



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:58 AM UTC

PDB ID : 1GT8 / pdb_00001gt8
Title : DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG,
TERNARY COMPLEX WITH NADPH AND URACIL-4-ACETIC ACID
Authors : Dobritsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2002-01-14
Resolution : 3.30 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

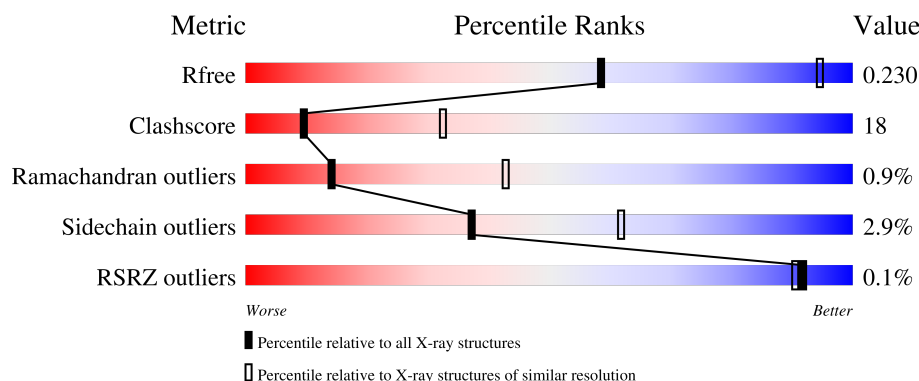
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	 67% 30% ..
1	B	1025	 65% 30% ..
1	C	1025	 63% 33% ..
1	D	1025	 60% 36% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	A	1027	-	-	X	-
2	SF4	A	1028	-	-	X	-
2	SF4	B	1026	-	-	X	-
2	SF4	B	1027	-	-	X	-
2	SF4	B	1028	-	-	X	-
2	SF4	B	1029	-	-	X	-
2	SF4	C	1027	-	-	X	-
2	SF4	C	1028	-	-	X	-
2	SF4	D	1027	-	-	X	-
2	SF4	D	1028	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31588 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.

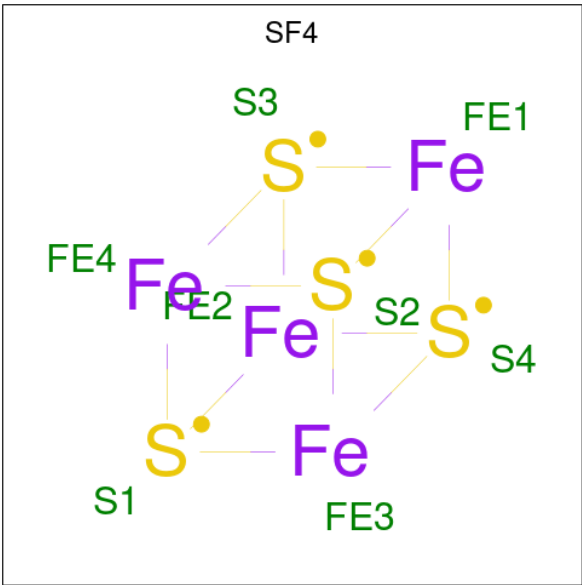
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			7755	4919	1312	1468	56			
1	B	1010	Total	C	N	O	S	0	0	0
			7703	4885	1304	1458	56			
1	C	1010	Total	C	N	O	S	0	0	0
			7708	4892	1303	1459	54			
1	D	1012	Total	C	N	O	S	0	0	0
			7718	4894	1307	1461	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).



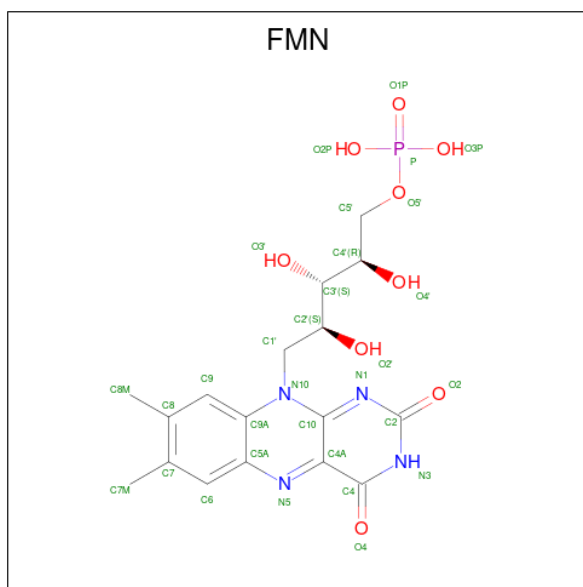
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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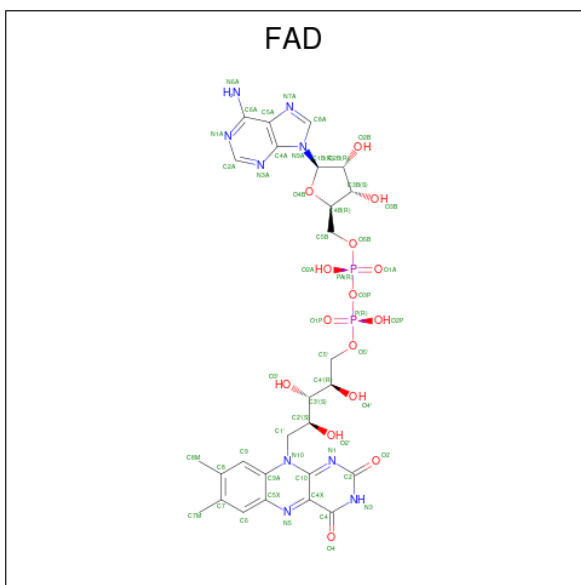
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

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



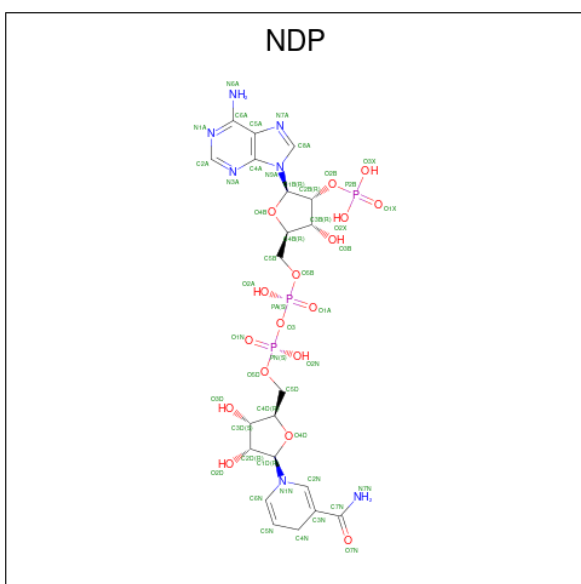
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



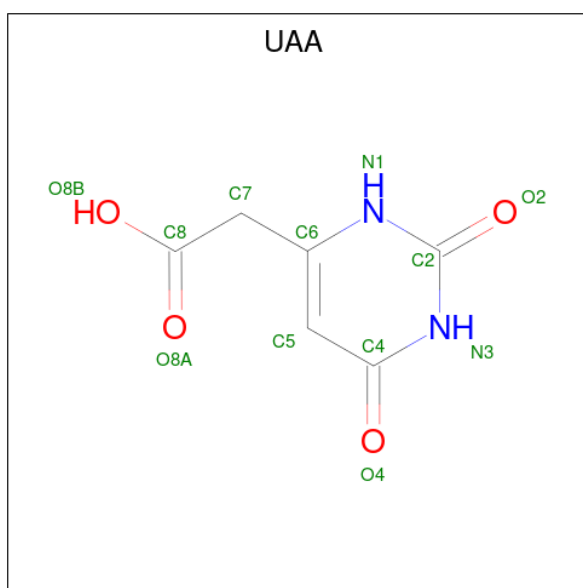
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- 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 URACIL-6-ACETIC ACID (CCD ID: UAA) (formula: $C_6H_6N_2O_4$).

