B:912:PHE:CD2	2.52	0.45
1:C:410:ARG:HH21	1:D:410:ARG:NE	2.15	0.45
1:C:608:LEU:HB2	1:C:742:MET:HE2	1.99	0.45
1:D:621:TRP:O	1:D:625:VAL:HG23	2.17	0.45
1:D:934:THR:OG1	1:D:937:GLU:HG3	2.17	0.45
1:A:533:ILE:O	1:A:545:PRO:HD3	2.17	0.44
1:B:643:CYS:C	1:B:680:MET:HE2	2.42	0.44
1:B:759:ARG:HG2	1:B:759:ARG:HH11	1.82	0.44
1:D:19:ASN:OD1	1:D:20:PRO:HD2	2.17	0.44
1:D:242:ASN:ND2	9:D:2215:HOH:O	2.50	0.44
1:A:750:PRO:O	1:A:753:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:ALA:HB3	1:C:553:PRO:HD3	2.00	0.44
1:A:783:ARG:NE	9:A:2624:HOH:O	2.49	0.44
1:C:574:LYS:HE3	9:C:2386:HOH:O	2.17	0.44
1:A:722:ARG:HD3	1:D:300:ASP:HB3	1.98	0.44
1:C:572:LEU:HD13	1:C:638:ILE:HB	1.99	0.44
1:D:699:ARG:NE	1:D:699:ARG:HA	2.32	0.44
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.56	0.44
1:A:309:PHE:CE1	1:A:331:ILE:HD11	2.53	0.44
1:A:776:ARG:O	1:A:780:THR:HG22	2.17	0.44
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.87	0.44
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.57	0.44
1:D:326:SER:HA	1:D:327:PRO:HD3	1.83	0.44
1:C:132:THR:HB	1:C:137:VAL:HG23	1.99	0.44
1:C:375:GLU:HG2	9:C:2151:HOH:O	2.17	0.44
1:D:703:GLN:HG3	9:D:2461:HOH:O	2.18	0.44
1:A:28:LEU:HD22	1:B:519:PRO:HB3	1.98	0.44
1:C:845:GLU:CD	1:C:845:GLU:H	2.25	0.44
1:D:225:GLY:HA2	4:D:1031:FAD:H3B	2.00	0.44
1:A:146:GLU:HG2	1:B:67:LEU:HD23	2.00	0.44
1:A:375:GLU:H	1:A:375:GLU:CD	2.26	0.44
1:A:771:ARG:N	1:A:772:PRO:CD	2.80	0.44
1:A:7:LYS:HE3	9:B:2563:HOH:O	2.17	0.44
1:B:150:ILE:HB	2:B:1027:SF4:S4	2.58	0.44
1:B:793:THR:HB	1:B:814:GLN:HB2	1.99	0.44
1:D:301:GLN:HA	1:D:402:ARG:HA	2.00	0.44
1:D:413:GLN:HA	1:D:418:LYS:O	2.18	0.44
1:B:692:ARG:HD2	9:B:2615:HOH:O	2.18	0.43
1:C:191:ALA:O	1:C:279:ALA:HA	2.18	0.43
1:C:675:MET:HE3	1:C:678:ARG:HD3	2.00	0.43
1:B:570:PHE:CB	1:B:636:ILE:HB	2.48	0.43
1:D:265:GLU:HB3	1:D:266:ILE:H	1.48	0.43
1:C:779:THR:O	1:C:783:ARG:HG3	2.17	0.43
1:D:451:LEU:O	1:D:454:ILE:HG12	2.19	0.43
1:D:900:GLN:HB3	9:D:2570:HOH:O	2.17	0.43
1:B:934:THR:OG1	1:B:937:GLU:HG3	2.18	0.43
1:D:293:ILE:HG21	1:D:394:ARG:C	2.43	0.43
1:A:371:ARG:NH1	1:A:371:ARG:HB2	2.33	0.43
1:C:427:VAL:HG21	1:D:410:ARG:NH2	2.10	0.43
1:C:915:LYS:HG3	9:C:2560:HOH:O	2.19	0.43
1:D:375:GLU:H	1:D:375:GLU:CD	2.27	0.43
1:D:570:PHE:HB3	1:D:636:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:THR:HB	1:B:677:GLU:CD	2.43	0.43
1:B:83:ALA:O	1:B:84:ASP:C	2.62	0.43
1:B:219:LYS:HG3	1:B:260:SER:OG	2.19	0.43
1:B:373:VAL:HG22	1:B:376:GLU:H	1.84	0.43
1:C:771:ARG:N	1:C:772:PRO:CD	2.82	0.43
1:C:793:THR:HB	1:C:814:GLN:HB2	2.00	0.43
1:D:759:ARG:HG2	1:D:759:ARG:NH1	2.33	0.43
1:A:7:LYS:HE2	9:B:2259:HOH:O	2.19	0.43
1:A:570:PHE:HB3	1:A:636:ILE:HB	2.00	0.43
1:A:905:PRO:HA	1:A:906:PRO:HD3	1.92	0.43
1:B:201:SER:HB2	1:B:493:VAL:HG13	2.00	0.43
1:C:140:CYS:HA	2:C:1027:SF4:S3	2.59	0.43
1:C:342:ASP:CB	5:C:1032:NDP:C5N	2.97	0.43
1:D:845:GLU:CD	1:D:845:GLU:H	2.26	0.43
1:B:847:GLN:HG2	9:B:2706:HOH:O	2.19	0.43
1:C:651:MET:HE3	1:C:700:GLN:HG3	2.01	0.43
1:D:998:ILE:HB	1:D:1001:CYS:HB2	2.01	0.43
1:B:859:HIS:HA	1:B:865:VAL:HG23	2.01	0.42
1:D:779:THR:O	1:D:783:ARG:HG3	2.19	0.42
1:C:342:ASP:HB2	5:C:1032:NDP:C5N	2.50	0.42
1:D:734:ALA:HA	1:D:735:THR:HA	1.71	0.42
1:A:342:ASP:HB3	5:A:1032:NDP:C4N	2.41	0.42
1:B:670:SER:N	9:B:2602:HOH:O	2.52	0.42
1:C:248:MET:HE1	1:C:255:ILE:HD11	2.02	0.42
1:C:378:GLU:O	1:C:382:GLU:CG	2.66	0.42
1:D:459:TRP:O	1:D:460:ASP:HB2	2.19	0.42
1:D:533:ILE:O	1:D:545:PRO:HD3	2.18	0.42
1:A:916:LYS:HB2	1:A:917:PRO:HD2	2.01	0.42
1:B:88:GLN:HG3	1:B:95:LEU:O	2.19	0.42
1:C:577:SER:HB2	9:C:2405:HOH:O	2.19	0.42
1:C:893:GLU:O	1:C:897:LEU:HG	2.19	0.42
1:D:97:ILE:HA	1:D:100:PHE:CD2	2.53	0.42
1:B:342:ASP:CB	5:B:1032:NDP:C5N	2.97	0.42
1:B:608:LEU:C	1:B:608:LEU:HD23	2.44	0.42
1:C:90:SER:HB2	1:C:136:CYS:HA	2.00	0.42
1:C:267:THR:HG21	9:C:2320:HOH:O	2.20	0.42
1:C:570:PHE:HB3	1:C:636:ILE:HB	2.01	0.42
1:D:319:ALA:HB2	1:D:904:PHE:CB	2.49	0.42
1:B:311:PRO:O	1:B:315:LYS:HG3	2.20	0.42
1:C:150:ILE:HB	2:C:1027:SF4:S4	2.60	0.42
1:B:541:LYS:HB3	9:B:2499:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.20	0.42
1:C:877:PRO:CG	1:C:977:THR:HB	2.48	0.42
1:D:132:THR:HB	1:D:137:VAL:CG2	2.49	0.42
1:D:711:THR:CG2	9:D:2454:HOH:O	2.58	0.42
1:D:836:ALA:O	1:D:840:LEU:HG	2.19	0.42
1:A:367:PHE:HB2	1:B:386:GLU:OE1	2.20	0.42
1:D:398:VAL:HG13	1:D:402:ARG:C	2.43	0.42
1:A:836:ALA:O	1:A:840:LEU:HG	2.19	0.42
1:C:699:ARG:HA	1:C:699:ARG:NE	2.33	0.42
1:C:771:ARG:HD2	9:D:2384:HOH:O	2.18	0.42
1:D:150:ILE:HB	2:D:1027:SF4:S4	2.60	0.42
1:D:342:ASP:CB	5:D:1032:NDP:C5N	2.98	0.42
1:B:671:CYS:SG	1:B:673:HIS:O	2.78	0.42
1:C:64:HIS:CE1	1:C:382:GLU:OE2	2.73	0.42
1:C:262:SER:CB	1:C:264:ASN:ND2	2.83	0.42
1:B:442:LEU:HD22	1:B:482:ILE:CD1	2.48	0.41
1:C:342:ASP:HB3	5:C:1032:NDP:C4N	2.43	0.41
1:D:574:LYS:HE3	9:D:2358:HOH:O	2.20	0.41
1:A:97:ILE:HD11	2:A:1026:SF4:S4	2.60	0.41
1:A:142:LEU:HD12	1:A:150:ILE:HG12	2.02	0.41
1:A:297:LEU:HA	1:A:301:GLN:OE1	2.21	0.41
1:B:647:LYS:O	1:B:651:MET:HG3	2.20	0.41
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.55	0.41
1:D:164:LYS:O	1:D:909:ARG:NH2	2.53	0.41
1:A:962:THR:OG1	1:A:995:VAL:HG21	2.20	0.41
1:B:106:ASN:O	1:B:107:LYS:HB2	2.20	0.41
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.87	0.41
1:C:116:ILE:HD13	1:C:156:GLN:HG3	2.02	0.41
1:C:541:LYS:HD3	9:C:2096:HOH:O	2.20	0.41
1:C:816:CYS:HB3	3:C:1030:FMN:O1P	2.20	0.41
1:D:44:ASN:HB2	1:D:45:PRO:HD2	2.02	0.41
1:D:261:LEU:HD21	1:D:451:LEU:HD21	2.00	0.41
1:B:49:CYS:SG	1:B:51:HIS:CE1	3.13	0.41
1:D:243:PHE:HD1	1:D:909:ARG:HE	1.68	0.41
1:D:400:GLY:C	1:D:402:ARG:H	2.29	0.41
1:D:910:LYS:HA	1:D:911:PRO:HD3	1.93	0.41
1:A:241:VAL:O	1:A:245:ILE:HG12	2.21	0.41
1:A:651:MET:HG2	1:A:701:ALA:HB2	2.02	0.41
1:D:124:LEU:HG	1:D:240:VAL:HG13	2.03	0.41
1:D:126:CYS:HB3	1:D:130:CYS:SG	2.61	0.41
1:D:402:ARG:HG3	9:D:2286:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:VAL:HG21	1:A:720:ILE:CG2	2.50	0.41
1:B:452:SER:HA	1:B:453:PRO:HA	1.87	0.41
1:B:644:SER:HA	1:B:680:MET:HG2	2.03	0.41
1:C:83:ALA:O	1:C:84:ASP:C	2.61	0.41
1:C:831:CYS:O	1:C:835:LYS:HG3	2.20	0.41
1:A:672:PRO:HG3	1:A:737:THR:OG1	2.21	0.41
1:A:709:LYS:HA	1:A:733:THR:HB	2.03	0.41
1:C:589:ARG:O	1:C:609:ASN:HA	2.21	0.41
1:D:83:ALA:O	1:D:84:ASP:C	2.63	0.41
1:D:331:ILE:HG23	1:D:433:VAL:HG21	2.02	0.41
1:D:608:LEU:HD23	1:D:608:LEU:C	2.46	0.41
1:C:132:THR:HB	1:C:137:VAL:CG2	2.49	0.41
1:D:319:ALA:CB	1:D:904:PHE:CB	2.90	0.41
1:A:18:LEU:HD11	1:A:975:PRO:HB3	2.02	0.41
1:A:371:ARG:HB2	1:A:371:ARG:HH11	1.86	0.41
1:A:489:THR:O	1:A:493:VAL:HG23	2.20	0.41
1:B:100:PHE:O	1:B:104:ILE:HG13	2.21	0.41
1:B:262:SER:HG	1:B:446:LYS:HB3	1.85	0.41
1:B:911:PRO:HG2	9:B:2760:HOH:O	2.21	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.03	0.41
1:C:44:ASN:HB2	1:C:45:PRO:HD2	2.02	0.41
1:C:264:ASN:HD22	1:C:264:ASN:N	1.95	0.41
1:C:413:GLN:HA	1:C:418:LYS:O	2.21	0.41
1:C:921:ILE:O	1:C:925:ILE:HG13	2.21	0.41
1:D:100:PHE:CD1	1:D:100:PHE:C	2.99	0.41
1:D:692:ARG:HG2	9:D:2458:HOH:O	2.20	0.41
1:A:722:ARG:O	1:A:726:GLU:HG3	2.21	0.41
1:A:762:TYR:CE1	1:B:780:THR:HG22	2.55	0.41
1:B:671:CYS:O	1:B:682:LEU:HG	2.22	0.41
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.56	0.41
1:A:703:GLN:HG3	9:A:2578:HOH:O	2.20	0.40
1:B:225:GLY:HA2	4:B:1031:FAD:H3B	2.04	0.40
1:B:776:ARG:NE	9:B:2663:HOH:O	2.53	0.40
1:B:807:HIS:HB3	1:B:928:ALA:HB2	2.02	0.40
1:C:124:LEU:HD13	1:C:160:SER:HB2	2.03	0.40
1:C:410:ARG:NH1	1:D:427:VAL:CG2	2.68	0.40
1:D:193:LEU:HD22	1:D:193:LEU:N	2.36	0.40
1:D:403:ILE:HD13	1:D:434:VAL:HG23	2.01	0.40
1:D:911:PRO:HG2	9:D:2220:HOH:O	2.20	0.40
1:C:248:MET:CE	1:C:255:ILE:HD11	2.51	0.40
1:A:124:LEU:HG	1:A:240:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:CYS:SG	1:B:97:ILE:HD12	2.61	0.40
1:B:193:LEU:N	1:B:193:LEU:HD22	2.36	0.40
1:D:577:SER:HB2	9:D:2415:HOH:O	2.21	0.40
1:C:297:LEU:HA	1:C:301:GLN:OE1	2.20	0.40
1:C:682:LEU:CD1	1:C:711:THR:HG21	2.51	0.40
1:D:311:PRO:O	1:D:315:LYS:HG3	2.21	0.40
1:D:403:ILE:HG12	1:D:404:VAL:N	2.36	0.40
1:D:410:ARG:NH1	1:D:410:ARG:CG	2.76	0.40
1:D:518:LYS:O	1:D:520:GLU:HG3	2.21	0.40
1:C:489:THR:O	1:C:493:VAL:HG23	2.21	0.40
1:C:608:LEU:C	1:C:608:LEU:HD23	2.45	0.40
1:D:152:ILE:HD11	2:D:1027:SF4:S4	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1017/1025 (99%)	974 (96%)	40 (4%)	3 (0%)	36	40
1	B	1008/1025 (98%)	961 (95%)	45 (4%)	2 (0%)	43	50
1	C	1011/1025 (99%)	973 (96%)	36 (4%)	2 (0%)	43	50
1	D	1017/1025 (99%)	968 (95%)	48 (5%)	1 (0%)	48	56
All	All	4053/4100 (99%)	3876 (96%)	169 (4%)	8 (0%)	43	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	GLU
1	A	53	GLU
1	A	906	PRO