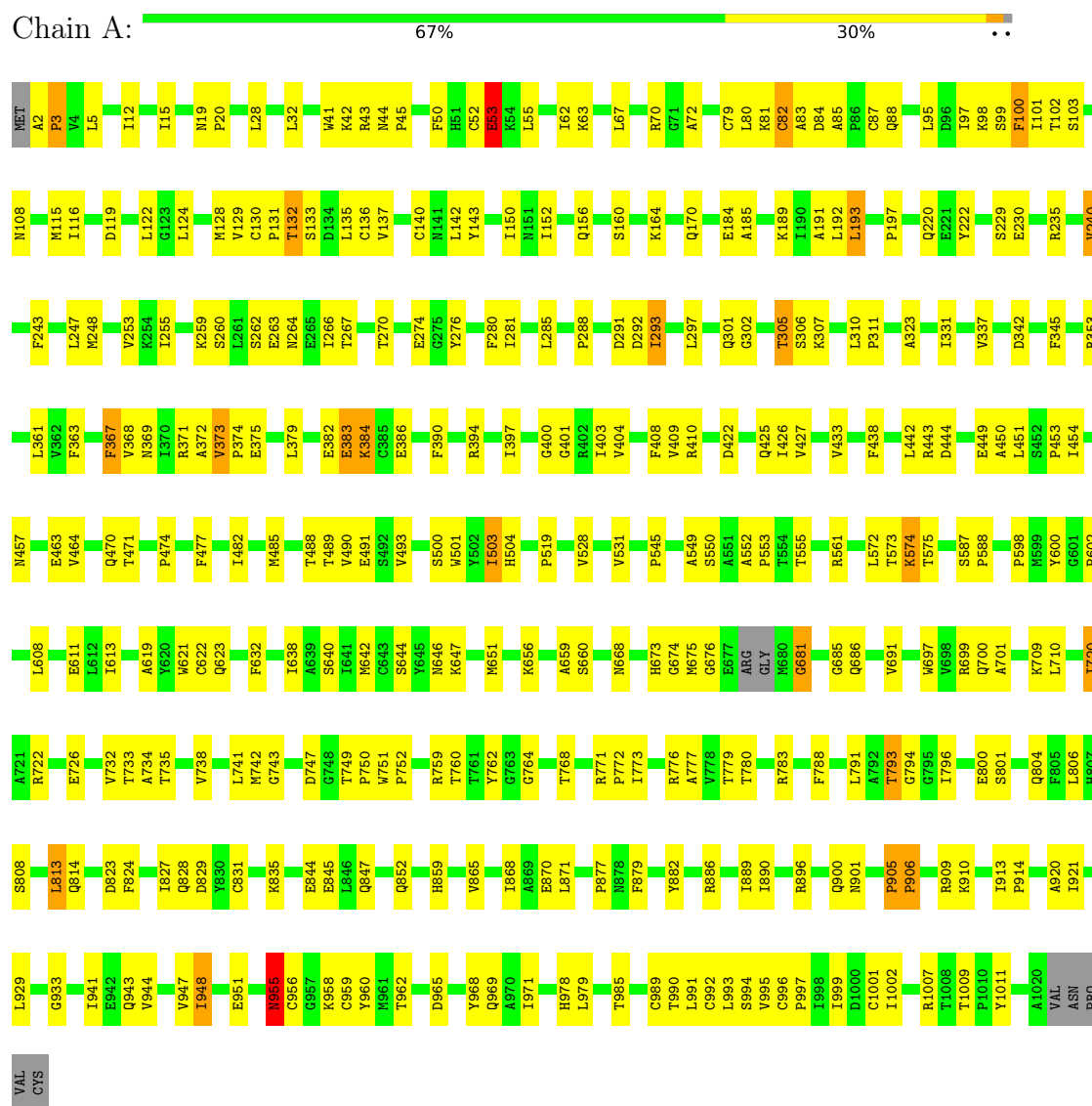


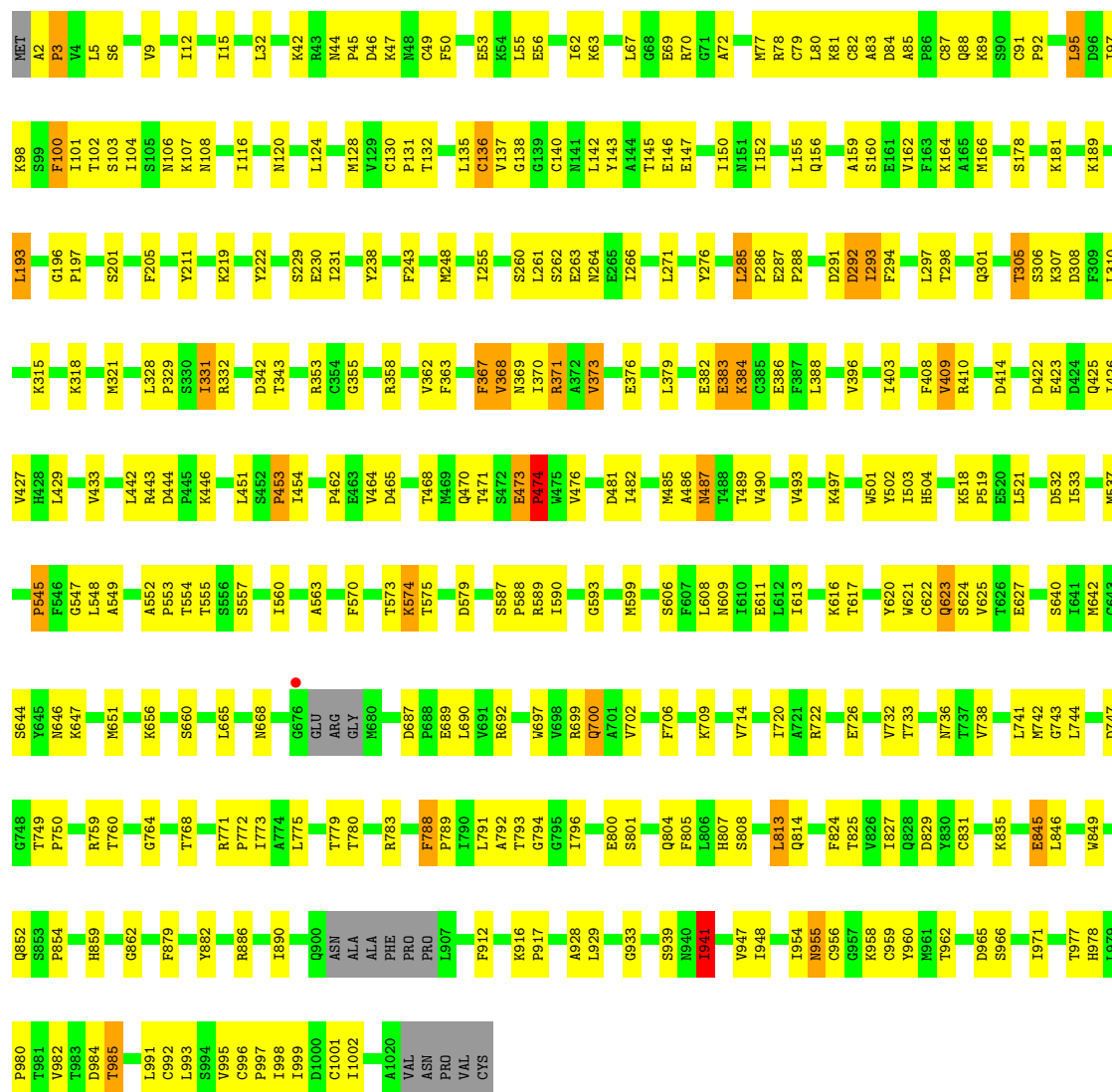
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	2	4		
6	B	1	Total	C	N	O	0	0
			12	6	2	4		
6	C	1	Total	C	N	O	0	0
			12	6	2	4		
6	D	1	Total	C	N	O	0	0
			12	6	2	4		

3 Residue-property plots

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

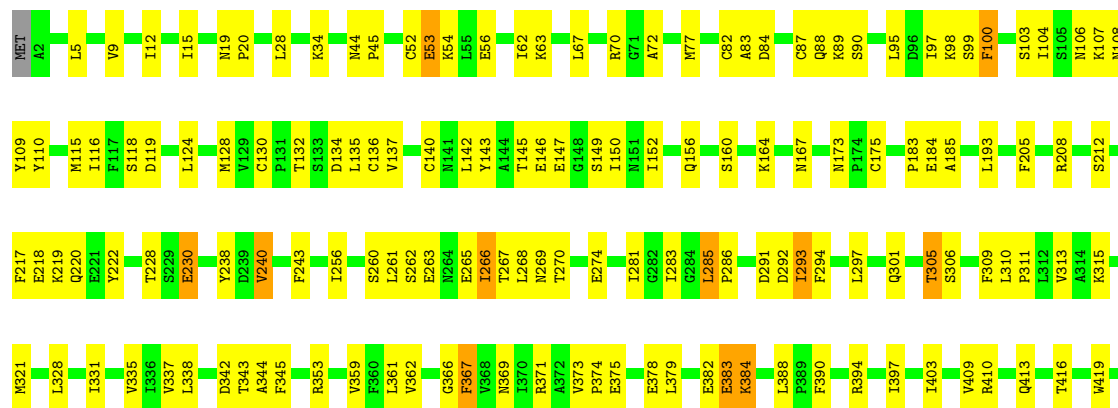
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

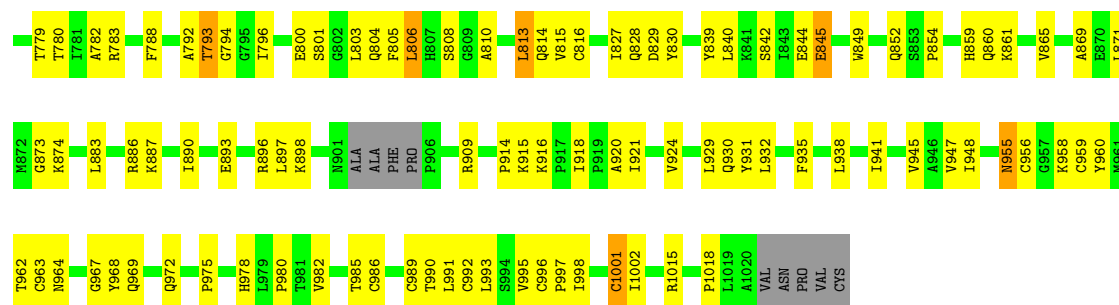




• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain C: 63% 33%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.03Å 159.53Å 166.02Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	29.75 – 3.30 29.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.75-3.30) 98.3 (29.75-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.269 (Not available) , 0.230	Depositor DCC
R_{free} test set	1247 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31588	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: FMN, FAD, SF4, NDP, UAA

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	0.58	0/7916	1.00	37/10729 (0.3%)
1	B	0.57	0/7860	1.00	37/10649 (0.3%)
1	C	0.52	0/7868	1.00	33/10667 (0.3%)
1	D	0.50	0/7876	0.98	28/10671 (0.3%)
All	All	0.54	0/31520	0.99	135/42716 (0.3%)