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Mol	Chain	Res	Type
1	C	674	GLY
1	B	3	PRO
1	D	902	ALA
1	A	674	GLY
1	C	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	848/854 (99%)	837 (99%)	11 (1%)	61	72
1	B	843/854 (99%)	826 (98%)	17 (2%)	48	59
1	C	845/854 (99%)	829 (98%)	16 (2%)	50	61
1	D	848/854 (99%)	832 (98%)	16 (2%)	50	61
All	All	3384/3416 (99%)	3324 (98%)	60 (2%)	51	63

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	100	PHE
1	A	265	GLU
1	A	367	PHE
1	A	373	VAL
1	A	453	PRO
1	A	667	LEU
1	A	793	THR
1	A	800	GLU
1	A	845	GLU
1	A	896	ARG
1	B	15	ILE
1	B	100	PHE
1	B	292	ASP
1	B	367	PHE
1	B	368	VAL

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Mol	Chain	Res	Type
1	B	373	VAL
1	B	378	GLU
1	B	394	ARG
1	B	412	GLU
1	B	426	ILE
1	B	453	PRO
1	B	599	MET
1	B	793	THR
1	B	800	GLU
1	B	845	GLU
1	B	916	LYS
1	B	984	ASP
1	C	15	ILE
1	C	100	PHE
1	C	184	GLU
1	C	264	ASN
1	C	330	SER
1	C	367	PHE
1	C	373	VAL
1	C	382	GLU
1	C	453	PRO
1	C	667	LEU
1	C	678	ARG
1	C	703	GLN
1	C	793	THR
1	C	800	GLU
1	C	845	GLU
1	C	1009	THR
1	D	11	ASP
1	D	15	ILE
1	D	100	PHE
1	D	179	GLN
1	D	263	GLU
1	D	293	ILE
1	D	373	VAL
1	D	376	GLU
1	D	410	ARG
1	D	428	HIS
1	D	453	PRO
1	D	680	MET
1	D	741	LEU
1	D	793	THR

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Mol	Chain	Res	Type
1	D	800	GLU
1	D	845	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	299	GLN
1	A	703	GLN
1	A	878	ASN
1	A	885	GLN
1	A	900	GLN
1	A	901	ASN
1	B	51	HIS
1	B	64	HIS
1	B	170	GLN
1	B	407	GLN
1	B	498	GLN
1	B	673	HIS
1	B	859	HIS
1	B	878	ASN
1	B	885	GLN
1	C	25	HIS
1	C	64	HIS
1	C	170	GLN
1	C	264	ASN
1	C	299	GLN
1	C	498	GLN
1	C	859	HIS
1	D	57	ASN
1	D	179	GLN
1	D	325	HIS
1	D	494	ASN
1	D	498	GLN
1	D	686	GLN
1	D	703	GLN

5.3.3 RNA ⓘ

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](#)

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$
5	NDP	D	1032	-	51,52,52	1.60	8 (15%)	71,80,80	1.49	14 (19%)
2	SF4	A	1029	-	0,12,12	-	-	-		
2	SF4	D	1027	-	0,12,12	-	-	-		
2	SF4	A	1028	-	0,12,12	-	-	-		
5	NDP	A	1032	-	51,52,52	1.61	8 (15%)	71,80,80	1.52	15 (21%)
2	SF4	B	1028	-	0,12,12	-	-	-		
2	SF4	A	1027	-	0,12,12	-	-	-		
8	URA	D	1034	-	8,8,8	1.43	1 (12%)	10,10,10	1.85	4 (40%)
2	SF4	B	1029	-	0,12,12	-	-	-		
7	IUR	C	1034	-	9,9,9	1.79	3 (33%)	11,12,12	2.09	3 (27%)
2	SF4	C	1028	-	0,12,12	-	-	-		
6	IDH	B	1034	-	6,9,9	1.92	2 (33%)	9,12,12	2.49	4 (44%)
4	FAD	D	1031	-	58,58,58	2.44	24 (41%)	85,89,89	1.69	9 (10%)
4	FAD	A	1031	-	58,58,58	2.38	25 (43%)	85,89,89	1.69	9 (10%)
2	SF4	D	1029	-	0,12,12	-	-	-		
2	SF4	C	1027	-	0,12,12	-	-	-		
5	NDP	B	1032	-	51,52,52	1.55	7 (13%)	71,80,80	1.48	14 (19%)
3	FMN	B	1030	-	33,33,33	1.94	10 (30%)	48,50,50	1.90	13 (27%)
2	SF4	C	1029	-	0,12,12	-	-	-		
3	FMN	A	1030	-	33,33,33	1.95	9 (27%)	48,50,50	1.85	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	B	1031	-	58,58,58	2.38	21 (36%)	85,89,89	1.68	11 (12%)
4	FAD	C	1031	-	58,58,58	2.37	23 (39%)	85,89,89	1.69	10 (11%)
3	FMN	D	1030	-	33,33,33	1.96	9 (27%)	48,50,50	1.87	13 (27%)
2	SF4	C	1026	-	0,12,12	-	-	-	-	-
2	SF4	D	1026	-	0,12,12	-	-	-	-	-
6	IDH	A	1033	-	8,8,9	2.24	3 (37%)	10,10,12	1.12	0
5	NDP	C	1032	-	51,52,52	1.63	9 (17%)	71,80,80	1.49	14 (19%)
2	SF4	B	1027	-	0,12,12	-	-	-	-	-
2	SF4	A	1026	-	0,12,12	-	-	-	-	-
3	FMN	C	1030	-	33,33,33	1.99	9 (27%)	48,50,50	1.88	12 (25%)
2	SF4	D	1028	-	0,12,12	-	-	-	-	-
2	SF4	B	1026	-	0,12,12	-	-	-	-	-

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
5	NDP	D	1032	-	-	6/34/77/77	0/5/5/5
2	SF4	A	1029	-	-	-	0/6/5/5
2	SF4	D	1027	-	-	-	0/6/5/5
2	SF4	A	1028	-	-	-	0/6/5/5
5	NDP	A	1032	-	-	6/34/77/77	0/5/5/5
2	SF4	B	1028	-	-	-	0/6/5/5
2	SF4	A	1027	-	-	-	0/6/5/5
8	URA	D	1034	-	-	-	0/1/1/1
2	SF4	B	1029	-	-	-	0/6/5/5
7	IUR	C	1034	-	-	-	0/1/1/1
2	SF4	C	1028	-	-	-	0/6/5/5
6	IDH	B	1034	-	-	-	0/1/1/1
4	FAD	D	1031	-	-	3/34/50/50	0/6/6/6
4	FAD	A	1031	-	-	3/34/50/50	0/6/6/6
2	SF4	D	1029	-	-	-	0/6/5/5
2	SF4	C	1027	-	-	-	0/6/5/5
5	NDP	B	1032	-	-	6/34/77/77	0/5/5/5
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1029	-	-	-	0/6/5/5
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
4	FAD	B	1031	-	-	6/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	C	1031	-	-	5/34/50/50	0/6/6/6
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1026	-	-	-	0/6/5/5
2	SF4	D	1026	-	-	-	0/6/5/5
6	IDH	A	1033	-	-	-	0/1/1/1
5	NDP	C	1032	-	-	5/34/77/77	0/5/5/5
2	SF4	B	1027	-	-	-	0/6/5/5
2	SF4	A	1026	-	-	-	0/6/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1028	-	-	-	0/6/5/5
2	SF4	B	1026	-	-	-	0/6/5/5

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	PA-O3P	9.95	1.70	1.59
4	C	1031	FAD	P-O3P	-8.47	1.50	1.59
4	A	1031	FAD	PA-O3P	8.36	1.68	1.59
4	B	1031	FAD	P-O3P	-8.23	1.50	1.59
4	B	1031	FAD	PA-O3P	8.18	1.68	1.59
4	A	1031	FAD	P-O3P	-8.11	1.50	1.59
4	C	1031	FAD	PA-O3P	7.64	1.67	1.59
4	D	1031	FAD	P-O3P	-7.22	1.51	1.59
5	B	1032	NDP	C4N-C3N	-5.25	1.40	1.50
5	D	1032	NDP	C4N-C3N	-5.07	1.40	1.50
5	A	1032	NDP	C4N-C3N	-5.07	1.40	1.50
5	C	1032	NDP	C4N-C3N	-5.06	1.40	1.50
3	C	1030	FMN	C4A-N5	4.59	1.40	1.30
3	A	1030	FMN	C4A-N5	4.58	1.40	1.30
3	D	1030	FMN	C4A-N5	4.58	1.40	1.30
3	C	1030	FMN	C7M-C7	4.53	1.59	1.51
3	A	1030	FMN	C7M-C7	4.39	1.59	1.51
5	B	1032	NDP	C4N-C5N	-4.31	1.37	1.49
3	B	1030	FMN	C4A-N5	4.30	1.40	1.30
3	D	1030	FMN	C7M-C7	4.29	1.59	1.51
5	C	1032	NDP	C4N-C5N	-4.29	1.37	1.49
5	A	1032	NDP	C4N-C5N	-4.24	1.38	1.49
4	B	1031	FAD	PA-O2A	-4.23	1.35	1.55
3	B	1030	FMN	C7M-C7	4.22	1.58	1.51
5	D	1032	NDP	C4N-C5N	-4.21	1.38	1.49
4	D	1031	FAD	PA-O2A	-4.08	1.36	1.55
4	A	1031	FAD	PA-O2A	-4.06	1.36	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1031	FAD	PA-O2A	-4.04	1.36	1.55
6	A	1033	IDH	O4-C4	3.80	1.30	1.23
6	A	1033	IDH	O2-C2	3.78	1.31	1.23
3	B	1030	FMN	C1'-N10	-3.77	1.38	1.47
5	D	1032	NDP	C2N-C3N	3.74	1.45	1.35
3	D	1030	FMN	C4'-C3'	3.68	1.59	1.53
5	A	1032	NDP	C2N-C3N	3.68	1.45	1.35
4	D	1031	FAD	C9A-N10	3.67	1.47	1.41
3	A	1030	FMN	C1'-N10	-3.67	1.39	1.47
4	C	1031	FAD	C9A-N10	3.66	1.47	1.41
5	B	1032	NDP	C2N-C3N	3.66	1.45	1.35
5	C	1032	NDP	C2N-C3N	3.65	1.45	1.35
4	B	1031	FAD	C9A-N10	3.65	1.47	1.41
3	A	1030	FMN	C4'-C3'	3.60	1.59	1.53
3	C	1030	FMN	C4'-C3'	3.57	1.59	1.53
4	D	1031	FAD	C4X-N5	3.56	1.38	1.30
7	C	1034	IUR	C2-N1	3.56	1.41	1.36
3	D	1030	FMN	C1'-N10	-3.54	1.39	1.47
3	C	1030	FMN	C1'-N10	-3.53	1.39	1.47
4	A	1031	FAD	C9A-N10	3.49	1.47	1.41
4	B	1031	FAD	P-O2P	-3.48	1.39	1.55
4	B	1031	FAD	C4X-N5	3.48	1.38	1.30
4	C	1031	FAD	P-O2P	-3.43	1.39	1.55
4	C	1031	FAD	C4X-N5	3.36	1.38	1.30
4	A	1031	FAD	P-O2P	-3.34	1.39	1.55
4	A	1031	FAD	C4X-N5	3.33	1.38	1.30
4	D	1031	FAD	P-O2P	-3.31	1.40	1.55
3	C	1030	FMN	C9A-N10	3.22	1.46	1.41
3	B	1030	FMN	C4'-C3'	3.20	1.59	1.53
4	B	1031	FAD	C8-C7	3.19	1.48	1.40
4	D	1031	FAD	C9A-C5X	3.18	1.46	1.41
4	C	1031	FAD	C9A-C5X	3.16	1.46	1.41
3	B	1030	FMN	C9A-C5A	3.16	1.46	1.41
3	B	1030	FMN	C9A-N10	3.15	1.46	1.41
3	C	1030	FMN	C9A-C5A	3.14	1.46	1.41
4	B	1031	FAD	C9A-C5X	3.12	1.46	1.41
4	A	1031	FAD	C8-C7	3.11	1.48	1.40
4	C	1031	FAD	C8-C7	3.08	1.48	1.40
4	C	1031	FAD	O5'-C5'	3.06	1.56	1.44
4	A	1031	FAD	O5'-C5'	3.05	1.56	1.44
4	A	1031	FAD	C6-C5X	3.03	1.44	1.40
3	A	1030	FMN	C9A-C5A	3.00	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	C8-C7	2.97	1.48	1.40
3	D	1030	FMN	C9A-N10	2.97	1.46	1.41
3	D	1030	FMN	C9A-C5A	2.95	1.45	1.41
3	A	1030	FMN	C9A-N10	2.91	1.46	1.41
4	A	1031	FAD	C9A-C5X	2.91	1.45	1.41
3	C	1030	FMN	C1'-C2'	2.91	1.56	1.52
4	B	1031	FAD	O5'-C5'	2.89	1.55	1.44
4	B	1031	FAD	C2A-N1A	2.87	1.39	1.33
7	C	1034	IUR	C6-C5	2.84	1.38	1.35
4	D	1031	FAD	O5'-C5'	2.83	1.55	1.44
4	C	1031	FAD	C6-C5X	2.81	1.44	1.40
6	B	1034	IDH	C6-N1	2.80	1.49	1.46
3	B	1030	FMN	C1'-C2'	2.79	1.56	1.52
4	B	1031	FAD	C6-C5X	2.78	1.44	1.40
4	B	1031	FAD	C4A-N3A	2.77	1.39	1.34
4	D	1031	FAD	O4B-C4B	2.76	1.51	1.45
4	C	1031	FAD	C5A-C6A	2.74	1.48	1.41
4	D	1031	FAD	C2A-N1A	2.71	1.38	1.33
4	C	1031	FAD	O4B-C4B	2.71	1.51	1.45
4	D	1031	FAD	C6-C5X	2.70	1.44	1.40
4	C	1031	FAD	C5A-C4A	2.70	1.43	1.39
4	A	1031	FAD	O4B-C4B	2.70	1.51	1.45
5	A	1032	NDP	PA-O3	-2.70	1.56	1.59
6	B	1034	IDH	O4-C4	-2.69	1.18	1.23
4	B	1031	FAD	O4B-C4B	2.68	1.51	1.45
3	D	1030	FMN	C1'-C2'	2.64	1.56	1.52
4	A	1031	FAD	C4A-N3A	2.64	1.39	1.34
4	A	1031	FAD	C2A-N1A	2.60	1.38	1.33
4	D	1031	FAD	C5A-C6A	2.58	1.48	1.41
4	C	1031	FAD	C4A-N3A	2.55	1.39	1.34
4	A	1031	FAD	C5A-C6A	2.54	1.48	1.41
4	B	1031	FAD	C5A-C6A	2.53	1.48	1.41
5	C	1032	NDP	PA-O3	-2.52	1.56	1.59
5	D	1032	NDP	C8A-N9A	2.52	1.41	1.37
4	D	1031	FAD	C4A-N3A	2.51	1.39	1.34
4	D	1031	FAD	C1'-C2'	2.51	1.56	1.52
5	A	1032	NDP	C8A-N9A	2.51	1.41	1.37
4	D	1031	FAD	C9-C9A	2.50	1.43	1.39
4	C	1031	FAD	C2A-N1A	2.50	1.38	1.33
3	C	1030	FMN	C6-C7	2.50	1.43	1.39
5	C	1032	NDP	C8A-N9A	2.48	1.41	1.37
3	A	1030	FMN	C6-C7	2.48	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1032	NDP	C4A-N3A	2.47	1.39	1.34
4	B	1031	FAD	C5A-C4A	2.47	1.43	1.39
6	A	1033	IDH	C5-C4	2.45	1.55	1.50
5	D	1032	NDP	C4A-N3A	2.44	1.39	1.34
4	A	1031	FAD	C9-C9A	2.43	1.43	1.39
4	A	1031	FAD	C9-C8	2.42	1.42	1.39
5	C	1032	NDP	P2B-O2B	-2.42	1.55	1.59
4	C	1031	FAD	C9-C9A	2.41	1.43	1.39
4	D	1031	FAD	C10-N1	2.40	1.38	1.33
5	B	1032	NDP	C8A-N9A	2.40	1.41	1.37
4	D	1031	FAD	O4B-C1B	2.39	1.47	1.42
5	C	1032	NDP	C5D-C4D	2.39	1.58	1.51
5	C	1032	NDP	C4A-N3A	2.38	1.38	1.34
5	C	1032	NDP	PN-O3	-2.38	1.56	1.59
4	A	1031	FAD	C2-N3	2.37	1.44	1.39
5	A	1032	NDP	P2B-O2B	-2.35	1.55	1.59
5	A	1032	NDP	C5D-C4D	2.34	1.58	1.51
4	C	1031	FAD	C1'-C2'	2.31	1.55	1.52
4	C	1031	FAD	C9-C8	2.28	1.42	1.39
4	B	1031	FAD	C10-N1	2.26	1.37	1.33
5	B	1032	NDP	C5D-C4D	2.24	1.58	1.51
4	A	1031	FAD	C5A-C4A	2.24	1.43	1.39
5	D	1032	NDP	P2B-O2B	-2.23	1.55	1.59
5	B	1032	NDP	C4A-N3A	2.23	1.38	1.34
4	C	1031	FAD	C2-N3	2.22	1.43	1.39
4	B	1031	FAD	C2-N3	2.20	1.43	1.39
4	A	1031	FAD	C10-N1	2.19	1.37	1.33
3	A	1030	FMN	C10-N1	2.19	1.37	1.33
5	D	1032	NDP	C5D-C4D	2.19	1.58	1.51
4	B	1031	FAD	C9-C9A	2.18	1.43	1.39
4	D	1031	FAD	P-O5'	-2.17	1.50	1.59
4	B	1031	FAD	C5B-C4B	2.17	1.58	1.51
4	D	1031	FAD	C9-C8	2.17	1.42	1.39
4	A	1031	FAD	O4B-C1B	2.16	1.47	1.42
4	D	1031	FAD	PA-O5B	-2.16	1.50	1.59
3	D	1030	FMN	C10-N1	2.16	1.37	1.33
3	B	1030	FMN	C6-C7	2.15	1.42	1.39
4	B	1031	FAD	C1'-C2'	2.15	1.55	1.52
4	C	1031	FAD	PA-O5B	-2.15	1.51	1.59
4	C	1031	FAD	O4B-C1B	2.14	1.47	1.42
4	C	1031	FAD	C10-N1	2.12	1.37	1.33
4	A	1031	FAD	C5B-C4B	2.12	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1032	NDP	PA-O1A	-2.10	1.43	1.50
4	A	1031	FAD	C1'-C2'	2.10	1.55	1.52
5	D	1032	NDP	PA-O3	-2.09	1.57	1.59
4	C	1031	FAD	C5B-C4B	2.09	1.57	1.51
4	D	1031	FAD	C2-N3	2.08	1.43	1.39
3	C	1030	FMN	C10-N1	2.08	1.37	1.33
8	D	1034	URA	C2-N3	2.08	1.40	1.37
4	D	1031	FAD	C5A-C4A	2.07	1.42	1.39
3	B	1030	FMN	C10-N1	2.07	1.37	1.33
3	A	1030	FMN	C1'-C2'	2.06	1.55	1.52
4	A	1031	FAD	PA-O5B	-2.05	1.51	1.59
3	D	1030	FMN	C6-C7	2.05	1.42	1.39
4	A	1031	FAD	P-O5'	-2.03	1.51	1.59
3	B	1030	FMN	C8M-C8	2.03	1.54	1.51
7	C	1034	IUR	C4-C5	-2.03	1.41	1.45
4	D	1031	FAD	C5B-C4B	2.02	1.57	1.51
4	A	1031	FAD	C3B-C4B	2.02	1.58	1.53
4	B	1031	FAD	P-O5'	-2.01	1.51	1.59

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1031	FAD	O3P-PA-O1A	-8.96	83.74	110.70
4	D	1031	FAD	O3P-PA-O1A	-8.93	83.85	110.70
4	B	1031	FAD	O3P-PA-O1A	-8.88	83.98	110.70
4	C	1031	FAD	O3P-PA-O1A	-8.80	84.23	110.70
4	C	1031	FAD	O2A-PA-O3P	-7.48	87.06	107.27
4	A	1031	FAD	O2A-PA-O3P	-7.28	87.60	107.27
4	D	1031	FAD	O2A-PA-O3P	-7.22	87.75	107.27
4	B	1031	FAD	O2A-PA-O3P	-7.08	88.14	107.27
6	B	1034	IDH	C4-N3-C2	-5.11	119.81	126.23
7	C	1034	IUR	O2-C2-N1	4.79	127.72	122.79
3	B	1030	FMN	C10-N1-C2	4.73	127.09	116.85
5	A	1032	NDP	C3N-C2N-N1N	-4.71	116.28	123.20
3	C	1030	FMN	C10-N1-C2	4.71	127.04	116.85
5	B	1032	NDP	C3N-C2N-N1N	-4.70	116.30	123.20
3	D	1030	FMN	C10-N1-C2	4.69	127.00	116.85
5	C	1032	NDP	C3N-C2N-N1N	-4.66	116.36	123.20
5	D	1032	NDP	C3N-C2N-N1N	-4.61	116.43	123.20
3	A	1030	FMN	C10-N1-C2	4.60	126.80	116.85
3	D	1030	FMN	C4-C4A-C10	4.26	124.23	116.93
3	A	1030	FMN	C4-C4A-C10	4.22	124.17	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1030	FMN	C4-C4A-C10	4.19	124.12	116.93
3	B	1030	FMN	C4-C4A-C10	4.16	124.07	116.93
3	A	1030	FMN	O4'-C4'-C3'	4.15	118.97	109.25
3	C	1030	FMN	O3'-C3'-C2'	-4.15	99.51	108.93
3	B	1030	FMN	O3'-C3'-C2'	-4.08	99.65	108.93
3	B	1030	FMN	O4'-C4'-C3'	4.06	118.75	109.25
3	B	1030	FMN	C4A-C10-N1	-3.91	115.00	124.59
3	D	1030	FMN	C4A-C10-N1	-3.88	115.08	124.59
3	D	1030	FMN	O4'-C4'-C3'	3.87	118.31	109.25
3	A	1030	FMN	C4A-C10-N1	-3.86	115.12	124.59
3	C	1030	FMN	C4A-C10-N1	-3.86	115.13	124.59
3	C	1030	FMN	O4'-C4'-C3'	3.81	118.17	109.25
6	B	1034	IDH	C5-C4-N3	3.79	121.76	116.19
3	D	1030	FMN	O3'-C3'-C2'	-3.76	100.39	108.93
4	A	1031	FAD	O2A-PA-O1A	3.66	129.48	112.44
4	D	1031	FAD	O2A-PA-O1A	3.65	129.44	112.44
5	D	1032	NDP	C1D-N1N-C2N	-3.65	115.12	121.14
5	B	1032	NDP	C1D-N1N-C2N	-3.64	115.14	121.14
4	B	1031	FAD	O2A-PA-O1A	3.61	129.26	112.44
3	A	1030	FMN	O3'-C3'-C2'	-3.61	100.74	108.93
4	C	1031	FAD	O2A-PA-O1A	3.60	129.19	112.44
5	A	1032	NDP	C1D-N1N-C2N	-3.56	115.27	121.14
5	C	1032	NDP	C1D-N1N-C2N	-3.50	115.37	121.14
3	B	1030	FMN	C5'-C4'-C3'	-3.15	106.27	112.22
8	D	1034	URA	C4-N3-C2	3.14	128.59	125.55
3	C	1030	FMN	C5'-C4'-C3'	-3.09	106.39	112.22
3	A	1030	FMN	C5'-C4'-C3'	-3.02	106.53	112.22
4	B	1031	FAD	O4B-C1B-N9A	-2.93	102.47	108.09
3	D	1030	FMN	C5'-C4'-C3'	-2.91	106.73	112.22
7	C	1034	IUR	C6-N1-C2	-2.81	120.08	122.69
8	D	1034	URA	C6-C5-C4	2.79	121.74	119.30
3	C	1030	FMN	C4A-C10-N10	2.79	120.47	116.48
3	A	1030	FMN	C4A-C10-N10	2.76	120.44	116.48
5	A	1032	NDP	C6N-N1N-C2N	2.75	122.26	119.32
3	B	1030	FMN	C4A-C10-N10	2.72	120.38	116.48
5	D	1032	NDP	O7N-C7N-N7N	-2.72	116.79	122.89
8	D	1034	URA	C5-C4-N3	-2.71	111.00	114.80
4	A	1031	FAD	O4B-C1B-N9A	-2.70	102.91	108.09
4	C	1031	FAD	C5X-C9A-N10	-2.70	115.53	117.97
3	D	1030	FMN	C4A-C10-N10	2.69	120.34	116.48
5	B	1032	NDP	C6N-N1N-C2N	2.69	122.20	119.32
4	D	1031	FAD	O4B-C1B-N9A	-2.69	102.93	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1032	NDP	O7N-C7N-N7N	-2.68	116.89	122.89
5	C	1032	NDP	O7N-C7N-N7N	-2.66	116.94	122.89
5	C	1032	NDP	C6N-N1N-C2N	2.63	122.13	119.32
8	D	1034	URA	O4-C4-N3	2.63	123.08	119.27
4	C	1031	FAD	O4B-C1B-N9A	-2.61	103.08	108.09
5	A	1032	NDP	O7N-C7N-N7N	-2.60	117.06	122.89
3	D	1030	FMN	O3'-C3'-C4'	2.60	114.84	108.93
5	D	1032	NDP	C6N-N1N-C2N	2.59	122.09	119.32
5	C	1032	NDP	O5B-C5B-C4B	-2.58	100.19	108.99
5	B	1032	NDP	O3-PA-O1A	-2.57	102.97	110.70
4	A	1031	FAD	C5X-C9A-N10	-2.54	115.67	117.97
5	A	1032	NDP	O2A-PA-O1A	2.54	124.28	112.44
4	D	1031	FAD	C5X-C9A-N10	-2.52	115.69	117.97
5	C	1032	NDP	O4B-C1B-N9A	2.51	112.91	108.09
7	C	1034	IUR	C4-N3-C2	2.51	129.82	126.37
3	C	1030	FMN	O3'-C3'-C4'	2.51	114.63	108.93
5	A	1032	NDP	O4B-C1B-N9A	2.50	112.90	108.09
6	B	1034	IDH	N3-C2-N1	2.48	119.46	116.61
5	C	1032	NDP	C2B-C1B-N9A	-2.48	109.67	113.75
5	D	1032	NDP	O5B-C5B-C4B	-2.47	100.60	108.99
4	D	1031	FAD	C2A-N1A-C6A	2.46	122.78	118.73
5	D	1032	NDP	O2A-PA-O1A	2.46	123.88	112.44
5	A	1032	NDP	C2B-C1B-N9A	-2.45	109.72	113.75
5	A	1032	NDP	O5B-C5B-C4B	-2.44	100.67	108.99
6	B	1034	IDH	C6-C5-I5	-2.44	107.52	110.58
4	B	1031	FAD	C5X-C9A-N10	-2.44	115.77	117.97
4	A	1031	FAD	C5'-C4'-C3'	-2.44	107.62	112.22
4	C	1031	FAD	C2A-N1A-C6A	2.43	122.72	118.73
5	B	1032	NDP	O5B-C5B-C4B	-2.43	100.73	108.99
5	A	1032	NDP	O2B-C2B-C3B	2.41	120.31	111.68
4	B	1031	FAD	C2A-N1A-C6A	2.41	122.68	118.73
4	D	1031	FAD	C5'-C4'-C3'	-2.40	107.69	112.22
4	C	1031	FAD	C5'-C4'-C3'	-2.40	107.69	112.22
4	B	1031	FAD	C5'-C4'-C3'	-2.39	107.70	112.22
5	A	1032	NDP	O3-PA-O1A	-2.39	103.50	110.70
5	B	1032	NDP	O2A-PA-O1A	2.39	123.57	112.44
5	B	1032	NDP	O2B-C2B-C3B	2.39	120.25	111.68
3	B	1030	FMN	O3'-C3'-C4'	2.38	114.33	108.93
5	C	1032	NDP	O2B-C2B-C3B	2.38	120.20	111.68
5	C	1032	NDP	O2A-PA-O1A	2.37	123.49	112.44
5	D	1032	NDP	O4B-C1B-N9A	2.36	112.61	108.09
5	D	1032	NDP	C2B-C1B-N9A	-2.35	109.88	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1032	NDP	O2B-C2B-C3B	2.33	120.04	111.68
3	A	1030	FMN	O3'-C3'-C4'	2.31	114.18	108.93
5	D	1032	NDP	O3-PA-O1A	-2.31	103.75	110.70
5	B	1032	NDP	O4B-C1B-N9A	2.31	112.52	108.09
5	A	1032	NDP	O4B-C1B-C2B	2.30	110.55	106.59
4	A	1031	FAD	C4-N3-C2	-2.27	121.62	125.64
5	C	1032	NDP	O4B-C1B-C2B	2.24	110.45	106.59
5	A	1032	NDP	N3A-C2A-N1A	-2.23	125.20	128.58
4	D	1031	FAD	C4'-C3'-C2'	-2.23	109.86	113.57
4	C	1031	FAD	C4-N3-C2	-2.21	121.71	125.64
5	A	1032	NDP	N9A-C8A-N7A	-2.21	110.80	113.94
4	A	1031	FAD	C2A-N1A-C6A	2.20	122.35	118.73
5	B	1032	NDP	C2B-C1B-N9A	-2.20	110.14	113.75
4	B	1031	FAD	C4'-C3'-C2'	-2.19	109.92	113.57
5	A	1032	NDP	O5D-PN-O1N	2.18	117.58	108.94
3	B	1030	FMN	C4-C4A-N5	-2.18	115.20	118.21
5	D	1032	NDP	N3A-C2A-N1A	-2.17	125.30	128.58
3	D	1030	FMN	C10-C4A-N5	-2.17	120.38	124.81
3	D	1030	FMN	N3-C2-N1	-2.17	114.90	119.50
5	D	1032	NDP	O4B-C1B-C2B	2.16	110.31	106.59
3	A	1030	FMN	C10-C4A-N5	-2.15	120.42	124.81
3	B	1030	FMN	N3-C2-N1	-2.15	114.94	119.50
5	C	1032	NDP	N9A-C8A-N7A	-2.14	110.90	113.94
5	B	1032	NDP	O5D-PN-O1N	2.12	117.35	108.94
4	B	1031	FAD	C4-N3-C2	-2.12	121.88	125.64
5	D	1032	NDP	O5D-PN-O1N	2.11	117.30	108.94
5	C	1032	NDP	N3A-C2A-N1A	-2.11	125.39	128.58
5	B	1032	NDP	N3A-C2A-N1A	-2.10	125.40	128.58
3	C	1030	FMN	C10-C4A-N5	-2.10	120.52	124.81
5	C	1032	NDP	O5D-PN-O1N	2.09	117.20	108.94
5	D	1032	NDP	N9A-C8A-N7A	-2.08	110.98	113.94
3	A	1030	FMN	N3-C2-N1	-2.08	115.09	119.50
3	B	1030	FMN	N10-C10-N1	2.07	124.62	118.51
4	B	1031	FAD	C5A-C4A-N9A	-2.07	103.55	105.81
3	C	1030	FMN	N3-C2-N1	-2.06	115.11	119.50
4	D	1031	FAD	C4-N3-C2	-2.06	121.98	125.64
3	B	1030	FMN	C6-C5A-C9A	2.06	121.88	119.05
3	D	1030	FMN	N10-C10-N1	2.06	124.58	118.51
3	C	1030	FMN	C4-C4A-N5	-2.06	115.36	118.21
4	C	1031	FAD	C10-N1-C2	2.05	121.29	116.85
5	B	1032	NDP	N9A-C8A-N7A	-2.05	111.03	113.94
4	C	1031	FAD	C4'-C3'-C2'	-2.05	110.16	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1030	FMN	C4-C4A-N5	-2.04	115.39	118.21
4	B	1031	FAD	C10-N1-C2	2.04	121.27	116.85
3	B	1030	FMN	C9A-C5A-N5	-2.04	120.29	122.45
3	A	1030	FMN	C4-C4A-N5	-2.03	115.40	118.21
5	B	1032	NDP	O4B-C1B-C2B	2.02	110.07	106.59
4	A	1031	FAD	C4'-C3'-C2'	-2.02	110.20	113.57
3	C	1030	FMN	O2'-C2'-C1'	2.02	118.51	110.20
5	C	1032	NDP	C5A-N7A-C8A	2.02	106.62	103.45
5	A	1032	NDP	C5A-N7A-C8A	2.02	106.62	103.45
3	A	1030	FMN	N10-C10-N1	2.01	124.43	118.51
3	D	1030	FMN	C9A-C5A-N5	-2.00	120.33	122.45