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	LEU	CA-C-N	10.12	130.41	119.28
1	B	285	LEU	C-N-CA	10.12	130.41	119.28
1	A	285	LEU	CA-C-N	9.60	129.35	119.56
1	A	285	LEU	C-N-CA	9.60	129.35	119.56
1	C	904	PHE	CA-C-N	9.19	129.84	120.38
1	C	904	PHE	C-N-CA	9.19	129.84	120.38
1	C	285	LEU	CA-C-N	8.73	128.47	119.56
1	C	285	LEU	C-N-CA	8.73	128.47	119.56
1	D	285	LEU	CA-C-N	8.57	129.41	119.47
1	D	285	LEU	C-N-CA	8.57	129.41	119.47
1	C	788	PHE	CA-C-N	8.52	129.04	119.93
1	C	788	PHE	C-N-CA	8.52	129.04	119.93
1	C	143	TYR	N-CA-C	-8.12	102.63	112.54
1	A	503	ILE	N-CA-C	-8.03	102.44	110.62
1	C	743	GLY	N-CA-C	7.91	120.23	111.85
1	C	503	ILE	N-CA-C	-7.83	102.64	110.62
1	C	905	PRO	N-CA-C	7.68	120.07	110.70
1	D	521	LEU	CA-C-N	7.30	127.30	119.78
1	D	521	LEU	C-N-CA	7.30	127.30	119.78
1	C	521	LEU	CA-C-N	7.18	127.18	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	521	LEU	C-N-CA	7.18	127.18	119.78
1	C	632	PHE	CA-C-N	7.03	127.01	119.28
1	C	632	PHE	C-N-CA	7.03	127.01	119.28
1	B	788	PHE	CA-C-N	6.95	127.37	119.93
1	B	788	PHE	C-N-CA	6.95	127.37	119.93
1	C	574	LYS	N-CA-C	-6.93	101.24	110.24
1	B	143	TYR	N-CA-C	-6.88	104.15	112.54
1	A	574	LYS	N-CA-C	-6.87	101.31	110.24
1	C	305	THR	N-CA-C	-6.86	98.74	109.72
1	A	955	ASN	N-CA-C	6.85	120.94	111.90
1	B	743	GLY	N-CA-C	6.80	119.06	111.85
1	D	85	ALA	CA-C-N	6.77	126.36	119.19
1	D	85	ALA	C-N-CA	6.77	126.36	119.19
1	A	632	PHE	CA-C-N	6.75	126.71	119.28
1	A	632	PHE	C-N-CA	6.75	126.71	119.28
1	A	806	LEU	N-CA-C	-6.74	103.87	111.14
1	A	82	CYS	N-CA-C	6.71	119.21	110.43
1	D	1001	CYS	N-CA-C	-6.70	103.45	111.69
1	B	941	ILE	N-CA-C	-6.60	106.36	112.96
1	A	400	GLY	N-CA-C	-6.58	106.36	114.92
1	D	955	ASN	N-CA-C	6.57	120.61	112.47
1	A	1001	CYS	N-CA-C	-6.55	103.63	111.69
1	D	675	MET	N-CA-C	6.53	121.16	111.04
1	B	545	PRO	N-CA-C	6.50	122.36	113.98
1	C	941	ILE	N-CA-C	-6.47	106.49	112.96
1	D	788	PHE	CA-C-N	6.41	126.79	119.93
1	D	788	PHE	C-N-CA	6.41	126.79	119.93
1	B	574	LYS	N-CA-C	-6.37	101.97	110.24
1	A	788	PHE	CA-C-N	6.32	126.69	119.93
1	A	788	PHE	C-N-CA	6.32	126.69	119.93
1	D	806	LEU	N-CA-C	-6.32	104.32	111.14
1	C	955	ASN	N-CA-C	6.25	120.15	111.90
1	C	240	VAL	N-CA-C	-6.23	104.43	110.72
1	D	143	TYR	N-CA-C	-6.21	104.61	111.82
1	B	136	CYS	N-CA-C	6.17	117.68	111.07
1	B	955	ASN	N-CA-C	6.14	120.01	111.90
1	A	305	THR	N-CA-C	-6.14	99.90	109.72
1	B	1001	CYS	N-CA-C	-6.12	104.68	111.36
1	B	521	LEU	CA-C-N	6.12	126.47	119.92
1	B	521	LEU	C-N-CA	6.12	126.47	119.92
1	A	905	PRO	CA-C-N	6.10	127.46	119.84
1	A	905	PRO	C-N-CA	6.10	127.46	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	LYS	N-CA-C	6.09	120.04	112.24
1	D	305	THR	N-CA-C	-6.09	99.88	109.50
1	D	545	PRO	N-CA-C	6.08	121.75	113.84
1	B	305	THR	N-CA-C	-6.05	100.05	109.72
1	B	503	ILE	N-CA-C	-6.04	104.46	110.62
1	B	985	THR	N-CA-C	-6.00	105.96	113.28
1	A	545	PRO	N-CA-C	5.99	121.71	113.98
1	A	323	ALA	N-CA-C	-5.99	104.83	111.36
1	A	143	TYR	N-CA-C	-5.96	105.27	112.54
1	C	545	PRO	N-CA-C	5.90	121.59	113.98
1	D	574	LYS	N-CA-C	-5.88	102.35	110.35
1	A	941	ILE	N-CA-C	-5.88	106.54	113.42
1	B	5	LEU	N-CA-C	5.85	117.66	111.28
1	A	240	VAL	N-CA-C	-5.84	104.63	111.00
1	C	619	ALA	N-CA-C	-5.84	104.60	110.97
1	B	476	VAL	N-CA-C	5.82	116.25	107.75
1	A	85	ALA	N-CA-C	5.78	116.68	109.57
1	D	135	LEU	N-CA-C	5.76	114.28	108.75
1	D	632	PHE	CA-C-N	5.66	125.28	119.56
1	D	632	PHE	C-N-CA	5.66	125.28	119.56
1	B	623	GLN	N-CA-C	-5.62	105.07	111.14
1	A	135	LEU	CB-CA-C	-5.61	108.34	116.54
1	A	948	ILE	N-CA-C	5.55	117.31	108.87
1	D	503	ILE	N-CA-C	-5.53	104.98	110.62
1	D	148	GLY	N-CA-C	5.53	119.91	112.17
1	A	743	GLY	N-CA-C	5.50	117.67	111.85
1	C	904	PHE	CA-C-O	5.48	122.85	119.29
1	D	212	SER	N-CA-C	5.48	120.07	113.17
1	B	617	THR	N-CA-C	5.46	117.78	110.35
1	A	824	PHE	N-CA-C	5.46	118.73	111.75
1	B	287	GLU	CA-C-N	5.45	125.35	119.85
1	B	287	GLU	C-N-CA	5.45	125.35	119.85
1	A	623	GLN	N-CA-C	-5.44	105.43	111.36
1	D	68	GLY	N-CA-C	-5.43	104.01	112.58
1	C	230	GLU	N-CA-C	5.40	120.36	113.18
1	D	230	GLU	N-CA-C	5.39	120.35	113.18
1	C	806	LEU	N-CA-C	-5.39	105.48	111.36
1	D	5	LEU	N-CA-C	5.39	117.15	111.28
1	A	910	LYS	CA-C-N	5.36	125.30	119.78
1	A	910	LYS	C-N-CA	5.36	125.30	119.78
1	C	824	PHE	N-CA-C	5.36	118.61	111.75
1	A	384	LYS	N-CA-C	5.36	118.97	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	384	LYS	N-CA-C	5.35	119.09	112.24
1	B	231	ILE	CA-C-N	5.35	125.36	119.90
1	B	231	ILE	C-N-CA	5.35	125.36	119.90
1	D	131	PRO	N-CA-C	-5.35	105.26	112.48
1	A	85	ALA	CA-C-N	5.34	124.85	119.19
1	A	85	ALA	C-N-CA	5.34	124.85	119.19
1	C	383	GLU	N-CA-C	-5.34	106.95	112.93
1	B	473	GLU	CA-C-N	5.34	126.51	119.84
1	B	473	GLU	C-N-CA	5.34	126.51	119.84
1	B	383	GLU	N-CA-C	-5.33	106.96	112.93
1	B	518	LYS	CA-C-N	5.32	126.49	119.84
1	B	518	LYS	C-N-CA	5.32	126.49	119.84
1	B	85	ALA	CA-C-N	5.24	126.39	119.84
1	B	85	ALA	C-N-CA	5.24	126.39	119.84
1	A	383	GLU	N-CA-C	-5.24	107.06	112.93
1	A	229	SER	N-CA-C	5.23	118.92	112.54
1	B	579	ASP	N-CA-C	5.22	117.65	111.33
1	C	617	THR	N-CA-C	5.22	117.45	110.35
1	C	1001	CYS	N-CA-C	-5.21	105.68	111.36
1	C	948	ILE	N-CA-C	5.21	116.47	108.71
1	B	120	ASN	CA-C-N	5.17	126.30	119.84
1	B	120	ASN	C-N-CA	5.17	126.30	119.84
1	D	615	GLU	N-CA-C	-5.14	106.69	113.17
1	D	383	GLU	N-CA-C	-5.11	107.20	112.93
1	C	579	ASP	N-CA-C	5.11	117.24	111.11
1	A	401	GLY	N-CA-C	-5.10	107.56	115.67
1	A	619	ALA	N-CA-C	-5.08	105.63	111.07
1	C	212	SER	N-CA-C	5.08	119.63	113.38
1	B	229	SER	N-CA-C	5.08	118.74	112.54
1	C	971	ILE	N-CA-C	5.04	115.17	108.11
1	A	397	ILE	N-CA-C	5.00	115.78	108.58

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	7755	0	7781	279	0
1	B	7703	0	7735	286	0
1	C	7708	0	7743	331	0
1	D	7718	0	7750	335	0
2	A	32	0	0	6	0
2	B	32	0	0	8	0
2	C	32	0	0	6	0
2	D	32	0	0	8	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	1	0
4	B	53	0	31	1	0
4	C	53	0	31	2	0
4	D	53	0	31	5	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	6	0
6	A	12	0	5	1	0
6	B	12	0	5	1	0
6	C	12	0	5	1	0
6	D	12	0	5	0	0
All	All	31588	0	31333	1120	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 18.