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	C5B-O5B-PA-O1A
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	D	1031	FAD	C5B-O5B-PA-O1A
5	A	1032	NDP	PN-O3-PA-O5B
5	A	1032	NDP	O4D-C1D-N1N-C2N
5	B	1032	NDP	PN-O3-PA-O5B
5	B	1032	NDP	O4D-C1D-N1N-C2N
5	C	1032	NDP	PN-O3-PA-O5B
5	C	1032	NDP	O4D-C1D-N1N-C2N
5	D	1032	NDP	PN-O3-PA-O5B
5	D	1032	NDP	O4D-C1D-N1N-C2N
5	A	1032	NDP	C3B-C2B-O2B-P2B
5	B	1032	NDP	C3B-C2B-O2B-P2B
5	C	1032	NDP	C3B-C2B-O2B-P2B
5	D	1032	NDP	C3B-C2B-O2B-P2B
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
4	A	1031	FAD	PA-O3P-P-O5'
4	C	1031	FAD	PA-O3P-P-O5'
4	D	1031	FAD	PA-O3P-P-O5'
4	A	1031	FAD	C2B-C1B-N9A-C8A
4	B	1031	FAD	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
4	C	1031	FAD	C2B-C1B-N9A-C8A
4	D	1031	FAD	C2B-C1B-N9A-C8A
4	B	1031	FAD	C5B-O5B-PA-O3P
4	C	1031	FAD	C5B-O5B-PA-O3P
3	A	1030	FMN	C4'-C5'-O5'-P
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	O4D-C4D-C5D-O5D
5	D	1032	NDP	O4D-C4D-C5D-O5D
4	B	1031	FAD	P-O3P-PA-O2A
4	B	1031	FAD	O4B-C4B-C5B-O5B
4	C	1031	FAD	O4B-C4B-C5B-O5B
5	B	1032	NDP	O4D-C4D-C5D-O5D
5	C	1032	NDP	O4D-C4D-C5D-O5D
5	A	1032	NDP	PN-O3-PA-O1A
5	B	1032	NDP	PN-O3-PA-O1A
5	D	1032	NDP	PN-O3-PA-O1A

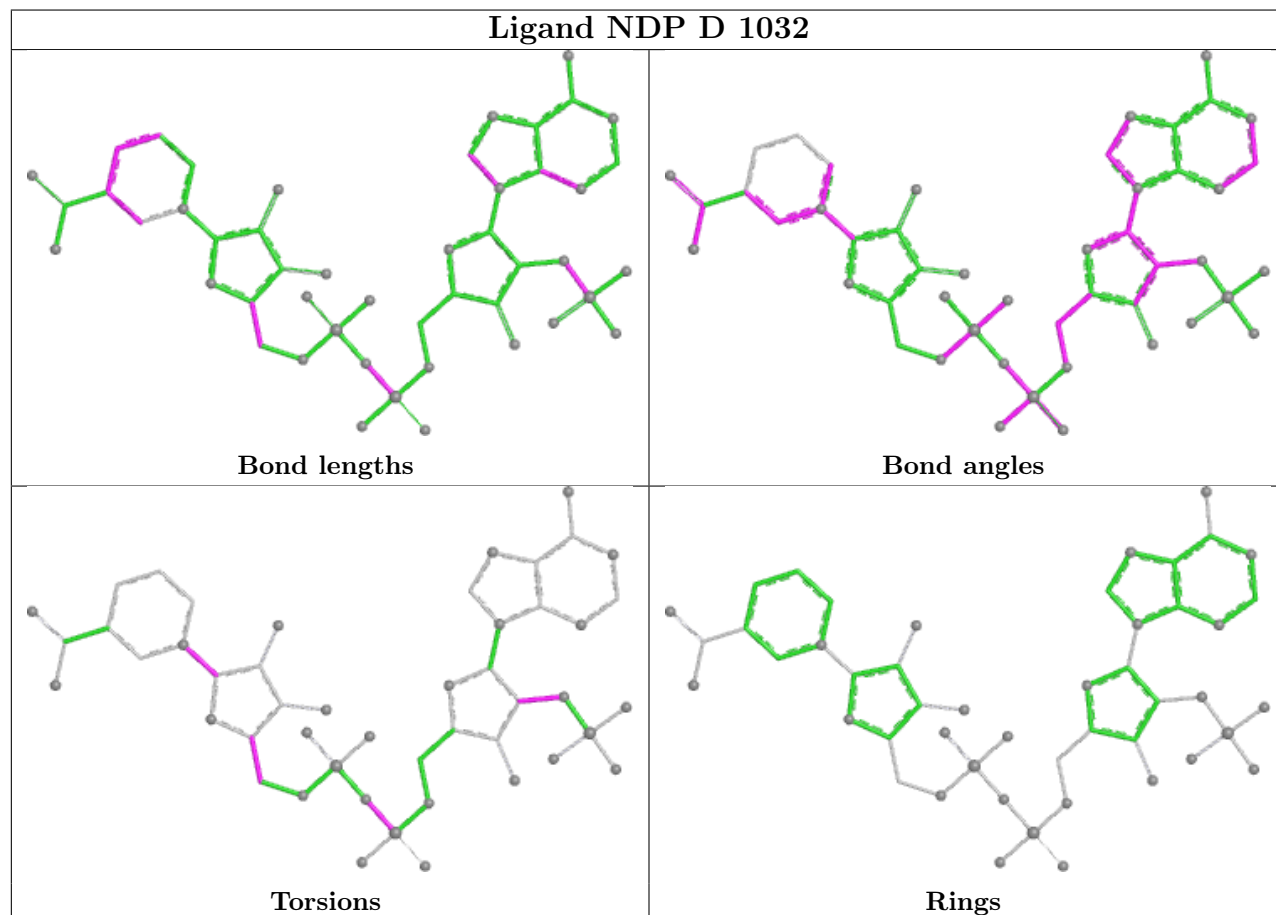
There are no ring outliers.

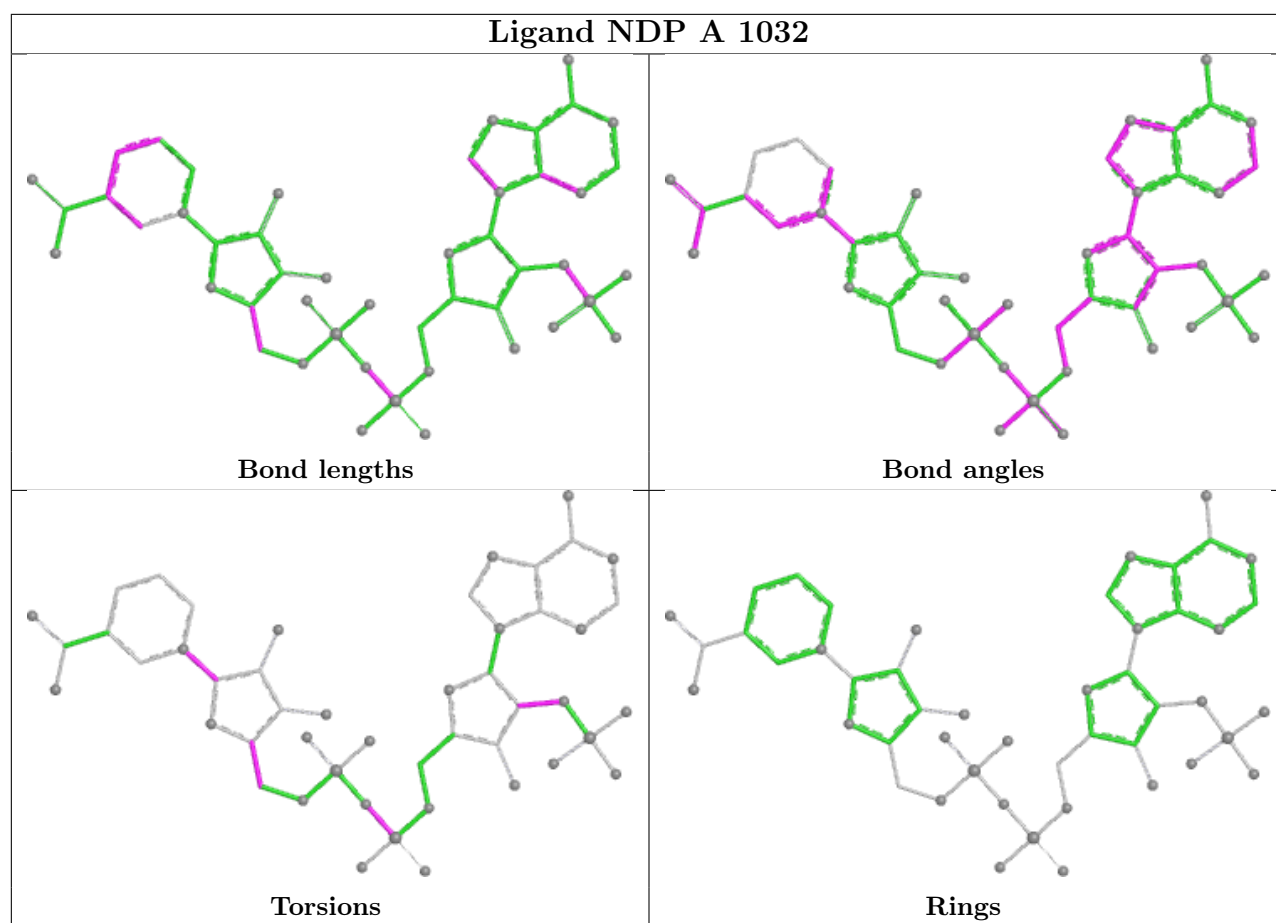
16 monomers are involved in 43 short contacts:

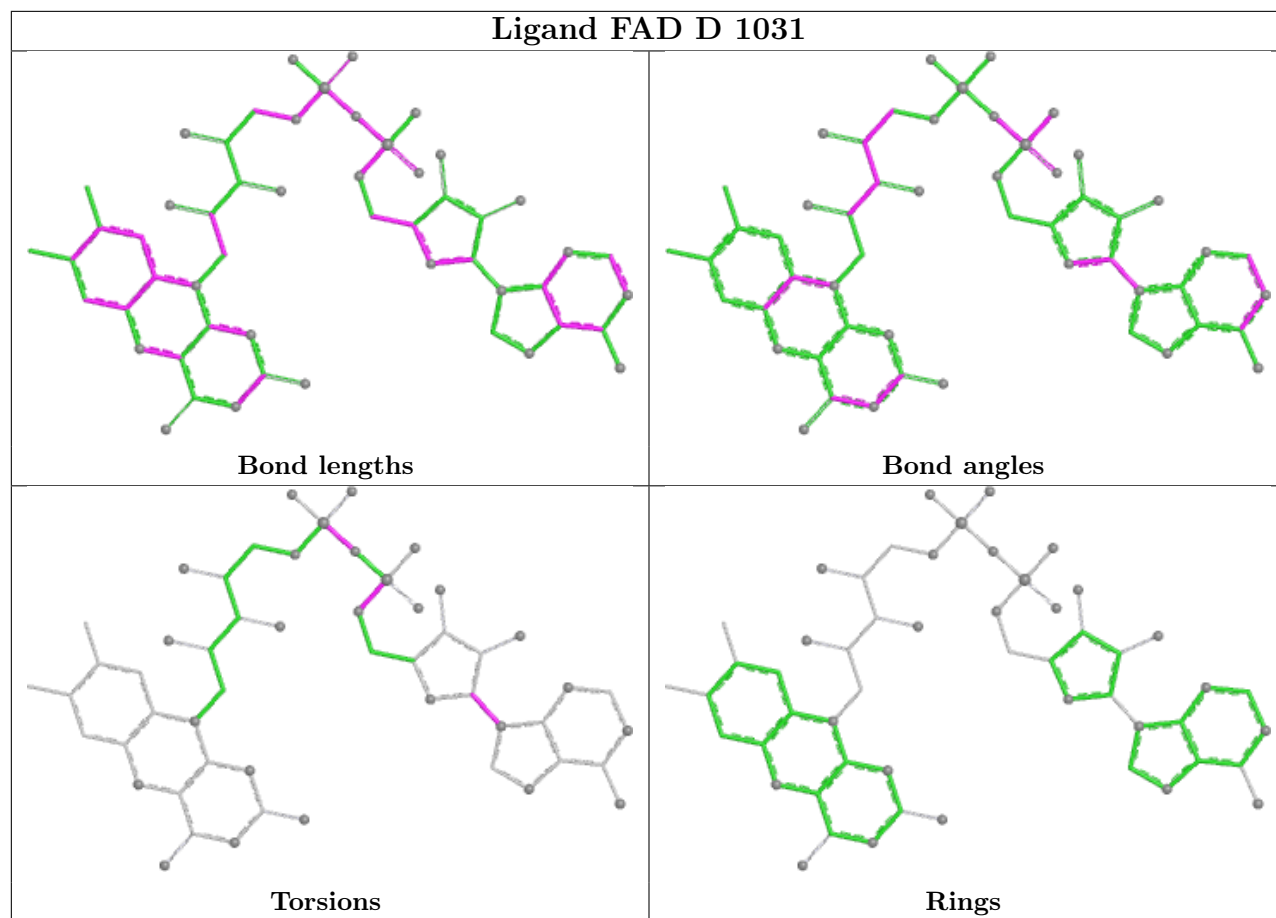
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1032	NDP	5	0
2	D	1027	SF4	3	0
5	A	1032	NDP	6	0
2	A	1027	SF4	1	0
7	C	1034	IUR	4	0
6	B	1034	IDH	4	0
4	D	1031	FAD	1	0
2	C	1027	SF4	2	0
5	B	1032	NDP	5	0
3	B	1030	FMN	1	0
4	B	1031	FAD	1	0
6	A	1033	IDH	1	0
5	C	1032	NDP	6	0
2	B	1027	SF4	2	0
2	A	1026	SF4	1	0
3	C	1030	FMN	1	0