All (1120) 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:136:CYS:SG	1:C:137:VAL:HG23	2.02	1.00
1:C:116:ILE:HD13	1:C:156:GLN:HG3	1.43	0.99
1:A:485:MET:HE1	1:B:32:LEU:HB2	1.46	0.97
1:C:410:ARG:NH1	1:D:427:VAL:HG13	1.84	0.92
1:A:32:LEU:HB2	1:B:485:MET:HE1	1.50	0.91
1:C:776:ARG:O	1:C:780:THR:HG22	1.71	0.90
1:A:608:LEU:HB2	1:A:742:MET:HE2	1.54	0.90
1:C:173:ASN:HD21	1:C:175:CYS:HB2	1.36	0.90
1:C:136:CYS:SG	1:C:137:VAL:N	2.44	0.88
1:A:608:LEU:HD13	1:A:742:MET:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:HIS:HD2	1:D:690:LEU:HD11	1.39	0.87
1:A:501:TRP:O	1:A:504:HIS:HB3	1.75	0.86
1:C:608:LEU:HD13	1:C:742:MET:HB2	1.58	0.86
1:D:116:ILE:HD13	1:D:156:GLN:HG3	1.57	0.85
1:D:608:LEU:HD13	1:D:742:MET:HB2	1.59	0.85
1:D:651:MET:HE3	1:D:700:GLN:HG3	1.58	0.85
1:B:95:LEU:HD21	1:B:116:ILE:HG23	1.59	0.84
1:B:549:ALA:HB2	1:B:814:GLN:HB3	1.59	0.84
1:C:485:MET:HE1	1:D:32:LEU:HB2	1.58	0.84
1:A:63:LYS:HE3	1:A:128:MET:HG2	1.59	0.84
1:D:673:HIS:CD2	1:D:690:LEU:HD11	2.13	0.84
1:C:410:ARG:NH2	1:D:427:VAL:HG22	1.93	0.83
1:A:896:ARG:HH21	1:A:900:GLN:HE22	1.22	0.83
1:C:410:ARG:HH22	1:D:427:VAL:HG22	1.42	0.83
1:C:362:VAL:HG22	1:C:388:LEU:HB2	1.61	0.83
1:A:549:ALA:HB2	1:A:814:GLN:HB3	1.61	0.82
1:C:291:ASP:OD1	1:C:293:ILE:HG12	1.79	0.82
1:D:572:LEU:HD13	1:D:638:ILE:HB	1.60	0.81
1:D:839:TYR:HA	1:D:918:ILE:HD12	1.62	0.81
1:B:342:ASP:HB3	5:B:1032:NDP:H42N	1.63	0.81
1:A:427:VAL:HG22	1:B:410:ARG:HH21	1.47	0.80
1:C:410:ARG:HE	1:D:410:ARG:NH2	1.79	0.80
1:D:124:LEU:HD23	1:D:240:VAL:HG13	1.63	0.80
1:D:842:SER:HB3	1:D:918:ILE:HD13	1.65	0.79
1:D:410:ARG:HH11	1:D:410:ARG:HG3	1.46	0.79
1:D:342:ASP:HB3	5:D:1032:NDP:H42N	1.65	0.78
1:C:501:TRP:O	1:C:504:HIS:HB3	1.83	0.78
1:B:193:LEU:HG	1:B:261:LEU:HD22	1.67	0.77
1:C:651:MET:HE3	1:C:700:GLN:HG3	1.66	0.77
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.64	0.77
1:D:673:HIS:HD2	1:D:690:LEU:CD1	1.97	0.77
1:C:173:ASN:ND2	1:C:175:CYS:HB2	2.00	0.77
1:C:549:ALA:HB2	1:C:814:GLN:HB3	1.64	0.77
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.66	0.77
1:B:608:LEU:HD13	1:B:742:MET:HB2	1.67	0.76
1:C:369:ASN:HA	1:D:50:PHE:HE2	1.50	0.76
1:C:343:THR:HG23	4:C:1031:FAD:HM72	1.67	0.76
1:A:962:THR:HG21	1:A:991:LEU:HB3	1.68	0.75
1:C:820:GLN:O	1:D:962:THR:HG22	1.86	0.75
1:A:611:GLU:O	6:A:1035:UAA:H5	1.85	0.75
1:B:193:LEU:HD12	1:B:261:LEU:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:ASP:HB3	1:B:690:LEU:HD12	1.69	0.75
1:A:747:ASP:OD2	1:A:749:THR:HG23	1.86	0.74
1:B:487:ASN:N	1:B:487:ASN:HD22	1.85	0.74
1:C:369:ASN:HA	1:D:50:PHE:CE2	2.24	0.73
1:B:768:THR:HG22	1:B:771:ARG:HH21	1.53	0.73
1:D:87:CYS:SG	1:D:97:ILE:HD12	2.28	0.73
1:A:451:LEU:O	1:A:454:ILE:HG12	1.88	0.73
1:B:422:ASP:OD2	1:B:425:GLN:HG3	1.88	0.73
1:A:342:ASP:HB3	5:A:1032:NDP:H42N	1.69	0.73
1:A:451:LEU:HB3	1:A:454:ILE:HD11	1.71	0.73
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.71	0.73
1:B:62:ILE:HD12	1:B:379:LEU:HD22	1.70	0.73
1:C:647:LYS:HA	1:C:697:TRP:CE3	2.24	0.73
1:B:343:THR:HG23	4:B:1031:FAD:HM72	1.71	0.72
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.70	0.72
1:D:331:ILE:HG23	1:D:433:VAL:HG21	1.70	0.72
1:C:477:PHE:CD1	1:C:503:ILE:HG12	2.24	0.72
1:A:133:SER:HB3	1:A:375:GLU:OE1	1.90	0.72
1:A:427:VAL:HG22	1:B:410:ARG:NH2	2.05	0.72
1:A:410:ARG:NH2	1:B:427:VAL:CG2	2.53	0.72
1:C:146:GLU:HG2	1:D:67:LEU:HD23	1.70	0.72
1:D:78:ARG:NH2	1:D:150:ILE:HD13	2.05	0.71
1:A:410:ARG:HH21	1:B:427:VAL:HG22	1.55	0.71
1:C:573:THR:OG1	1:C:639:ALA:HA	1.89	0.71
1:C:962:THR:OG1	1:C:995:VAL:HG21	1.90	0.71
1:C:394:ARG:HG3	1:C:409:VAL:HG13	1.71	0.71
1:C:762:TYR:CZ	1:D:780:THR:HG22	2.26	0.71
1:B:294:PHE:HA	1:B:297:LEU:HD12	1.73	0.71
1:C:779:THR:O	1:C:783:ARG:HG3	1.90	0.71
1:A:87:CYS:SG	1:A:97:ILE:HD12	2.30	0.71
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.72	0.71
1:D:337:VAL:HB	1:D:361:LEU:HD23	1.72	0.70
1:D:451:LEU:HD13	1:D:454:ILE:HD11	1.73	0.70
1:A:267:THR:OG1	1:A:270:THR:HG23	1.91	0.70
1:D:410:ARG:HH11	1:D:410:ARG:CG	2.04	0.70
1:A:367:PHE:HB2	1:B:386:GLU:OE1	1.91	0.70
1:D:549:ALA:HB2	1:D:814:GLN:HB3	1.74	0.70
1:D:201:SER:HB2	1:D:493:VAL:HG13	1.73	0.70
1:D:259:LYS:HB3	1:D:266:ILE:HD11	1.73	0.70
1:B:608:LEU:HB2	1:B:742:MET:HE2	1.73	0.69
1:C:150:ILE:HB	2:C:1027:SF4:S4	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:THR:HB	1:D:814:GLN:HB2	1.72	0.69
1:A:62:ILE:HD12	1:A:379:LEU:HD22	1.74	0.69
1:B:470:GLN:NE2	1:B:474:PRO:HA	2.07	0.69
1:A:95:LEU:HD23	1:A:119:ASP:HB2	1.72	0.69
1:A:779:THR:HG22	1:A:808:SER:HB3	1.73	0.69
1:B:608:LEU:HD23	1:B:609:ASN:N	2.07	0.69
1:C:9:VAL:HG22	1:C:12:ILE:HG12	1.74	0.69
1:D:394:ARG:HG3	1:D:409:VAL:HG13	1.73	0.69
1:C:959:CYS:HB2	1:C:992:CYS:HB2	1.73	0.69
1:D:52:CYS:HB3	1:D:384:LYS:HG2	1.75	0.69
1:A:651:MET:HE3	1:A:700:GLN:HG3	1.74	0.69
1:D:108:ASN:HA	1:D:852:GLN:NE2	2.08	0.69
1:D:776:ARG:O	1:D:780:THR:HG23	1.93	0.69
1:B:116:ILE:HD13	1:B:156:GLN:HG3	1.75	0.68
1:C:427:VAL:HG21	1:D:410:ARG:HH21	1.57	0.68
1:A:52:CYS:HB2	1:A:384:LYS:HG2	1.74	0.68
1:B:992:CYS:SG	1:B:993:LEU:N	2.66	0.68
1:B:993:LEU:C	1:B:993:LEU:HD23	2.19	0.68
1:D:180:GLU:CD	1:D:180:GLU:H	2.01	0.68
1:D:722:ARG:O	1:D:726:GLU:HG3	1.94	0.68
1:B:779:THR:HG23	1:B:808:SER:HB3	1.75	0.68
1:C:342:ASP:HB3	5:C:1032:NDP:H42N	1.76	0.68
1:B:297:LEU:HA	1:B:301:GLN:OE1	1.94	0.68
1:A:896:ARG:HH21	1:A:900:GLN:NE2	1.93	0.67
1:A:422:ASP:OD2	1:A:425:GLN:HG3	1.95	0.67
1:D:996:CYS:HA	2:D:1028:SF4:S3	2.35	0.67
1:D:992:CYS:SG	1:D:993:LEU:N	2.68	0.67
1:D:699:ARG:HE	1:D:699:ARG:HA	1.60	0.67
1:B:747:ASP:OD2	1:B:749:THR:HG23	1.95	0.67
1:C:457:ASN:HB3	1:C:463:GLU:OE1	1.94	0.67
1:D:616:LYS:HD3	1:D:620:TYR:CE2	2.30	0.67
1:C:283:ILE:HG13	1:C:482:ILE:HD13	1.78	0.66
1:A:410:ARG:CZ	1:B:410:ARG:NH2	2.58	0.66
1:B:87:CYS:SG	1:B:97:ILE:HD12	2.35	0.66
1:C:811:SER:HA	1:C:925:ILE:HD13	1.77	0.66
1:B:219:LYS:HG3	1:B:260:SER:OG	1.93	0.66
1:C:193:LEU:HD23	1:C:281:ILE:HD13	1.76	0.66
1:A:342:ASP:HB2	5:A:1032:NDP:C5N	2.25	0.66
1:C:611:GLU:O	6:C:1035:UAA:H5	1.95	0.66
1:D:328:LEU:HD12	1:D:329:PRO:HD2	1.76	0.66
1:C:261:LEU:HD12	1:C:266:ILE:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:CYS:HA	2:B:1028:SF4:S3	2.35	0.66
1:A:80:LEU:HD11	1:B:954:ILE:HD11	1.78	0.66
1:C:578:LEU:HD23	1:C:653:LEU:HD13	1.78	0.66
1:D:291:ASP:OD1	1:D:293:ILE:HG13	1.96	0.66
1:C:557:SER:HA	1:C:560:ILE:HD12	1.77	0.66
1:C:427:VAL:HG13	1:D:410:ARG:HE	1.60	0.65
1:C:954:ILE:HD11	1:D:80:LEU:HD11	1.77	0.65
1:D:568:TRP:NE1	1:D:827:ILE:HB	2.12	0.65
1:B:150:ILE:HB	2:B:1027:SF4:S4	2.36	0.65
1:D:699:ARG:HA	1:D:699:ARG:NE	2.11	0.65
1:A:369:ASN:HD22	1:B:50:PHE:HE2	1.43	0.65
1:C:709:LYS:HA	1:C:733:THR:HB	1.79	0.65
1:C:294:PHE:HA	1:C:297:LEU:HD12	1.78	0.65
1:C:335:VAL:HB	1:C:359:VAL:HG22	1.79	0.65
1:D:873:GLY:O	1:D:874:LYS:HD3	1.97	0.65
1:B:859:HIS:HD2	1:B:862:GLY:H	1.45	0.65
1:C:378:GLU:O	1:C:382:GLU:HG2	1.97	0.65
1:A:342:ASP:CB	5:A:1032:NDP:H42N	2.27	0.64
1:A:342:ASP:OD1	1:A:372:ALA:HB1	1.96	0.64
1:D:860:GLN:O	1:D:861:LYS:HB2	1.95	0.64
1:C:130:CYS:SG	1:C:490:VAL:HB	2.38	0.64
1:D:82:CYS:O	1:D:98:LYS:HD2	1.97	0.64
1:B:408:PHE:CE1	1:B:429:LEU:HD12	2.32	0.64
1:C:410:ARG:CZ	1:D:427:VAL:HG22	2.28	0.64
1:D:150:ILE:HB	2:D:1027:SF4:S4	2.37	0.64
1:D:959:CYS:HB2	1:D:992:CYS:HB2	1.78	0.64
1:C:310:LEU:HB2	1:C:311:PRO:HD3	1.79	0.64
1:C:342:ASP:HB2	5:C:1032:NDP:C5N	2.27	0.64
1:C:615:GLU:O	1:D:1015:ARG:HD3	1.98	0.64
1:B:621:TRP:O	1:B:625:VAL:HG23	1.97	0.64
1:D:301:GLN:O	1:D:403:ILE:HG22	1.96	0.64
1:A:297:LEU:HA	1:A:301:GLN:OE1	1.98	0.64
1:B:537:MET:HE1	1:B:791:LEU:HD11	1.80	0.63
1:B:470:GLN:HE21	1:B:474:PRO:HA	1.60	0.63
1:B:709:LYS:HE2	1:B:736:ASN:ND2	2.12	0.63
1:D:311:PRO:O	1:D:315:LYS:HG3	1.99	0.63
1:A:647:LYS:HA	1:A:697:TRP:CE3	2.32	0.63
1:A:410:ARG:NH2	1:B:427:VAL:HG22	2.13	0.63
1:C:761:THR:HG22	1:D:938:LEU:HD11	1.81	0.63
1:C:768:THR:HG22	1:C:771:ARG:HH21	1.63	0.63
1:B:501:TRP:O	1:B:504:HIS:HB3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:VAL:HG12	1:D:471:THR:HG22	1.80	0.63
1:C:297:LEU:HA	1:C:301:GLN:OE1	1.99	0.63
1:D:651:MET:CE	1:D:700:GLN:HG3	2.29	0.63
1:B:79:CYS:SG	1:B:101:ILE:HG21	2.39	0.62
1:D:62:ILE:HD12	1:D:379:LEU:HD22	1.81	0.62
1:D:501:TRP:O	1:D:504:HIS:HB3	1.99	0.62
1:B:608:LEU:HD23	1:B:608:LEU:C	2.25	0.62
1:B:959:CYS:HB2	1:B:992:CYS:HB2	1.81	0.62
1:C:108:ASN:HA	1:C:852:GLN:NE2	2.15	0.62
1:C:859:HIS:HD2	1:C:862:GLY:H	1.46	0.62
1:C:99:SER:HB3	1:C:115:MET:HE3	1.82	0.62
1:C:410:ARG:NH1	1:D:427:VAL:HG22	2.15	0.62
1:C:451:LEU:HB3	1:C:454:ILE:CD1	2.30	0.62
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.82	0.62
1:C:747:ASP:OD2	1:C:749:THR:HG23	2.00	0.62
1:D:342:ASP:HB2	5:D:1032:NDP:C5N	2.29	0.62
1:A:796:ILE:CD1	1:A:813:LEU:HB3	2.29	0.61
1:B:95:LEU:HD13	2:B:1026:SF4:S2	2.40	0.61
1:C:87:CYS:SG	1:C:97:ILE:HD12	2.39	0.61
1:A:691:VAL:HG21	1:A:720:ILE:CG2	2.30	0.61
1:A:959:CYS:SG	1:A:960:TYR:N	2.73	0.61
1:B:92:PRO:HB2	1:B:490:VAL:HG22	1.82	0.61
1:C:124:LEU:HD23	1:C:240:VAL:HG13	1.80	0.61
1:C:451:LEU:HB3	1:C:454:ILE:HD11	1.82	0.61
1:A:561:ARG:NE	1:B:6:SER:O	2.27	0.61
1:A:996:CYS:HA	2:A:1028:SF4:S3	2.40	0.61
1:B:62:ILE:HD11	1:B:379:LEU:HD13	1.81	0.61
1:A:116:ILE:HD13	1:A:156:GLN:HG3	1.83	0.61
1:B:142:LEU:HD12	1:B:150:ILE:HD11	1.82	0.61
1:B:305:THR:O	1:B:306:SER:C	2.44	0.61
1:C:95:LEU:HD23	1:C:119:ASP:HB2	1.81	0.61
1:D:261:LEU:HD21	1:D:451:LEU:HD21	1.81	0.61
1:B:291:ASP:OD1	1:B:293:ILE:HG12	2.01	0.61
1:D:100:PHE:CD1	1:D:100:PHE:C	2.78	0.61
1:A:427:VAL:CG2	1:B:410:ARG:NH2	2.64	0.61
1:D:560:ILE:O	1:D:563:ALA:HB3	2.01	0.61
1:D:9:VAL:HG22	1:D:12:ILE:HG12	1.81	0.61
1:A:768:THR:HG22	1:A:771:ARG:HH21	1.64	0.60
1:D:883:LEU:HG	1:D:887:LYS:HE3	1.83	0.60
1:A:150:ILE:HB	2:A:1027:SF4:S4	2.41	0.60
1:B:589:ARG:HD2	1:B:611:GLU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:GLU:OE1	1:C:910:LYS:HE3	2.00	0.60
1:A:164:LYS:HD2	1:A:243:PHE:CD2	2.36	0.60
1:A:470:GLN:HE21	1:A:474:PRO:HA	1.66	0.60
1:C:261:LEU:HD21	1:C:451:LEU:HD21	1.83	0.60
1:B:709:LYS:HA	1:B:733:THR:HB	1.84	0.60
1:C:651:MET:CE	1:C:700:GLN:HG3	2.30	0.60
1:D:283:ILE:HG13	1:D:482:ILE:HD13	1.84	0.60
1:D:706:PHE:CZ	1:D:729:ALA:HA	2.37	0.60
1:D:108:ASN:HA	1:D:852:GLN:HE22	1.67	0.60
1:A:741:LEU:O	1:B:772:PRO:HA	2.02	0.60
1:B:362:VAL:HG22	1:B:388:LEU:HB2	1.84	0.60
1:D:998:ILE:CG2	1:D:1001:CYS:HB2	2.32	0.60
1:A:673:HIS:O	1:A:675:MET:N	2.34	0.59
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.85	0.59
1:A:651:MET:CE	1:A:700:GLN:HG3	2.32	0.59
1:D:261:LEU:HD21	1:D:451:LEU:CD2	2.33	0.59
1:B:608:LEU:CD1	1:B:742:MET:HB2	2.32	0.59
1:D:95:LEU:HD23	1:D:119:ASP:HB2	1.84	0.59
1:C:410:ARG:HH12	1:D:427:VAL:HA	1.66	0.59
1:D:621:TRP:O	1:D:625:VAL:HG23	2.02	0.59
1:D:641:ILE:HB	1:D:653:LEU:CD2	2.32	0.59
1:A:301:GLN:O	1:A:403:ILE:HG13	2.03	0.59
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.38	0.59
1:C:477:PHE:CE1	1:C:503:ILE:HG12	2.37	0.59
1:D:373:VAL:HG22	1:D:376:GLU:HB2	1.85	0.59
1:A:50:PHE:CE2	1:B:369:ASN:HA	2.38	0.58
1:A:192:LEU:HG	1:A:280:PHE:HB3	1.84	0.58
1:A:368:VAL:HG13	1:B:384:LYS:HD2	1.84	0.58
1:C:67:LEU:HD23	1:D:146:GLU:HG2	1.85	0.58
1:A:193:LEU:HD22	1:A:193:LEU:N	2.18	0.58
1:C:846:LEU:HD22	1:C:849:TRP:CE2	2.37	0.58
1:B:42:LYS:HE3	1:B:44:ASN:OD1	2.03	0.58
1:B:342:ASP:CB	5:B:1032:NDP:H42N	2.33	0.58
1:C:410:ARG:HE	1:D:410:ARG:CZ	2.16	0.58
1:A:489:THR:O	1:A:493:VAL:HG23	2.04	0.58
1:B:136:CYS:SG	1:B:137:VAL:N	2.77	0.58
1:B:916:LYS:HG3	1:B:917:PRO:HD2	1.84	0.58
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.39	0.58
1:A:189:LYS:HB3	1:A:276:TYR:CD2	2.39	0.58
1:A:962:THR:CG2	1:A:991:LEU:HB3	2.33	0.58
1:B:80:LEU:HD11	1:B:142:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:VAL:HG22	1:C:788:PHE:CE2	2.38	0.58
1:C:82:CYS:O	1:C:98:LYS:HD2	2.03	0.58
1:A:394:ARG:HG3	1:A:409:VAL:HG13	1.86	0.57
1:B:687:ASP:HB3	1:B:690:LEU:CD1	2.33	0.57
1:B:744:LEU:HD23	1:B:750:PRO:HA	1.85	0.57
1:C:394:ARG:HG3	1:C:409:VAL:CG1	2.34	0.57
1:C:458:ARG:HH11	1:C:458:ARG:HG2	1.68	0.57
1:D:342:ASP:CB	5:D:1032:NDP:H42N	2.33	0.57
1:A:451:LEU:HB3	1:A:454:ILE:CD1	2.34	0.57
1:C:451:LEU:O	1:C:454:ILE:HG12	2.05	0.57
1:C:561:ARG:NE	1:D:6:SER:O	2.34	0.57
1:D:87:CYS:SG	1:D:88:GLN:N	2.76	0.57
1:D:806:LEU:HD23	1:D:810:ALA:O	2.04	0.57
1:B:982:VAL:HG13	2:B:1029:SF4:S2	2.44	0.57
1:D:997:PRO:HD2	2:D:1028:SF4:S3	2.45	0.57
1:B:722:ARG:O	1:B:726:GLU:HG3	2.04	0.57
1:C:53:GLU:OE2	1:C:887:LYS:O	2.23	0.57
1:D:294:PHE:HB3	1:D:303:PHE:CZ	2.40	0.57
1:A:947:VAL:O	1:A:947:VAL:HG13	2.05	0.57
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.35	0.57
1:D:962:THR:HG21	1:D:995:VAL:HG21	1.87	0.57
1:C:745:LYS:HG3	1:C:749:THR:OG1	2.05	0.57
1:C:772:PRO:HA	1:D:741:LEU:O	2.05	0.57
1:D:124:LEU:HD11	1:D:161:GLU:HG2	1.86	0.57
1:D:262:SER:OG	1:D:446:LYS:HB3	2.04	0.57
1:D:738:VAL:HG21	1:D:773:ILE:HD12	1.85	0.57
1:A:12:ILE:O	1:A:15:ILE:HG22	2.05	0.57
1:C:270:THR:O	1:C:274:GLU:HG3	2.05	0.57
1:C:410:ARG:NH2	1:D:410:ARG:NH1	2.52	0.57
1:D:956:CYS:SG	1:D:958:LYS:HG3	2.44	0.57
1:B:738:VAL:HG21	1:B:773:ILE:HD12	1.87	0.57
1:C:337:VAL:HB	1:C:361:LEU:HD23	1.86	0.57
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.87	0.57
1:C:108:ASN:HA	1:C:852:GLN:HE22	1.67	0.57
1:A:337:VAL:HB	1:A:361:LEU:HD23	1.87	0.56
1:C:844:GLU:O	1:C:847:GLN:HG3	2.05	0.56
1:A:2:ALA:O	1:A:3:PRO:O	2.23	0.56
1:A:259:LYS:HB3	1:A:266:ILE:HD11	1.87	0.56
1:C:501:TRP:CZ2	1:C:519:PRO:HA	2.39	0.56
1:C:642:MET:HB2	1:C:668:ASN:HB3	1.88	0.56
1:D:130:CYS:SG	1:D:490:VAL:HB	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASN:OD1	1:A:20:PRO:HD2	2.05	0.56
1:B:124:LEU:HD13	1:B:160:SER:HB2	1.85	0.56
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	1.88	0.56
1:C:410:ARG:HH21	1:D:410:ARG:CZ	2.18	0.56
1:D:709:LYS:HG3	1:D:733:THR:CG2	2.36	0.56
1:B:410:ARG:HD2	1:B:425:GLN:OE1	2.05	0.56
1:C:9:VAL:CG2	1:C:12:ILE:HG12	2.36	0.56
1:C:823:ASP:O	1:C:826:VAL:HG22	2.06	0.56
1:D:283:ILE:CG1	1:D:482:ILE:HD13	2.35	0.56