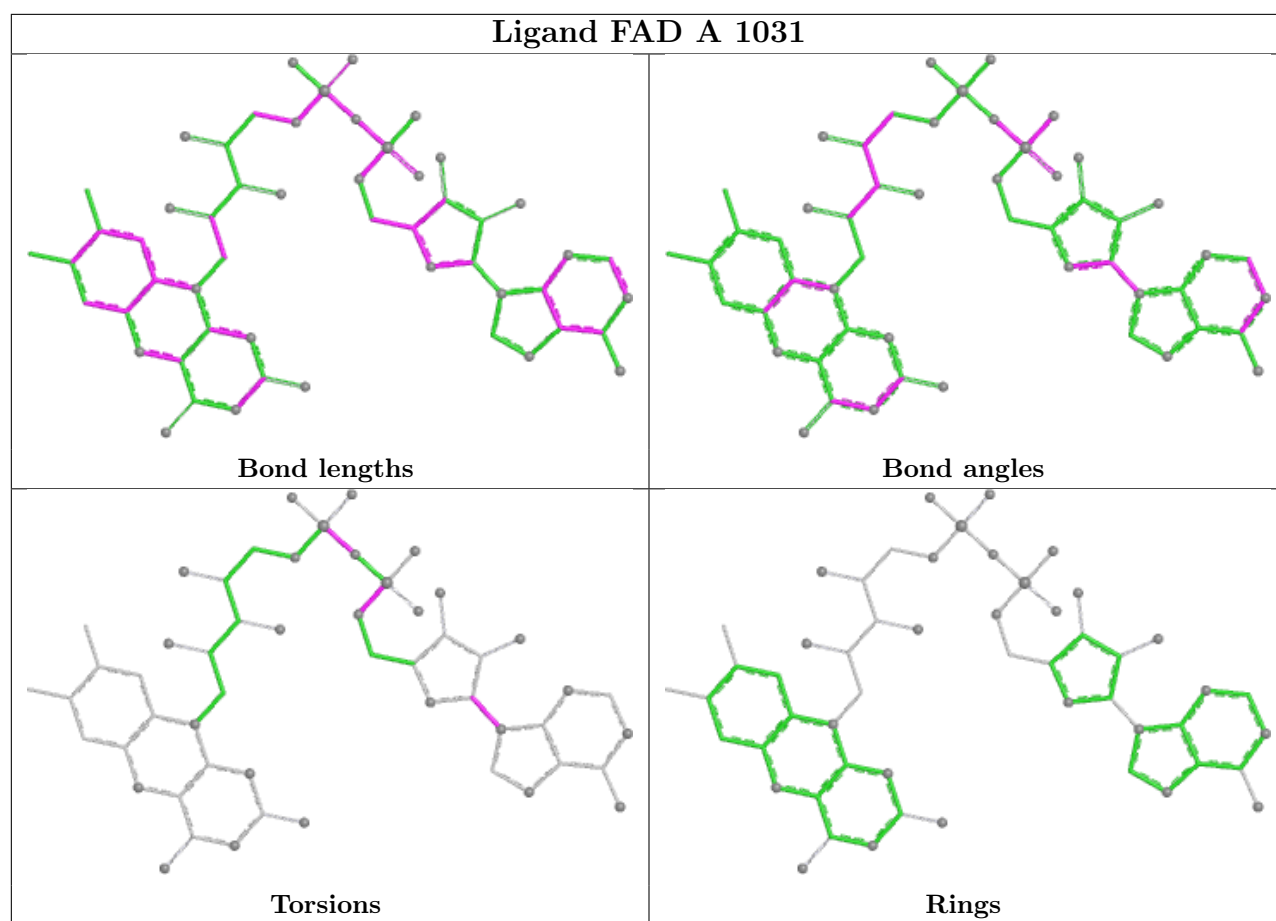
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

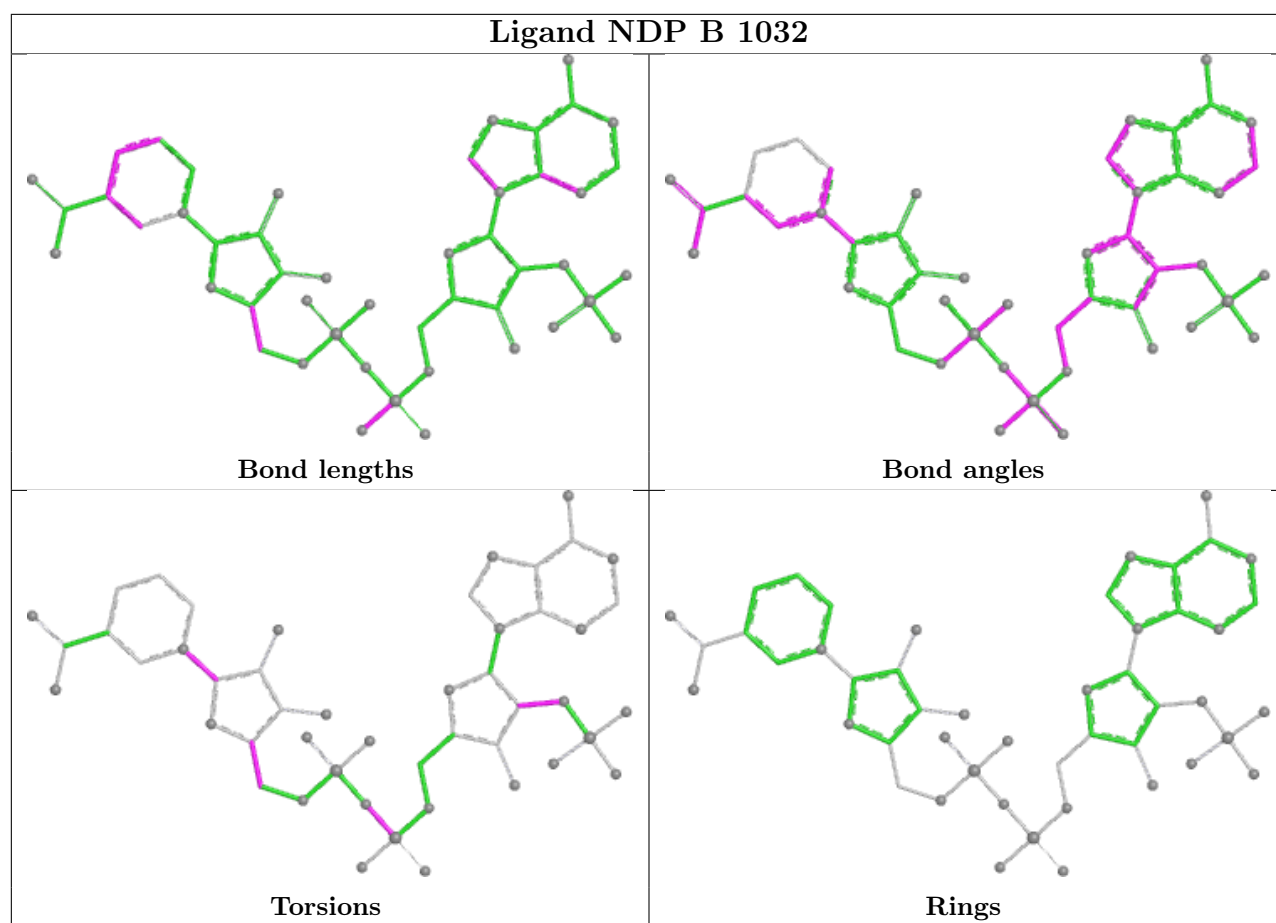
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