1:A:368:VAL:CG1	1:B:384:LYS:HD2	2.36	0.56
1:B:342:ASP:HB2	5:B:1032:NDP:C5N	2.36	0.56
1:B:993:LEU:HD23	1:B:993:LEU:O	2.05	0.56
1:A:734:ALA:HB1	1:A:735:THR:HG22	1.88	0.56
1:C:5:LEU:HG	1:D:623:GLN:HE22	1.71	0.56
1:C:5:LEU:HG	1:D:623:GLN:NE2	2.20	0.56
1:C:741:LEU:O	1:D:772:PRO:HA	2.05	0.56
1:D:343:THR:HG23	4:D:1031:FAD:HM72	1.88	0.56
1:A:464:VAL:HG12	1:A:471:THR:HG22	1.87	0.56
1:B:238:TYR:HB2	1:B:318:LYS:HD3	1.87	0.56
1:B:997:PRO:HD2	2:B:1028:SF4:S3	2.46	0.56
1:C:193:LEU:N	1:C:193:LEU:HD22	2.21	0.56
1:A:97:ILE:HA	1:A:100:PHE:CD2	2.41	0.55
1:C:410:ARG:HH12	1:D:427:VAL:HG22	1.71	0.55
1:A:779:THR:CG2	1:A:808:SER:HB3	2.37	0.55
1:C:519:PRO:HB3	1:D:28:LEU:HD22	1.87	0.55
1:D:451:LEU:HB3	1:D:454:ILE:CD1	2.36	0.55
1:D:709:LYS:HA	1:D:733:THR:HB	1.89	0.55
1:C:616:LYS:HB2	1:C:621:TRP:HE1	1.72	0.55
1:A:248:MET:HE3	1:A:253:VAL:HG11	1.88	0.55
1:B:486:ALA:C	1:B:487:ASN:HD22	2.13	0.55
1:C:427:VAL:CG1	1:D:410:ARG:HE	2.19	0.55
1:D:408:PHE:HB2	1:D:427:VAL:HB	1.89	0.55
1:D:792:ALA:HB1	1:D:805:PHE:CD2	2.41	0.55
1:B:261:LEU:HD12	1:B:266:ILE:O	2.06	0.55
1:D:573:THR:HB	1:D:621:TRP:CE3	2.42	0.55
1:D:714:VAL:HG21	1:D:720:ILE:HD11	1.88	0.55
1:B:189:LYS:HB3	1:B:276:TYR:CD2	2.42	0.55
1:B:651:MET:CE	1:B:700:GLN:HG2	2.37	0.55
1:B:948:ILE:HD13	1:B:980:PRO:HG2	1.89	0.55
1:C:97:ILE:HD13	1:C:152:ILE:HD13	1.88	0.55
1:C:147:GLU:OE1	1:C:147:GLU:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASN:HB2	1:B:45:PRO:HD2	1.89	0.55
1:C:996:CYS:HA	2:C:1028:SF4:S3	2.47	0.55
1:D:305:THR:O	1:D:306:SER:C	2.50	0.55
1:D:315:LYS:HA	1:D:321:MET:SD	2.47	0.55
1:D:444:ASP:OD1	1:D:446:LYS:HB2	2.07	0.55
1:C:62:ILE:HD11	1:C:379:LEU:HD13	1.89	0.54
1:D:451:LEU:HD12	1:D:456:PHE:HZ	1.70	0.54
1:B:104:ILE:HD11	1:B:159:ALA:HB2	1.89	0.54
1:C:1009:THR:CG2	1:C:1010:PRO:HD2	2.37	0.54
1:D:606:SER:HB2	1:D:766:SER:O	2.07	0.54
1:A:759:ARG:HH21	1:B:933:GLY:HA3	1.72	0.54
1:B:623:GLN:O	1:B:627:GLU:HG3	2.06	0.54
1:B:699:ARG:HA	1:B:699:ARG:NE	2.22	0.54
1:B:164:LYS:HD2	1:B:243:PHE:CG	2.43	0.54
1:C:19:ASN:OD1	1:C:20:PRO:HD2	2.08	0.54
1:C:228:THR:HG23	1:C:238:TYR:CD1	2.42	0.54
1:C:933:GLY:HA3	1:D:759:ARG:NH2	2.21	0.54
1:A:124:LEU:HD13	1:A:160:SER:HB2	1.88	0.54
1:A:394:ARG:HG3	1:A:409:VAL:CG1	2.38	0.54
1:A:709:LYS:HG3	1:A:733:THR:CG2	2.38	0.54
1:A:997:PRO:HD2	2:A:1028:SF4:S3	2.47	0.54
1:B:62:ILE:CD1	1:B:379:LEU:HD13	2.36	0.54
1:C:164:LYS:HD2	1:C:243:PHE:CG	2.43	0.54
1:D:656:LYS:O	1:D:659:ALA:HB3	2.08	0.54
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.88	0.54
1:D:886:ARG:O	1:D:890:ILE:HG13	2.08	0.54
1:C:97:ILE:HA	1:C:100:PHE:CD2	2.42	0.54
1:A:193:LEU:HD23	1:A:281:ILE:HD13	1.89	0.54
1:B:956:CYS:SG	1:B:958:LYS:HG3	2.48	0.54
1:A:699:ARG:HA	1:A:699:ARG:NE	2.23	0.54
1:C:67:LEU:HD13	1:C:72:ALA:HA	1.90	0.54
1:C:845:GLU:H	1:C:845:GLU:CD	2.15	0.54
1:D:136:CYS:SG	1:D:137:VAL:N	2.81	0.54
1:B:465:ASP:HB3	1:B:468:THR:OG1	2.08	0.53
1:C:145:THR:OG1	1:C:147:GLU:HG2	2.07	0.53
1:D:211:TYR:HE2	1:D:507:ILE:HG21	1.73	0.53
1:D:709:LYS:HG3	1:D:733:THR:HG22	1.90	0.53
1:C:219:LYS:HG3	1:C:260:SER:OG	2.08	0.53
1:C:708:ALA:HB3	1:C:732:VAL:HG12	1.90	0.53
1:A:709:LYS:HG3	1:A:733:THR:HG22	1.89	0.53
1:B:80:LEU:HD11	1:B:142:LEU:CD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:THR:HA	1:B:640:SER:O	2.08	0.53
1:B:962:THR:OG1	1:B:995:VAL:HG21	2.07	0.53
1:C:827:ILE:HG23	1:C:828:GLN:N	2.24	0.53
1:A:470:GLN:NE2	1:A:474:PRO:HA	2.24	0.53
1:B:468:THR:HA	1:B:502:TYR:CD1	2.44	0.53
1:C:311:PRO:O	1:C:315:LYS:HG3	2.08	0.53
1:C:608:LEU:HB2	1:C:742:MET:HE2	1.90	0.53
1:D:162:VAL:O	1:D:166:MET:HG3	2.08	0.53
1:C:589:ARG:HD2	1:C:611:GLU:HB2	1.91	0.53
1:A:573:THR:O	1:A:574:LYS:C	2.52	0.53
1:B:647:LYS:O	1:B:651:MET:HG3	2.09	0.53
1:B:947:VAL:O	1:B:947:VAL:HG13	2.08	0.53
1:D:608:LEU:CD1	1:D:742:MET:HB2	2.36	0.53
1:C:136:CYS:SG	1:C:152:ILE:HD12	2.48	0.53
1:D:267:THR:OG1	1:D:270:THR:HG23	2.09	0.53
1:D:390:PHE:O	1:D:391:LEU:HD23	2.09	0.53
1:D:990:THR:HG22	1:D:990:THR:O	2.07	0.53
1:B:78:ARG:NH2	1:B:150:ILE:HD13	2.24	0.53
1:B:315:LYS:HG2	1:B:321:MET:HE2	1.91	0.53
1:A:410:ARG:NH2	1:B:427:VAL:HG21	2.23	0.52
1:D:218:GLU:OE1	4:D:1031:FAD:H1B	2.09	0.52
1:C:999:ILE:O	1:C:1000:ASP:HB2	2.09	0.52
1:A:305:THR:O	1:A:306:SER:C	2.52	0.52
1:A:956:CYS:SG	1:A:958:LYS:HG3	2.49	0.52
1:C:642:MET:HA	1:C:650:TRP:CH2	2.45	0.52
1:D:470:GLN:NE2	1:D:474:PRO:HA	2.24	0.52
1:A:410:ARG:NE	1:B:410:ARG:NH2	2.56	0.52
1:B:230:GLU:HG2	1:B:310:LEU:HB2	1.92	0.52
1:D:78:ARG:CZ	1:D:150:ILE:HD13	2.39	0.52
1:D:379:LEU:O	1:D:383:GLU:HG3	2.10	0.52
1:B:489:THR:O	1:B:493:VAL:HG23	2.10	0.52
1:C:942:GLU:OE2	1:D:756:ALA:N	2.39	0.52
1:D:451:LEU:O	1:D:454:ILE:HG12	2.10	0.52
1:D:842:SER:CB	1:D:918:ILE:HD13	2.37	0.52
1:A:944:VAL:HG22	1:B:587:SER:OG	2.09	0.52
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.92	0.52
1:B:747:ASP:CG	1:B:749:THR:HG23	2.35	0.52
1:B:831:CYS:O	1:B:835:LYS:HG3	2.09	0.52
1:C:110:TYR:OH	1:C:529:ASP:OD2	2.26	0.52
1:A:136:CYS:SG	1:A:137:VAL:N	2.83	0.52
1:A:990:THR:HG22	1:A:990:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LYS:HD2	1:D:41:TRP:CE2	2.45	0.52
1:C:465:ASP:HB3	1:C:468:THR:OG1	2.10	0.52
1:D:783:ARG:HG3	1:D:929:LEU:HD22	1.91	0.52
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.91	0.52
1:D:99:SER:HB3	1:D:115:MET:HE3	1.92	0.52
1:D:404:VAL:O	1:D:405:ALA:HB2	2.08	0.52
1:D:449:GLU:C	1:D:451:LEU:H	2.17	0.52
1:B:83:ALA:O	1:B:84:ASP:C	2.53	0.52
1:B:971:ILE:HG13	2:B:1029:SF4:S2	2.50	0.52
1:D:451:LEU:HB3	1:D:454:ILE:HD11	1.91	0.52
1:A:831:CYS:O	1:A:835:LYS:HG3	2.10	0.51
1:A:772:PRO:HA	1:B:741:LEU:O	2.09	0.51
1:C:410:ARG:NH1	1:D:427:VAL:CG1	2.66	0.51
1:C:622:CYS:O	1:C:660:SER:HB2	2.09	0.51
1:C:1009:THR:HG22	1:C:1010:PRO:HD2	1.92	0.51
1:A:136:CYS:SG	1:A:152:ILE:HD12	2.50	0.51
1:A:248:MET:HE3	1:A:253:VAL:CG1	2.39	0.51
1:A:575:THR:HA	1:A:640:SER:O	2.10	0.51
1:B:9:VAL:HG22	1:B:12:ILE:HG12	1.91	0.51
1:B:82:CYS:O	1:B:98:LYS:HD2	2.10	0.51
1:B:779:THR:CG2	1:B:808:SER:HB3	2.39	0.51
1:D:398:VAL:HG13	1:D:402:ARG:O	2.09	0.51
1:B:331:ILE:HG23	1:B:433:VAL:HG21	1.91	0.51
1:B:948:ILE:HD13	1:B:980:PRO:CG	2.41	0.51
1:C:575:THR:HA	1:C:640:SER:HB3	1.92	0.51
1:B:647:LYS:HA	1:B:697:TRP:CE3	2.46	0.51
1:B:647:LYS:HG3	1:B:697:TRP:CG	2.45	0.51
1:C:100:PHE:O	1:C:104:ILE:HG13	2.10	0.51
1:C:342:ASP:CB	5:C:1032:NDP:H42N	2.39	0.51
1:C:664:ALA:HB1	1:C:705:PRO:O	2.11	0.51
1:D:394:ARG:HG3	1:D:409:VAL:CG1	2.39	0.51
1:D:477:PHE:CD1	1:D:503:ILE:HG12	2.45	0.51
1:D:945:VAL:HB	1:D:986:CYS:SG	2.50	0.51
1:C:53:GLU:HG2	1:C:54:LYS:N	2.25	0.51
1:A:587:SER:HA	1:A:588:PRO:C	2.36	0.51
1:A:673:HIS:CE1	1:A:675:MET:CB	2.94	0.51
1:A:992:CYS:SG	1:A:993:LEU:N	2.84	0.51
1:C:443:ARG:O	1:C:444:ASP:C	2.54	0.51
1:C:959:CYS:SG	1:C:960:TYR:N	2.84	0.51
1:A:776:ARG:HH11	1:A:776:ARG:HG2	1.74	0.51
1:B:845:GLU:CD	1:B:845:GLU:H	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:LEU:HD22	1:B:849:TRP:CE2	2.45	0.51
1:D:243:PHE:CZ	1:D:247:LEU:HD11	2.46	0.51
1:A:80:LEU:CD1	1:B:954:ILE:HD11	2.40	0.51
1:A:288:PRO:HB3	1:A:307:LYS:HB2	1.92	0.51
1:A:573:THR:HB	1:A:621:TRP:CE3	2.46	0.51
1:C:616:LYS:HD3	1:C:620:TYR:CE2	2.46	0.51
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.92	0.51
1:A:100:PHE:CD1	1:A:100:PHE:C	2.88	0.50
1:A:933:GLY:HA3	1:B:759:ARG:NH2	2.25	0.50
1:C:70:ARG:HH22	1:D:147:GLU:CD	2.19	0.50
1:C:577:SER:HA	1:C:653:LEU:HD21	1.92	0.50
1:D:19:ASN:OD1	1:D:964:ASN:ND2	2.38	0.50
1:D:219:LYS:HG3	1:D:260:SER:OG	2.10	0.50
1:D:578:LEU:HD23	1:D:653:LEU:HD13	1.93	0.50
1:A:909:ARG:HG3	1:A:909:ARG:HH11	1.76	0.50
1:B:271:LEU:HD22	1:B:276:TYR:CD1	2.47	0.50
1:C:90:SER:HB3	1:C:135:LEU:O	2.11	0.50
1:C:342:ASP:CB	5:C:1032:NDP:C5N	2.88	0.50
1:C:856:THR:HG21	1:C:952:MET:HE1	1.92	0.50
1:D:124:LEU:CD2	1:D:240:VAL:HG13	2.34	0.50
1:A:108:ASN:HA	1:A:852:GLN:NE2	2.26	0.50
1:A:699:ARG:HA	1:A:699:ARG:HE	1.76	0.50
1:C:375:GLU:CD	1:C:375:GLU:H	2.19	0.50
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.94	0.50
1:B:100:PHE:CD1	1:B:100:PHE:C	2.89	0.50
1:C:997:PRO:HD2	2:C:1028:SF4:S3	2.52	0.50
1:D:449:GLU:C	1:D:451:LEU:N	2.69	0.50
1:D:658:GLU:HB2	1:D:704:ILE:HD11	1.94	0.50
1:D:962:THR:HG21	1:D:995:VAL:HG11	1.94	0.50
1:B:886:ARG:O	1:B:890:ILE:HG13	2.12	0.50
1:C:991:LEU:O	1:C:995:VAL:HG22	2.11	0.50
1:C:132:THR:HB	1:C:137:VAL:HG23	1.94	0.50
1:C:294:PHE:HZ	1:C:338:LEU:HD12	1.77	0.50
1:D:470:GLN:HB2	1:D:477:PHE:CE2	2.46	0.50
1:D:578:LEU:HD21	1:D:653:LEU:HB2	1.92	0.50
1:B:201:SER:HB2	1:B:493:VAL:HG13	1.93	0.50
1:B:622:CYS:O	1:B:660:SER:HB2	2.11	0.50
1:C:768:THR:HG22	1:C:771:ARG:NH2	2.27	0.50
1:B:140:CYS:HA	2:B:1027:SF4:S3	2.52	0.49
1:B:487:ASN:N	1:B:487:ASN:ND2	2.56	0.49
1:C:53:GLU:CG	1:C:54:LYS:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:547:GLY:HA3	1:C:570:PHE:CZ	2.47	0.49
1:A:342:ASP:CB	5:A:1032:NDP:C5N	2.90	0.49
1:A:933:GLY:HA3	1:B:759:ARG:HH21	1.77	0.49
1:D:801:SER:O	1:D:804:GLN:HB2	2.11	0.49
1:A:81:LYS:HD3	1:A:102:THR:OG1	2.12	0.49
1:B:699:ARG:HA	1:B:699:ARG:HE	1.77	0.49
1:D:375:GLU:H	1:D:375:GLU:CD	2.21	0.49
1:D:827:ILE:HG23	1:D:828:GLN:N	2.26	0.49
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.42	0.49
1:A:759:ARG:NH2	1:B:933:GLY:HA3	2.28	0.49
1:C:315:LYS:HA	1:C:321:MET:SD	2.51	0.49
1:B:328:LEU:O	1:B:329:PRO:C	2.55	0.49
1:D:457:ASN:HB3	1:D:463:GLU:OE1	2.12	0.49
1:A:673:HIS:CE1	1:A:675:MET:HB3	2.48	0.49
1:B:87:CYS:SG	1:B:88:GLN:N	2.85	0.49
1:B:285:LEU:HG	1:B:481:ASP:HB3	1.94	0.49
1:D:103:SER:HA	1:D:829:ASP:OD1	2.12	0.49
1:D:362:VAL:HG22	1:D:388:LEU:HB2	1.94	0.49
1:D:396:VAL:HG13	1:D:403:ILE:CD1	2.42	0.49
1:D:557:SER:HB3	1:D:624:SER:HB3	1.94	0.49
1:D:815:VAL:HG12	1:D:816:CYS:N	2.27	0.49
1:D:842:SER:OG	1:D:914:PRO:HB3	2.12	0.49
1:A:67:LEU:HD13	1:A:72:ALA:HA	1.95	0.49
1:A:1007:ARG:HG2	1:A:1009:THR:O	2.12	0.49
1:B:130:CYS:SG	1:B:490:VAL:HB	2.52	0.49
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.95	0.49
1:C:699:ARG:HA	1:C:699:ARG:NE	2.28	0.49
1:C:990:THR:O	1:C:990:THR:HG22	2.13	0.49
1:D:56:GLU:OE2	1:D:898:LYS:NZ	2.43	0.49
1:A:97:ILE:HG22	1:A:101:ILE:CD1	2.42	0.49
1:A:868:ILE:HB	1:A:871:LEU:HD12	1.94	0.49
1:A:962:THR:OG1	1:A:995:VAL:HG21	2.12	0.49
1:C:305:THR:O	1:C:306:SER:C	2.56	0.49
1:C:553:PRO:O	1:C:559:MET:HE2	2.13	0.49
1:C:621:TRP:O	1:C:625:VAL:HG23	2.12	0.49
1:D:909:ARG:HG2	1:D:909:ARG:HH11	1.78	0.49
1:A:793:THR:HB	1:A:814:GLN:HB2	1.94	0.49
1:C:222:TYR:CD2	1:C:321:MET:HE2	2.48	0.49
1:C:582:ILE:HD11	1:D:1015:ARG:HH11	1.78	0.49
1:D:845:GLU:CD	1:D:845:GLU:H	2.17	0.49
1:A:968:TYR:O	1:A:969:GLN:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:ILE:HG13	2:A:1029:SF4:S4	2.53	0.48
1:D:189:LYS:HB3	1:D:276:TYR:CD2	2.47	0.48
1:A:122:LEU:HD22	1:A:493:VAL:HG22	1.96	0.48
1:C:77:MET:SD	1:D:598:PRO:HG2	2.53	0.48
1:C:954:ILE:HD11	1:D:80:LEU:CD1	2.42	0.48
1:D:193:LEU:N	1:D:193:LEU:HD22	2.28	0.48
1:D:545:PRO:O	1:D:570:PHE:HE2	1.95	0.48
1:B:732:VAL:HG13	1:B:788:PHE:CE2	2.48	0.48
1:C:367:PHE:HB2	1:D:386:GLU:OE1	2.13	0.48
1:A:776:ARG:O	1:A:780:THR:HG22	2.13	0.48
1:C:932:LEU:HD21	1:D:741:LEU:HD11	1.96	0.48
1:C:992:CYS:SG	1:C:993:LEU:N	2.86	0.48
1:D:97:ILE:HD13	1:D:152:ILE:HD13	1.95	0.48
1:A:220:GLN:HG3	1:A:222:TYR:CZ	2.48	0.48
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.13	0.48
1:A:410:ARG:CZ	1:B:410:ARG:CZ	2.92	0.48
1:A:779:THR:HG22	1:A:808:SER:CB	2.42	0.48
1:B:262:SER:O	1:B:263:GLU:C	2.57	0.48
1:C:933:GLY:HA3	1:D:759:ARG:HH21	1.78	0.48
1:C:1019:LEU:HD21	1:D:617:THR:HG22	1.96	0.48
1:D:42:LYS:HE3	1:D:44:ASN:OD1	2.14	0.48
1:D:947:VAL:HG13	1:D:947:VAL:O	2.12	0.48
1:A:270:THR:O	1:A:274:GLU:HG3	2.13	0.48
1:A:608:LEU:CD1	1:A:742:MET:HB2	2.36	0.48
1:B:453:PRO:HG2	1:B:473:GLU:OE1	2.14	0.48
1:B:642:MET:HB2	1:B:668:ASN:HB3	1.96	0.48
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.43	0.48
1:C:944:VAL:HG23	1:C:1004:MET:HE3	1.95	0.48
1:D:410:ARG:CG	1:D:410:ARG:NH1	2.70	0.48
1:D:647:LYS:O	1:D:651:MET:HG3	2.14	0.48
1:B:408:PHE:HB2	1:B:427:VAL:HB	1.95	0.48
1:B:485:MET:O	1:B:487:ASN:ND2	2.46	0.48
1:D:288:PRO:HB3	1:D:307:LYS:HB2	1.96	0.48
1:D:546:PHE:CE1	1:D:830:TYR:HB3	2.49	0.48
1:D:750:PRO:HG3	1:D:760:THR:HG22	1.95	0.48
1:C:487:ASN:O	5:C:1032:NDP:H1D	2.14	0.48
1:C:608:LEU:CD1	1:C:742:MET:HB2	2.37	0.48
1:C:647:LYS:O	1:C:651:MET:HG3	2.13	0.48
1:D:699:ARG:HE	1:D:699:ARG:CA	2.25	0.48
1:A:442:LEU:HD22	1:A:482:ILE:HD11	1.95	0.48
1:A:768:THR:HG22	1:A:771:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HA	1:B:852:GLN:HE22	1.79	0.48
1:B:371:ARG:HE	1:B:371:ARG:HB2	1.32	0.48
1:B:801:SER:O	1:B:804:GLN:HB2	2.14	0.48
1:C:828:GLN:O	1:C:832:THR:HG23	2.14	0.48
1:C:845:GLU:HG3	1:C:912:PHE:CE2	2.49	0.48
1:D:142:LEU:HD12	1:D:150:ILE:HD11	1.95	0.48
1:A:129:VAL:O	1:A:130:CYS:C	2.54	0.48
1:A:230:GLU:HG2	1:A:310:LEU:HB2	1.96	0.48
1:A:989:CYS:O	1:A:990:THR:HB	2.14	0.48
1:D:664:ALA:O	1:D:665:LEU:HD23	2.14	0.48
1:A:291:ASP:OD1	1:A:292:ASP:N	2.47	0.47
1:B:353:ARG:HH12	1:B:383:GLU:CD	2.22	0.47
1:C:963:CYS:HA	1:C:967:GLY:HA3	1.96	0.47
1:D:608:LEU:HD21	1:D:763:GLY:HA3	1.96	0.47
1:D:771:ARG:N	1:D:772:PRO:CD	2.77	0.47
1:B:81:LYS:HD3	1:B:102:THR:OG1	2.14	0.47
1:B:288:PRO:HB3	1:B:307:LYS:HB2	1.95	0.47
1:A:685:GLY:O	1:A:720:ILE:HD12	2.13	0.47
1:C:776:ARG:HB2	1:D:740:GLY:HA2	1.96	0.47
1:A:83:ALA:O	1:A:84:ASP:C	2.55	0.47
1:A:992:CYS:O	1:A:993:LEU:C	2.56	0.47
1:B:263:GLU:O	1:B:264:ASN:HB2	2.14	0.47
1:B:807:HIS:HB3	1:B:928:ALA:HB2	1.95	0.47
1:C:557:SER:HB3	1:C:624:SER:HB3	1.97	0.47
1:B:332:ARG:HG2	1:B:332:ARG:HH11	1.79	0.47
1:C:124:LEU:CD2	1:C:240:VAL:HG13	2.43	0.47
1:C:261:LEU:HD21	1:C:451:LEU:CD2	2.44	0.47
1:C:810:ALA:O	1:C:925:ILE:HG23	2.14	0.47
1:D:642:MET:HB2	1:D:668:ASN:HB3	1.96	0.47
1:B:261:LEU:HD21	1:B:451:LEU:HD21	1.96	0.47
1:C:87:CYS:SG	1:C:88:GLN:N	2.88	0.47
1:A:97:ILE:HA	1:A:100:PHE:CE2	2.49	0.47
1:A:371:ARG:NH1	1:A:371:ARG:HB2	2.30	0.47
1:A:709:LYS:HA	1:A:733:THR:HB	1.97	0.47
1:A:989:CYS:O	1:A:990:THR:CB	2.61	0.47