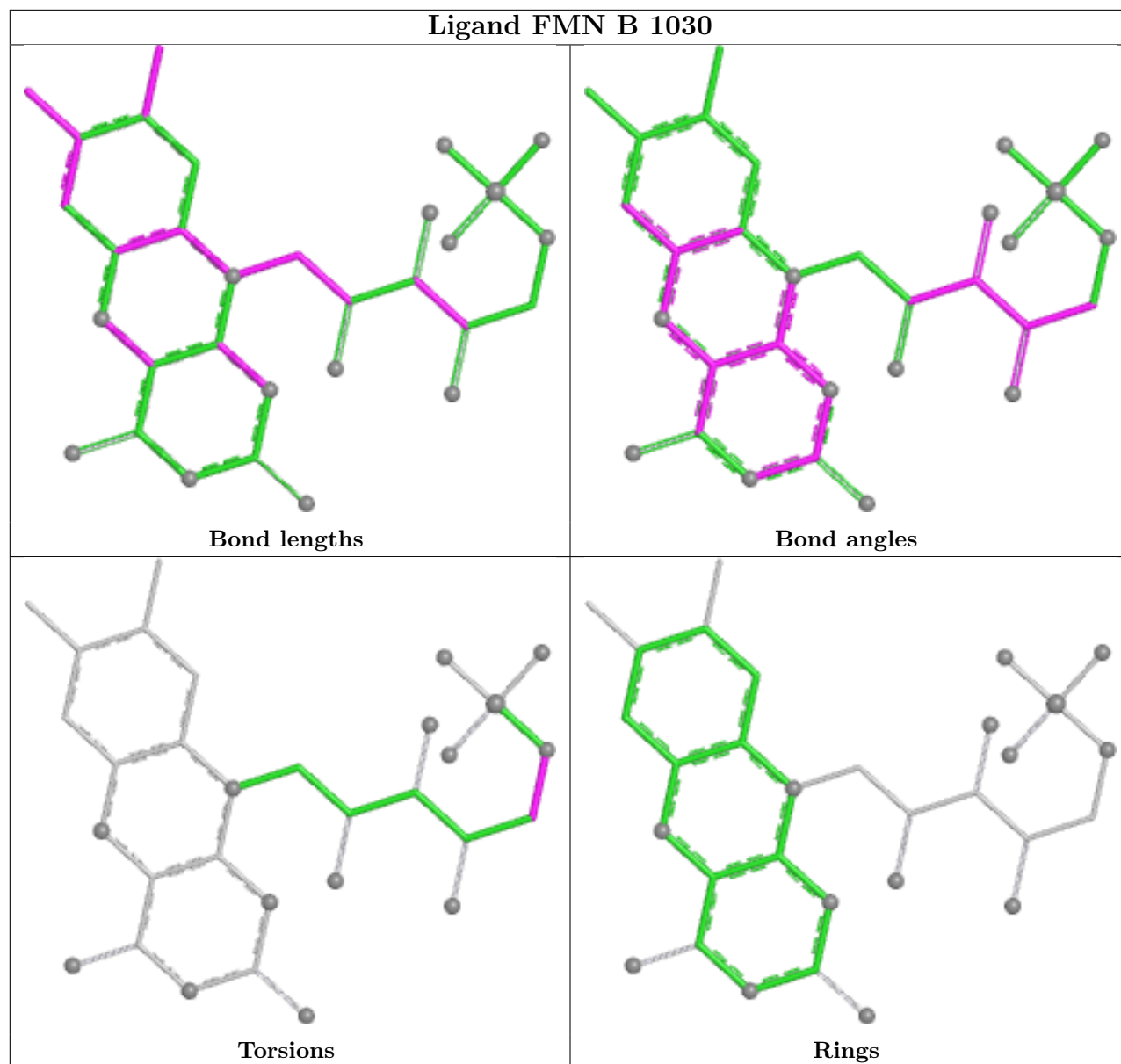




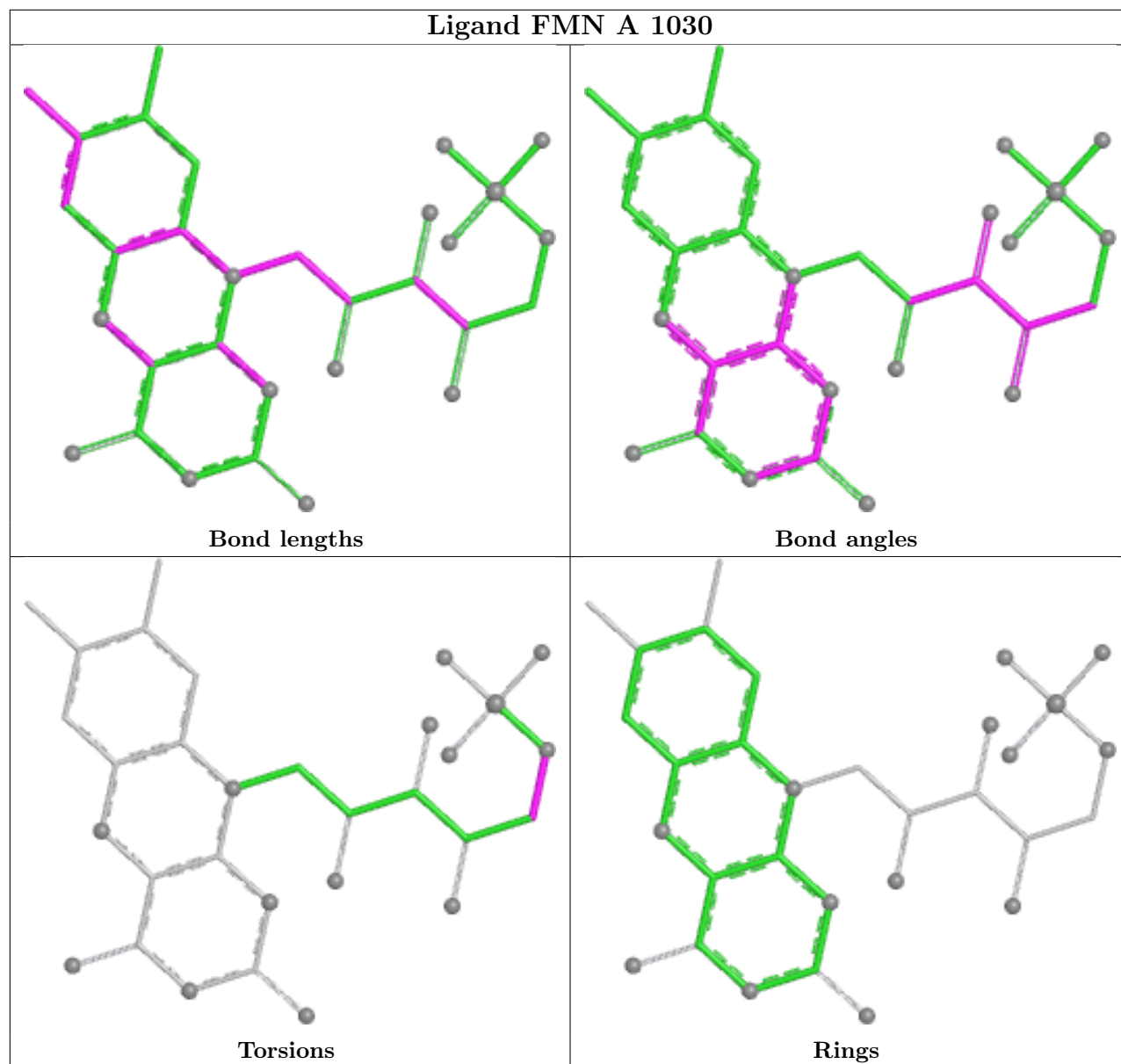


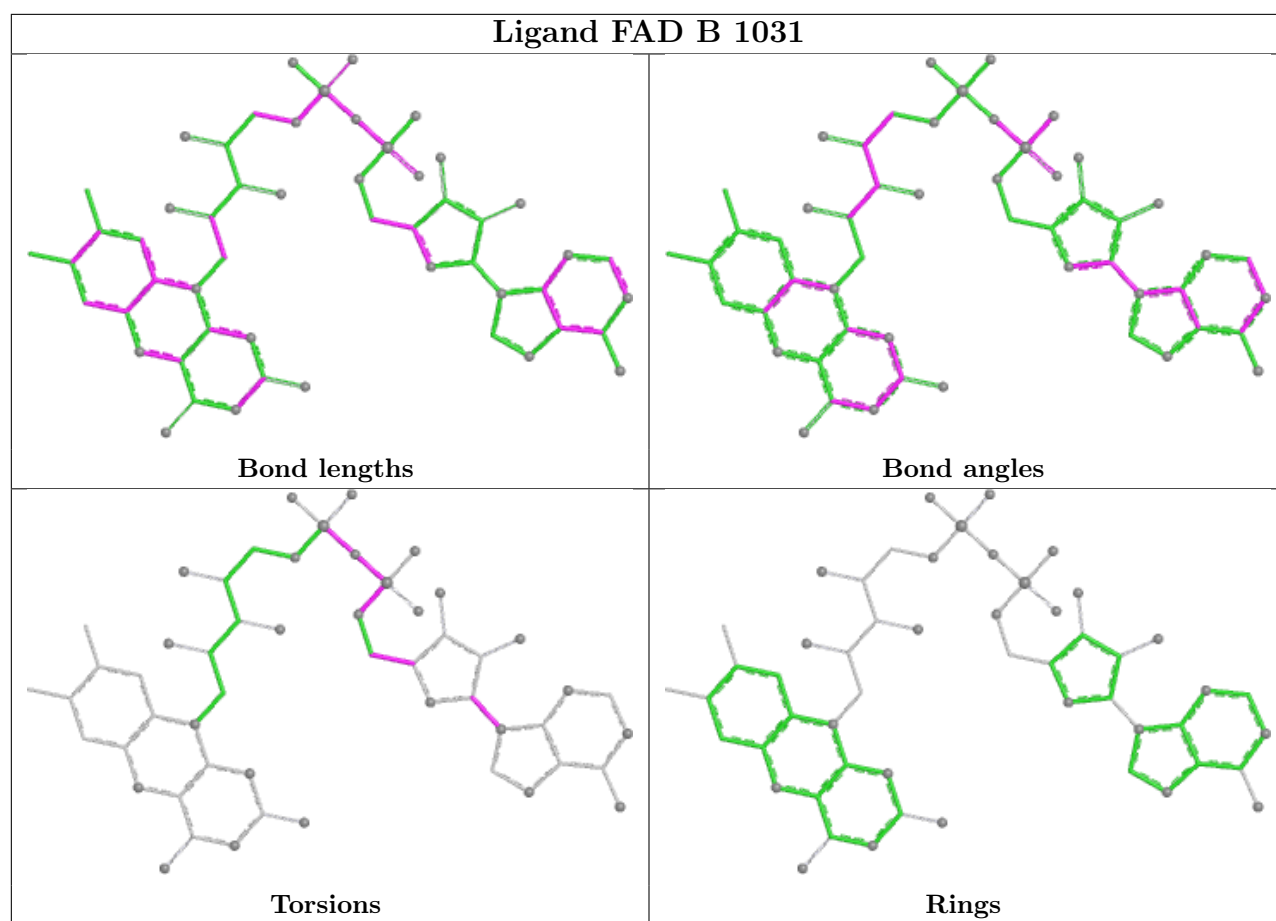


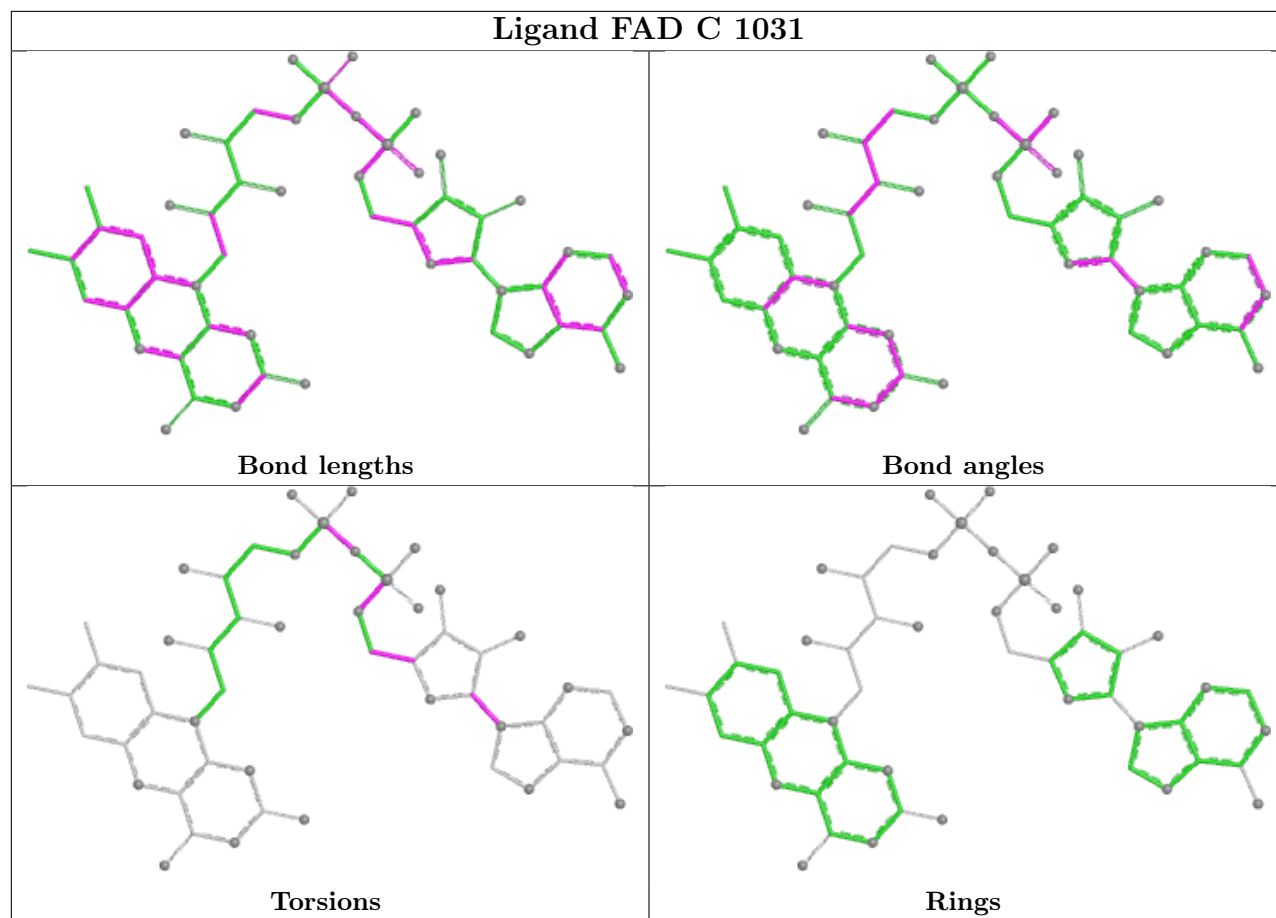
Ligand FMN B 1030

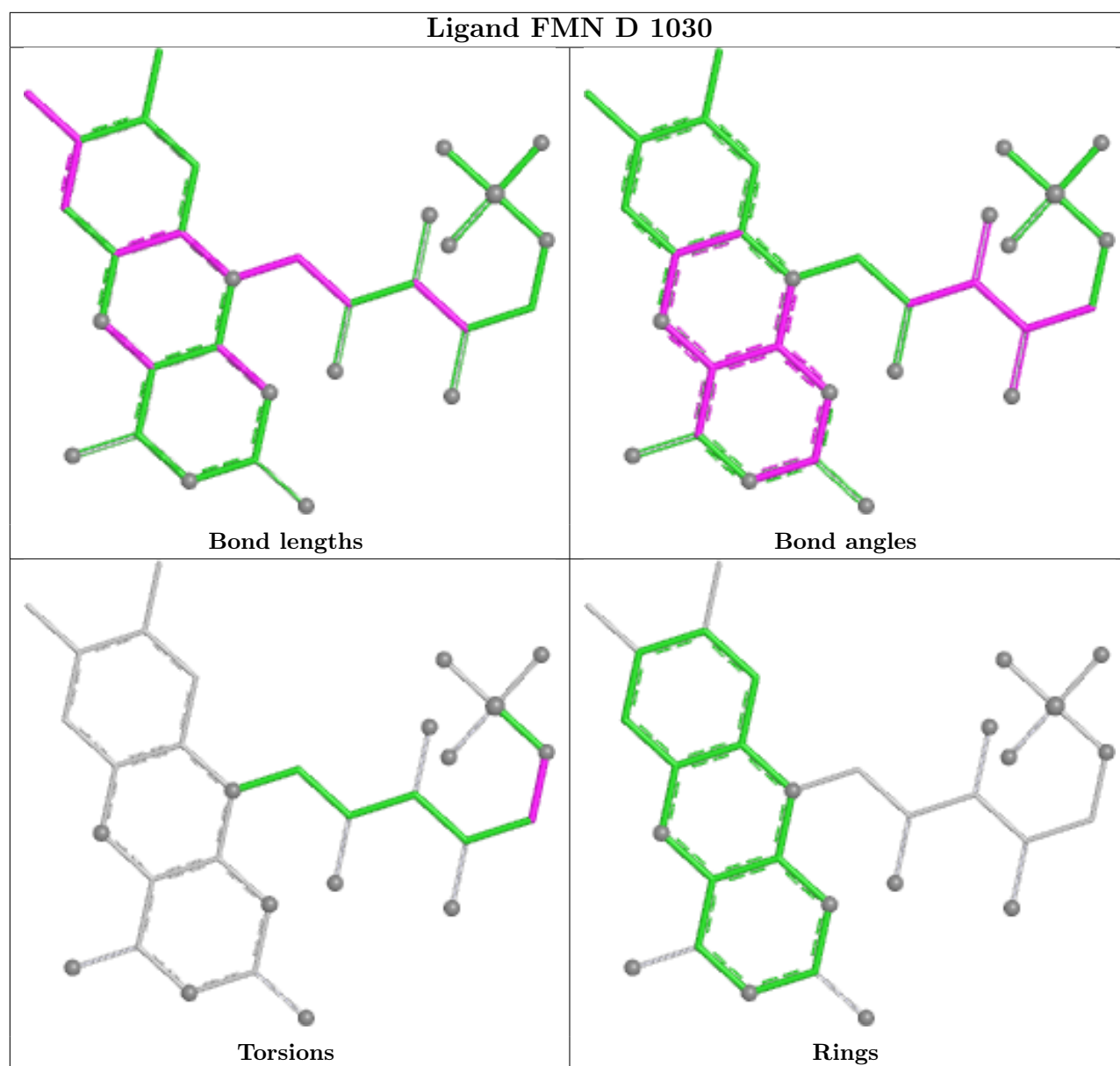


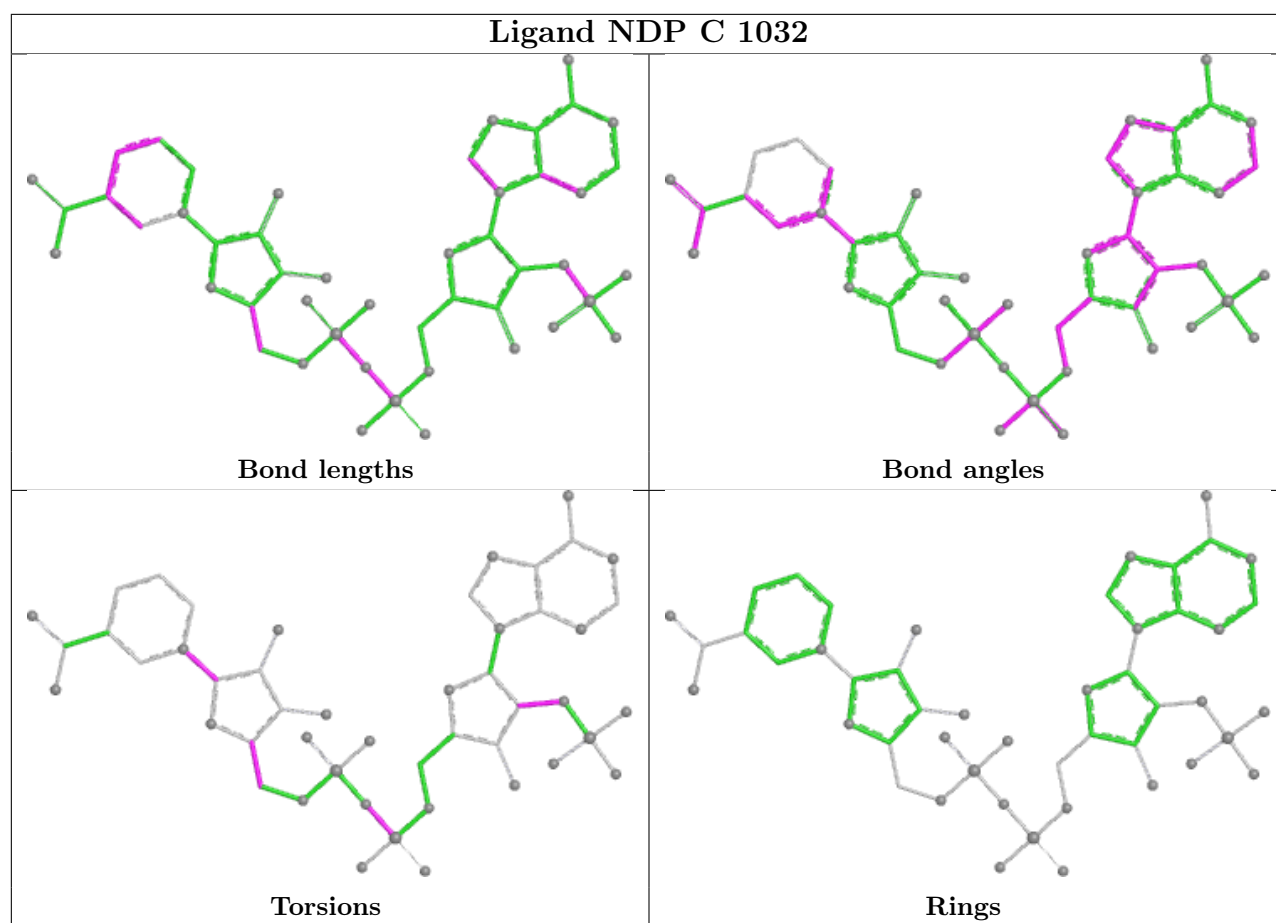
Ligand FMN A 1030

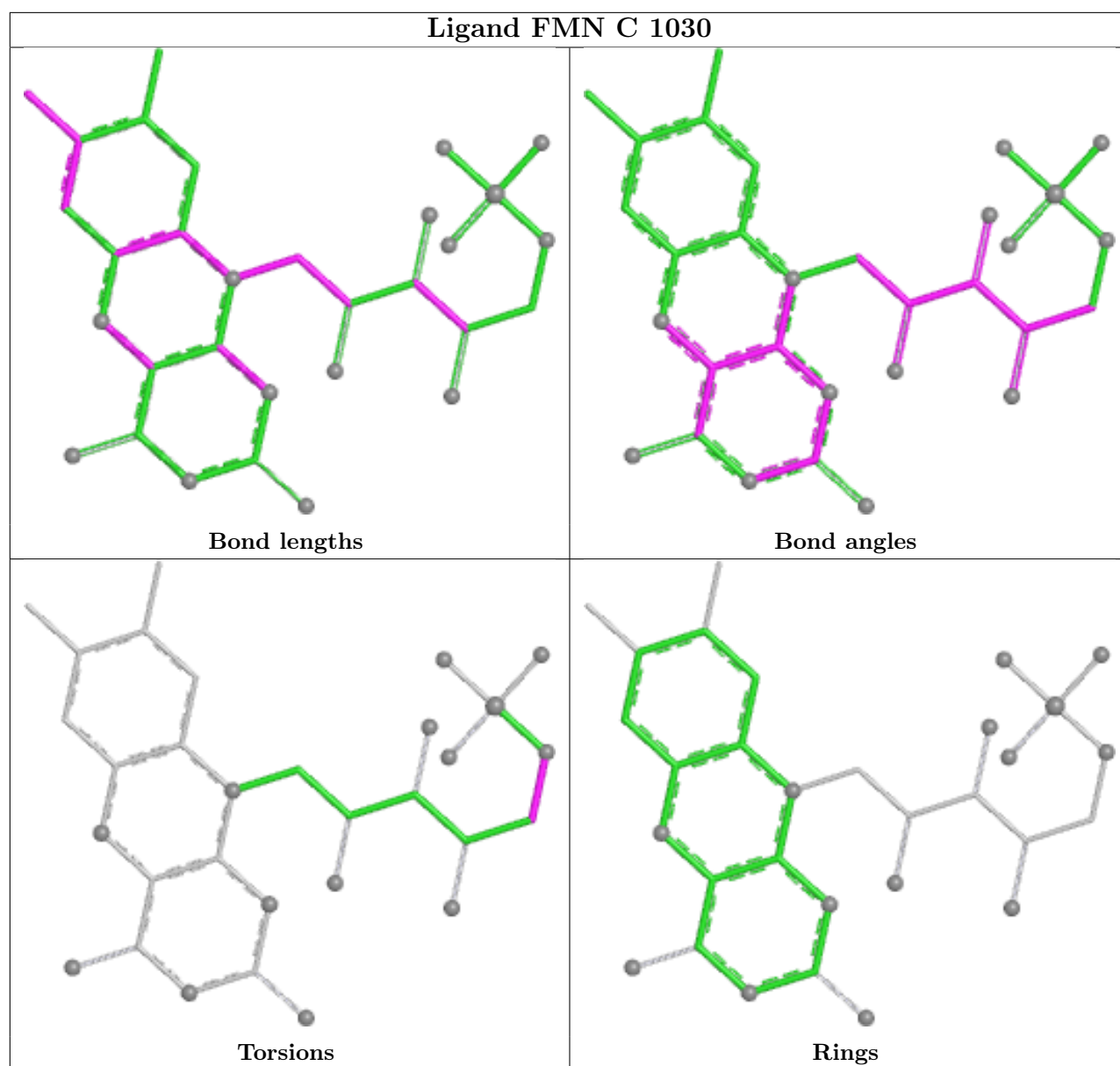












5.7 Other polymers [i](#)

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	1019/1025 (99%)	-0.16	40 (3%)	43	43	14, 27, 63, 83	0
1	B	1012/1025 (98%)	-0.15	28 (2%)	55	55	15, 27, 61, 83	0
1	C	1015/1025 (99%)	-0.06	32 (3%)	50	50	17, 29, 63, 85	0
1	D	1019/1025 (99%)	0.01	44 (4%)	40	39	17, 29, 67, 87	0
All	All	4065/4100 (99%)	-0.09	144 (3%)	47	47	14, 28, 64, 87	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	LEU	7.5
1	B	2	ALA	7.1
1	C	682	LEU	6.5
1	D	2	ALA	6.5
1	B	682	LEU	5.5
1	A	2	ALA	5.5
1	C	2	ALA	5.4
1	D	682	LEU	5.0
1	B	681	GLY	4.9
1	D	1010	PRO	4.9
1	C	681	GLY	4.8
1	D	904	PHE	4.6
1	C	1010	PRO	4.3
1	B	683	ALA	4.3
1	A	1010	PRO	4.3
1	A	904	PHE	4.2
1	A	52	CYS	4.1
1	C	907	LEU	4.1
1	C	683	ALA	4.0
1	D	681	GLY	4.0
1	B	679	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	51	HIS	3.8
1	D	401	GLY	3.8
1	A	1009	THR	3.7
1	B	1020	ALA	3.6
1	B	51	HIS	3.5
1	B	1010	PRO	3.5
1	D	400	GLY	3.5
1	D	296	GLY	3.4
1	D	302	GLY	3.4
1	A	50	PHE	3.4
1	A	427	VAL	3.3
1	C	679	GLY	3.2
1	B	371	ARG	3.2
1	C	1009	THR	3.2
1	A	907	LEU	3.2
1	B	410	ARG	3.2
1	A	1014	LYS	3.1
1	C	429	LEU	3.1
1	D	427	VAL	3.1
1	A	419	TRP	3.1
1	C	423	GLU	3.1
1	D	905	PRO	3.1
1	B	50	PHE	3.0
1	C	901	ASN	3.0
1	D	679	GLY	3.0
1	D	678	ARG	2.9
1	B	265	GLU	2.9
1	D	897	LEU	2.9
1	A	683	ALA	2.9
1	B	1019	LEU	2.9
1	D	396	VAL	2.9
1	D	676	GLY	2.9
1	A	671	CYS	2.8
1	A	681	GLY	2.8
1	D	429	LEU	2.8
1	A	902	ALA	2.8
1	A	325	HIS	2.7
1	D	330	SER	2.7
1	C	1018	PRO	2.7
1	D	1020	ALA	2.7
1	C	367	PHE	2.7
1	B	426	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	410	ARG	2.7
1	A	903	ALA	2.6
1	D	683	ALA	2.6
1	B	680	MET	2.6
1	C	427	VAL	2.6
1	D	428	HIS	2.6
1	C	52	CYS	2.6
1	B	367	PHE	2.5
1	A	329	PRO	2.5
1	B	427	VAL	2.5
1	C	331	ILE	2.5
1	A	679	GLY	2.5
1	C	398	VAL	2.5
1	D	899	GLU	2.5
1	D	292	ASP	2.5
1	A	1008	THR	2.4
1	A	331	ILE	2.4
1	D	397	ILE	2.4
1	D	426	ILE	2.4
1	A	429	LEU	2.4
1	D	907	LEU	2.4
1	D	680	MET	2.4
1	A	901	ASN	2.4
1	D	903	ALA	2.4
1	D	906	PRO	2.4
1	D	52	CYS	2.4
1	D	50	PHE	2.4
1	A	1019	LEU	2.4
1	C	51	HIS	2.4
1	C	357	ARG	2.4
1	B	324	CYS	2.4
1	D	398	VAL	2.4
1	C	872	MET	2.4
1	A	1011	TYR	2.4
1	B	428	HIS	2.4
1	D	423	GLU	2.4
1	A	367	PHE	2.4
1	B	900	GLN	2.4
1	D	1009	THR	2.3
1	C	1020	ALA	2.3
1	A	423	GLU	2.3
1	C	396	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	342	ASP	2.3
1	D	432	ASP	2.3
1	B	423	GLU	2.3
1	A	426	ILE	2.3
1	C	426	ILE	2.3
1	B	678	ARG	2.2
1	B	325	HIS	2.2
1	C	902	ALA	2.2
1	D	1011	TYR	2.2
1	D	871	LEU	2.2
1	A	264	ASN	2.2
1	C	333	GLY	2.2
1	D	403	ILE	2.2
1	A	1020	ALA	2.2
1	B	331	ILE	2.2
1	D	422	ASP	2.2
1	D	327	PRO	2.2
1	A	430	LYS	2.2
1	A	322	CYS	2.2
1	C	449	GLU	2.1
1	A	371	ARG	2.1
1	B	443	ARG	2.1
1	C	410	ARG	2.1
1	D	443	ARG	2.1
1	A	871	LEU	2.1
1	B	899	GLU	2.1
1	B	396	VAL	2.1
1	C	50	PHE	2.1
1	C	411	THR	2.1
1	C	428	HIS	2.1
1	C	871	LEU	2.1
1	A	868	ILE	2.1
1	A	905	PRO	2.1
1	A	678	ARG	2.0
1	D	402	ARG	2.0
1	D	404	VAL	2.0
1	D	320	GLY	2.0
1	B	290	THR	2.0
1	C	264	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	IUR	C	1034	9/9	0.87	0.09	27,28,32,38	1
6	IDH	B	1034	9/9	0.88	0.16	39,42,45,52	1
5	NDP	D	1032	48/48	0.90	0.12	40,47,57,58	0
6	IDH	A	1033	8/9	0.90	0.10	23,28,32,32	0
2	SF4	C	1026	8/8	0.92	0.08	26,28,29,29	0
5	NDP	C	1032	48/48	0.92	0.10	39,46,56,57	0
2	SF4	A	1026	8/8	0.92	0.09	21,23,23,24	0
5	NDP	B	1032	48/48	0.93	0.10	36,44,56,57	0
2	SF4	D	1026	8/8	0.93	0.08	26,28,28,28	0
5	NDP	A	1032	48/48	0.93	0.11	36,42,56,56	0
8	URA	D	1034	8/8	0.93	0.08	28,30,31,32	0
2	SF4	B	1028	8/8	0.94	0.07	20,22,23,23	0
2	SF4	B	1029	8/8	0.94	0.07	22,23,24,24	0
2	SF4	A	1029	8/8	0.94	0.07	21,22,23,23	0
2	SF4	C	1027	8/8	0.94	0.08	24,26,26,26	0
2	SF4	B	1026	8/8	0.94	0.07	19,23,24,24	0
2	SF4	D	1028	8/8	0.94	0.07	28,29,30,31	0
4	FAD	C	1031	53/53	0.94	0.08	26,31,33,34	0
4	FAD	D	1031	53/53	0.94	0.08	25,28,35,37	0
2	SF4	A	1028	8/8	0.95	0.07	21,23,24,24	0
2	SF4	D	1027	8/8	0.95	0.07	22,23,24,24	0
2	SF4	B	1027	8/8	0.95	0.07	18,19,21,21	0
2	SF4	D	1029	8/8	0.95	0.07	29,30,31,31	0
2	SF4	A	1027	8/8	0.95	0.07	17,20,20,21	0
2	SF4	C	1028	8/8	0.95	0.06	23,25,26,26	0
2	SF4	C	1029	8/8	0.95	0.07	24,25,27,27	0
4	FAD	B	1031	53/53	0.96	0.07	22,26,32,34	0

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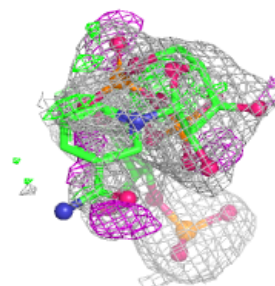
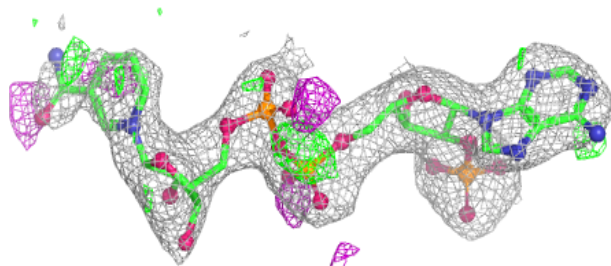
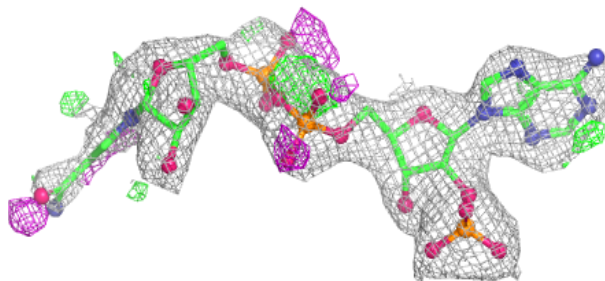
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FAD	A	1031	53/53	0.97	0.06	21,26,32,33	0
3	FMN	A	1030	31/31	0.97	0.06	16,19,21,22	0
3	FMN	B	1030	31/31	0.97	0.06	17,19,21,22	0
3	FMN	C	1030	31/31	0.97	0.05	16,20,22,22	0
3	FMN	D	1030	31/31	0.98	0.04	16,20,22,23	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.

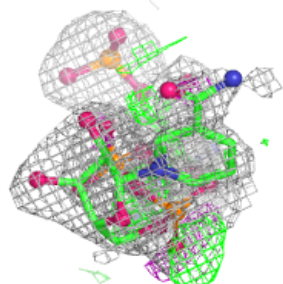
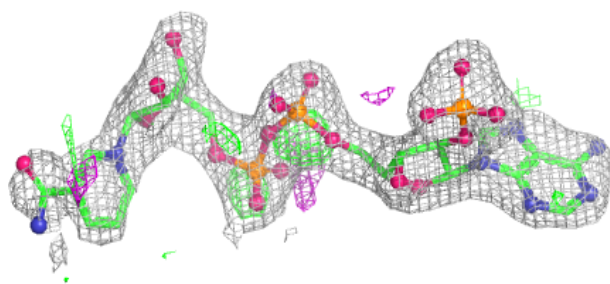
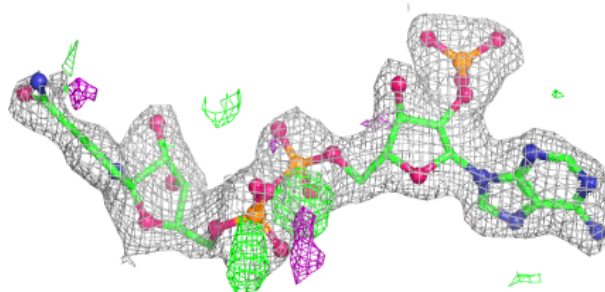
Electron density around NDP D 1032:

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

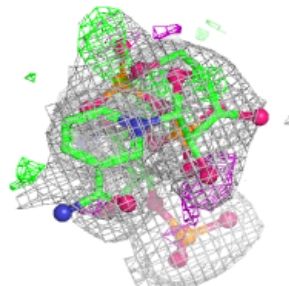
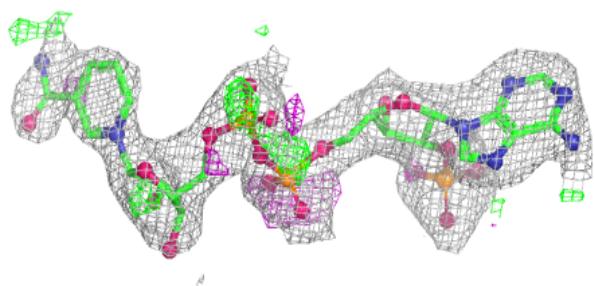
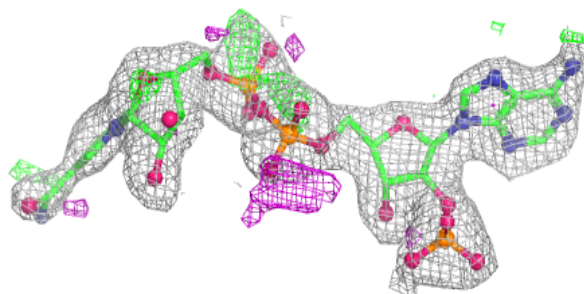


Electron density around NDP C 1032:

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

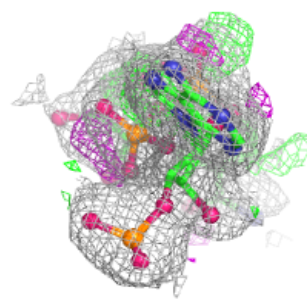
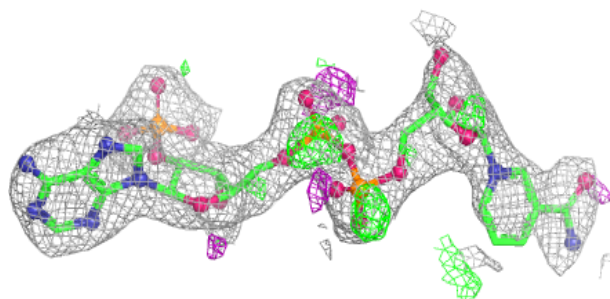
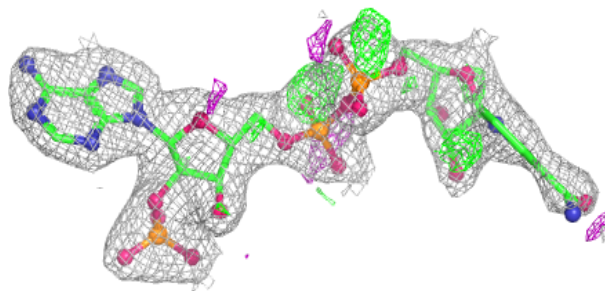
**Electron density around NDP B 1032:**

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and green (positive)

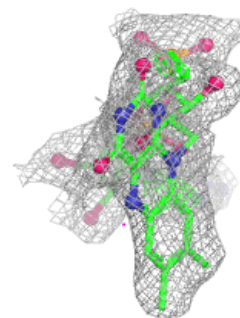
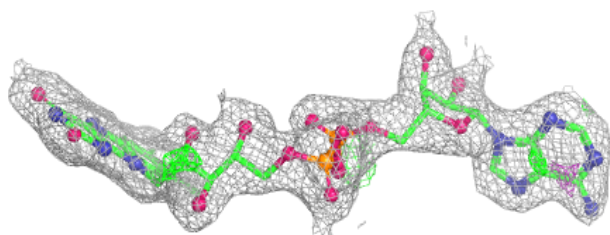
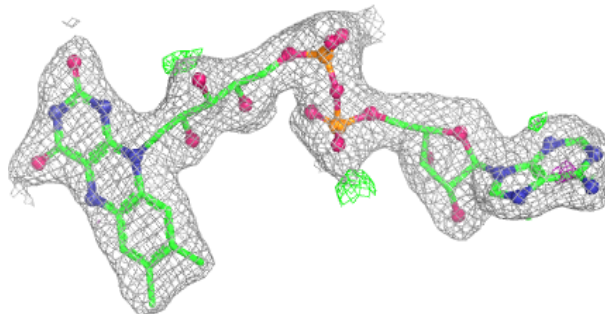


Electron density around NDP A 1032:

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

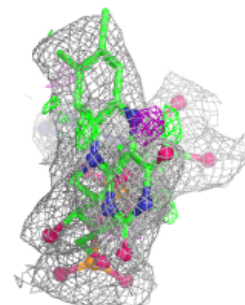
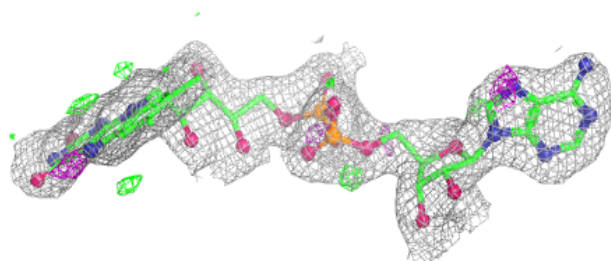
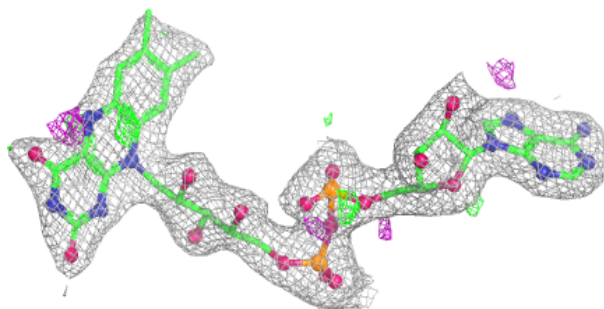
**Electron density around FAD C 1031:**

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

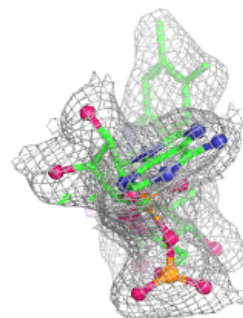
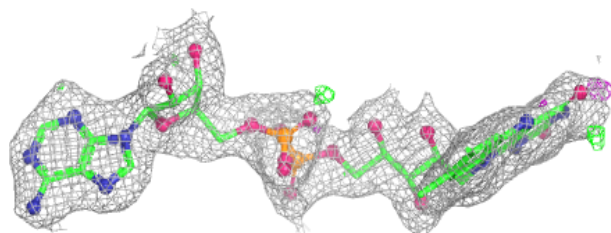
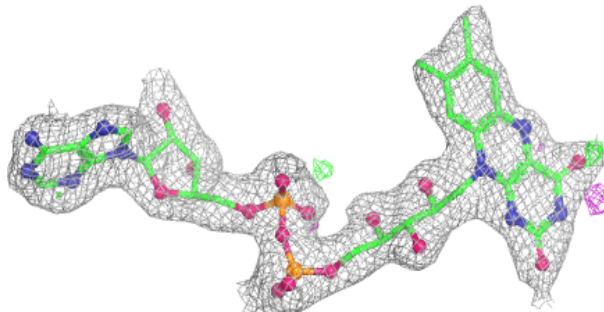


Electron density around FAD D 1031:

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

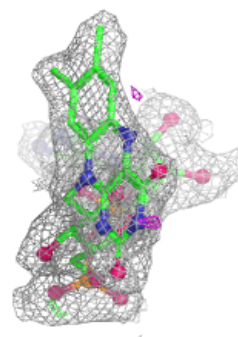
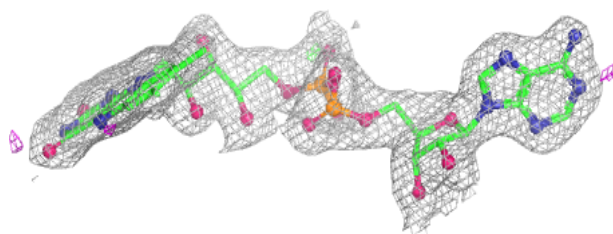
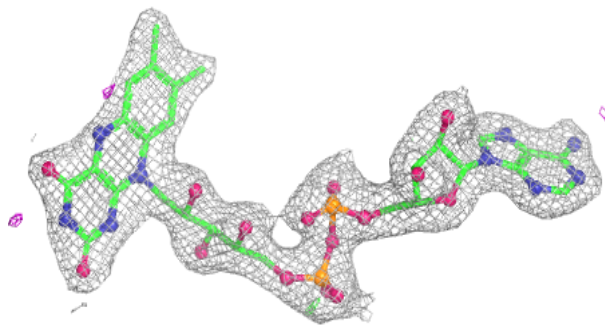
**Electron density around FAD B 1031:**

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



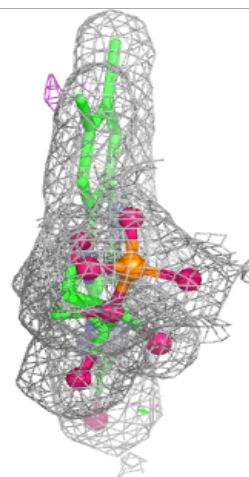
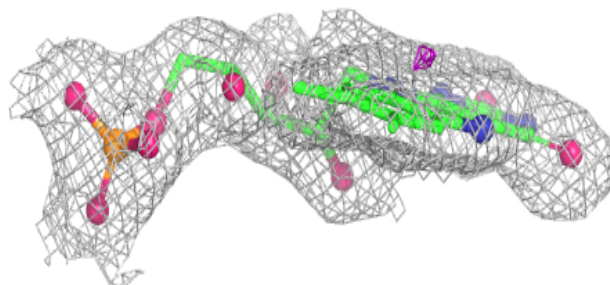
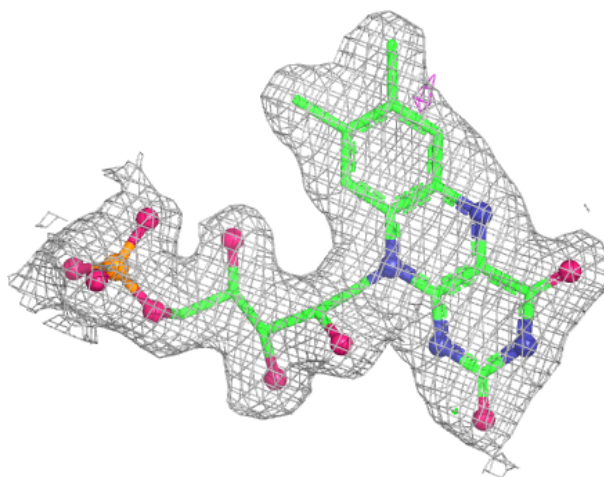
Electron density around FAD A 1031:

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and green (positive)



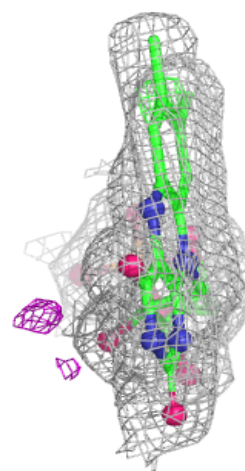
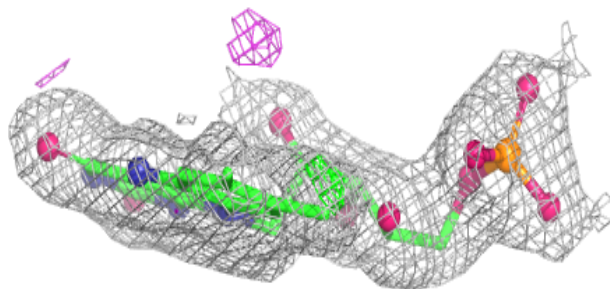
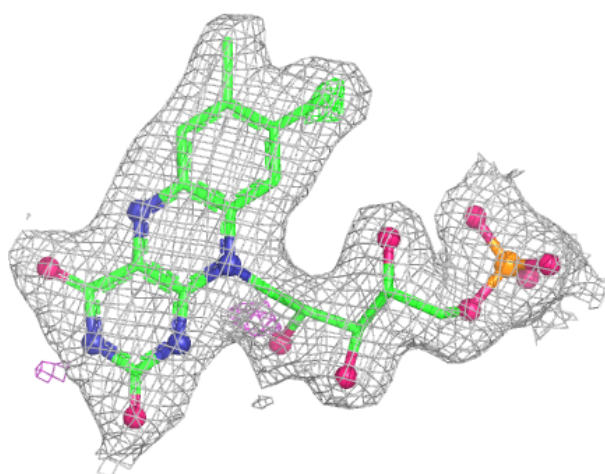
Electron density around FMN A 1030:

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



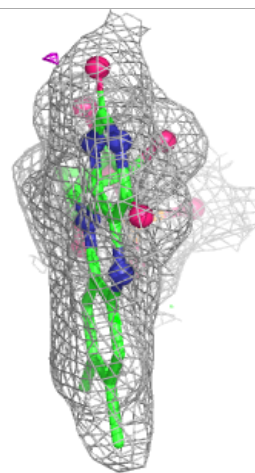
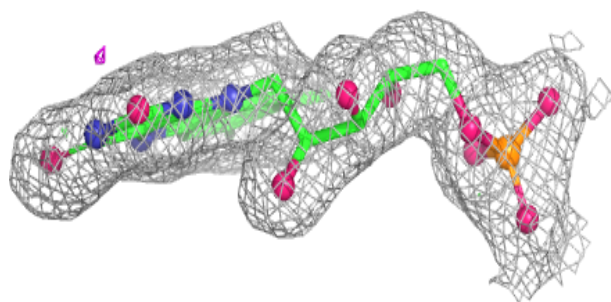
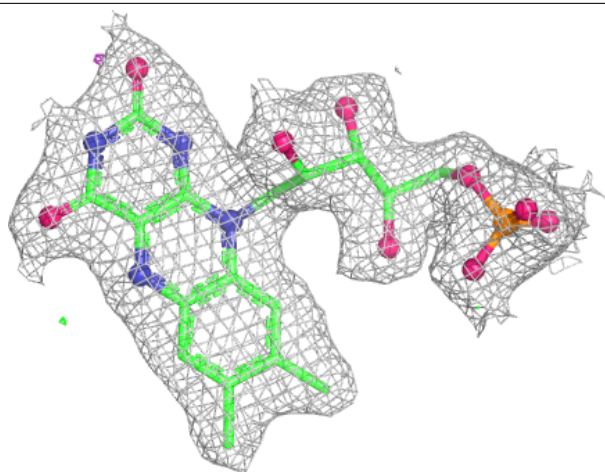
Electron density around FMN B 1030:

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



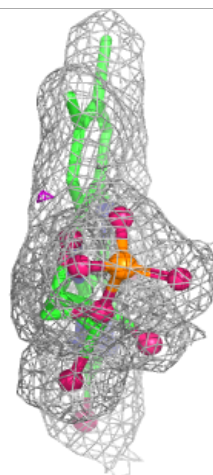
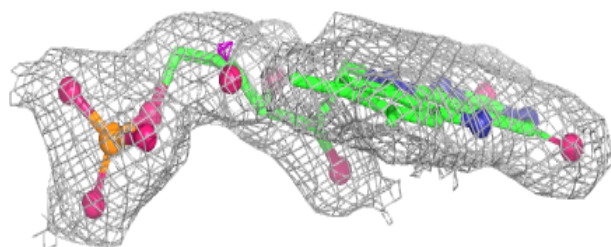
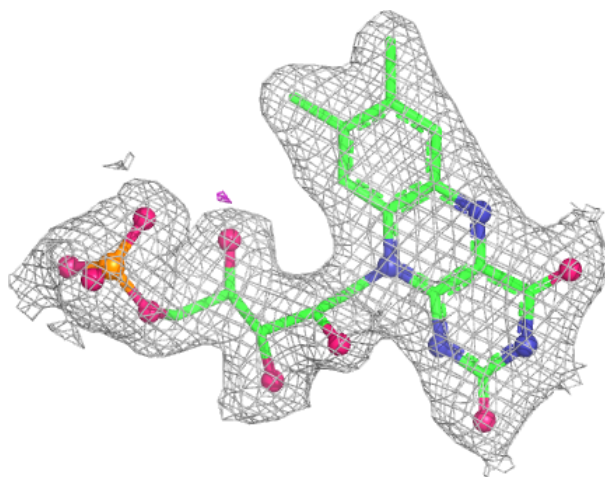
Electron density around FMN C 1030:

$2mF_o-DF_c$ (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.