1:B:533:ILE:O	1:B:545:PRO:HD3	2.14	0.47
1:B:646:ASN:C	1:B:646:ASN:OD1	2.58	0.47
1:B:651:MET:HE1	1:B:700:GLN:HG2	1.96	0.47
1:C:62:ILE:CD1	1:C:379:LEU:HD13	2.44	0.47
1:C:521:LEU:HA	1:C:522:PRO:HD3	1.79	0.47
1:D:307:LYS:O	1:D:311:PRO:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:744:LEU:HD23	1:D:750:PRO:HA	1.95	0.47
1:A:408:PHE:HB2	1:A:427:VAL:HB	1.97	0.47
1:A:738:VAL:HG21	1:A:773:ILE:HD12	1.97	0.47
1:A:909:ARG:HG3	1:A:909:ARG:NH1	2.29	0.47
1:B:622:CYS:HB3	1:B:660:SER:HB3	1.96	0.47
1:C:410:ARG:HH12	1:D:427:VAL:CA	2.27	0.47
1:D:108:ASN:ND2	1:D:111:GLY:HA3	2.29	0.47
1:D:454:ILE:HA	1:D:472:SER:OG	2.15	0.47
1:D:568:TRP:CE2	1:D:827:ILE:HB	2.49	0.47
1:C:292:ASP:O	1:C:294:PHE:N	2.48	0.47
1:C:587:SER:HA	1:C:588:PRO:C	2.39	0.47
1:A:386:GLU:OE2	1:B:368:VAL:HG23	2.15	0.47
1:A:699:ARG:HE	1:A:699:ARG:CA	2.29	0.47
1:A:859:HIS:C	1:A:859:HIS:ND1	2.73	0.47
1:B:46:ASP:HB3	1:B:49:CYS:HB2	1.96	0.47
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.15	0.47
1:A:827:ILE:HG23	1:A:828:GLN:N	2.29	0.46
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.50	0.46
1:C:267:THR:HG23	1:C:450:ALA:HA	1.96	0.46
1:C:301:GLN:O	1:C:403:ILE:HG13	2.15	0.46
1:C:806:LEU:CD2	1:C:813:LEU:HD21	2.45	0.46
1:D:687:ASP:HB3	1:D:690:LEU:HD12	1.96	0.46
1:B:414:ASP:OD1	1:B:414:ASP:C	2.59	0.46
1:B:451:LEU:O	1:B:454:ILE:HG23	2.15	0.46
1:A:99:SER:CB	1:A:115:MET:HE3	2.45	0.46
1:B:63:LYS:HE3	1:B:128:MET:HG2	1.97	0.46
1:B:103:SER:HA	1:B:829:ASP:OD1	2.15	0.46
1:B:193:LEU:N	1:B:193:LEU:HD22	2.30	0.46
1:A:477:PHE:CD1	1:A:503:ILE:HG12	2.51	0.46
1:C:943:GLN:HG3	1:C:1011:TYR:CD2	2.51	0.46
1:D:557:SER:CB	1:D:624:SER:HB3	2.46	0.46
1:D:921:ILE:O	1:D:924:VAL:HG22	2.15	0.46
1:C:345:PHE:CE2	1:C:361:LEU:HD13	2.51	0.46
1:C:971:ILE:HG13	2:C:1029:SF4:S4	2.56	0.46
1:D:839:TYR:C	1:D:839:TYR:CD2	2.93	0.46
1:B:824:PHE:O	1:B:827:ILE:HG22	2.16	0.46
1:C:124:LEU:HD13	1:C:160:SER:HB2	1.97	0.46
1:A:651:MET:HE2	1:A:701:ALA:HB2	1.97	0.46
1:B:136:CYS:SG	1:B:152:ILE:HD12	2.55	0.46
1:B:211:TYR:OH	1:B:504:HIS:ND1	2.38	0.46
1:C:77:MET:HE1	1:D:599:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:SER:OG	1:C:263:GLU:N	2.49	0.46
1:C:343:THR:O	1:C:344:ALA:C	2.58	0.46
1:C:410:ARG:HH11	1:D:427:VAL:HG13	1.76	0.46
1:D:959:CYS:SG	1:D:960:TYR:N	2.88	0.46
1:A:99:SER:HB3	1:A:115:MET:HE3	1.97	0.46
1:A:823:ASP:HB2	1:B:965:ASP:OD2	2.16	0.46
1:A:896:ARG:NH2	1:A:900:GLN:HE22	2.02	0.46
1:C:97:ILE:HD11	2:C:1026:SF4:S4	2.56	0.46
1:D:83:ALA:O	1:D:84:ASP:C	2.57	0.46
1:D:388:LEU:HD12	1:D:429:LEU:HD21	1.97	0.46
1:D:641:ILE:HB	1:D:653:LEU:HD21	1.98	0.46
1:A:103:SER:HA	1:A:829:ASP:OD1	2.16	0.46
1:A:457:ASN:HB3	1:A:463:GLU:OE1	2.16	0.46
1:C:132:THR:HB	1:C:137:VAL:CG2	2.45	0.46
1:C:575:THR:HA	1:C:640:SER:O	2.16	0.46
1:D:291:ASP:OD1	1:D:292:ASP:N	2.49	0.46
1:B:142:LEU:HD22	1:B:145:THR:HG21	1.98	0.46
1:B:699:ARG:HE	1:B:699:ARG:CA	2.29	0.46
1:C:218:GLU:OE1	4:C:1031:FAD:H1B	2.16	0.46
1:C:410:ARG:HH21	1:D:410:ARG:NH1	2.13	0.46
1:C:449:GLU:C	1:C:451:LEU:H	2.23	0.46
1:C:651:MET:HE2	1:C:701:ALA:HB2	1.98	0.46
1:A:70:ARG:HG3	1:A:999:ILE:HG13	1.97	0.45
1:A:193:LEU:N	1:A:193:LEU:CD2	2.80	0.45
1:A:747:ASP:OD2	1:A:747:ASP:C	2.59	0.45
1:B:548:LEU:HD11	1:B:563:ALA:CB	2.46	0.45
1:B:783:ARG:HG3	1:B:929:LEU:HD22	1.98	0.45
1:C:294:PHE:CZ	1:C:338:LEU:HD12	2.51	0.45
1:D:294:PHE:HA	1:D:297:LEU:HD12	1.97	0.45
1:D:297:LEU:HA	1:D:301:GLN:OE1	2.16	0.45
1:D:375:GLU:CD	1:D:375:GLU:N	2.74	0.45
1:D:608:LEU:HD23	1:D:609:ASN:N	2.31	0.45
1:D:962:THR:CG2	1:D:995:VAL:HG21	2.45	0.45
1:C:578:LEU:HD21	1:C:653:LEU:HB2	1.98	0.45
1:C:695:CYS:SG	1:C:729:ALA:HB2	2.56	0.45
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.51	0.45
1:A:651:MET:CE	1:A:701:ALA:HB2	2.46	0.45
1:A:673:HIS:C	1:A:675:MET:H	2.21	0.45
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.96	0.45
1:A:734:ALA:HA	1:A:735:THR:HA	1.57	0.45
1:A:750:PRO:HG3	1:A:760:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:MET:HE1	1:B:255:ILE:HD11	1.97	0.45
1:B:379:LEU:O	1:B:383:GLU:HG3	2.15	0.45
1:C:449:GLU:C	1:C:451:LEU:N	2.72	0.45
1:D:108:ASN:O	1:D:108:ASN:CG	2.60	0.45
1:A:310:LEU:HB2	1:A:311:PRO:HD3	1.98	0.45
1:B:205:PHE:CZ	1:B:497:LYS:HG3	2.52	0.45
1:B:464:VAL:HG12	1:B:471:THR:HG22	1.98	0.45
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.51	0.45
1:B:993:LEU:C	1:B:993:LEU:CD2	2.88	0.45
1:C:208:ARG:HB3	1:C:522:PRO:HB2	1.98	0.45
1:B:373:VAL:HG22	1:B:376:GLU:HB3	1.98	0.45
1:B:443:ARG:O	1:B:444:ASP:C	2.60	0.45
1:C:34:LYS:HG3	1:D:92:PRO:HA	1.99	0.45
1:C:544:ASN:HD21	1:C:569:GLY:N	2.14	0.45
1:D:958:LYS:HB2	2:D:1028:SF4:S3	2.57	0.45
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.57	0.45
1:A:488:THR:OG1	1:A:491:GLU:HG3	2.17	0.45
1:A:608:LEU:HA	1:A:764:GLY:O	2.17	0.45
1:A:710:LEU:HD11	1:A:732:VAL:HG11	1.98	0.45
1:C:791:LEU:HB3	1:C:814:GLN:HE21	1.81	0.45
1:C:877:PRO:CG	1:C:977:THR:HB	2.46	0.45
1:A:230:GLU:HB3	4:A:1031:FAD:HM72	1.99	0.45
1:C:962:THR:HG21	1:C:991:LEU:HB3	1.97	0.45
1:D:982:VAL:HG13	2:D:1029:SF4:S4	2.56	0.45
1:A:130:CYS:SG	1:A:490:VAL:HB	2.56	0.45
1:C:734:ALA:HA	1:C:735:THR:HA	1.64	0.45
1:D:859:HIS:HA	1:D:865:VAL:HG23	1.98	0.45
1:A:28:LEU:HD22	1:B:519:PRO:HB3	1.97	0.45
1:A:751:TRP:HA	1:A:752:PRO:C	2.42	0.45
1:A:773:ILE:HD11	1:B:738:VAL:HG11	1.98	0.45
1:A:791:LEU:HD12	1:A:791:LEU:N	2.32	0.45
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.69	0.45
1:D:99:SER:CB	1:D:115:MET:HE3	2.47	0.45
1:A:87:CYS:SG	1:A:88:GLN:N	2.89	0.45
1:A:622:CYS:O	1:A:660:SER:HB2	2.17	0.45
1:A:877:PRO:HD2	1:A:882:TYR:CD2	2.51	0.45
1:C:568:TRP:NE1	1:C:827:ILE:HB	2.31	0.45
1:C:744:LEU:HD23	1:C:750:PRO:HA	1.98	0.45
1:C:845:GLU:HG3	1:C:912:PHE:CD2	2.52	0.45
1:C:935:PHE:CZ	1:D:612:LEU:HD21	2.51	0.45
1:D:193:LEU:HD23	1:D:281:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HA	1:B:852:GLN:NE2	2.32	0.44
1:B:788:PHE:HA	1:B:789:PRO:HD3	1.84	0.44
1:D:44:ASN:HB2	1:D:45:PRO:CD	2.47	0.44
1:D:267:THR:HG22	1:D:450:ALA:CB	2.47	0.44
1:D:521:LEU:HA	1:D:522:PRO:HD3	1.77	0.44
1:D:929:LEU:HD23	1:D:932:LEU:HD12	1.98	0.44
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.98	0.44
1:A:771:ARG:N	1:A:772:PRO:CD	2.80	0.44
1:A:886:ARG:O	1:A:890:ILE:HG13	2.16	0.44
1:B:342:ASP:CB	5:B:1032:NDP:C5N	2.96	0.44
1:C:367:PHE:CE1	1:D:367:PHE:CE1	3.06	0.44
1:C:458:ARG:HG2	1:C:458:ARG:NH1	2.32	0.44
1:D:893:GLU:OE1	1:D:896:ARG:NH1	2.50	0.44
1:A:871:LEU:HG	1:A:889:ILE:HG21	2.00	0.44
1:B:162:VAL:O	1:B:166:MET:HG3	2.18	0.44
1:A:97:ILE:HD11	2:A:1026:SF4:S4	2.58	0.44
1:A:267:THR:HG22	1:A:450:ALA:CB	2.47	0.44
1:A:991:LEU:O	1:A:994:SER:HB2	2.17	0.44
1:B:292:ASP:O	1:B:294:PHE:N	2.51	0.44
1:B:294:PHE:HA	1:B:297:LEU:CD1	2.46	0.44
1:B:298:THR:N	1:B:301:GLN:OE1	2.48	0.44
1:C:140:CYS:SG	1:C:149:SER:HA	2.57	0.44
1:C:410:ARG:HD2	1:C:425:GLN:OE1	2.18	0.44
1:C:773:ILE:HD11	1:D:738:VAL:HG11	1.99	0.44
1:C:959:CYS:SG	1:C:971:ILE:HD13	2.57	0.44
1:D:201:SER:CB	1:D:493:VAL:HG13	2.44	0.44
1:D:248:MET:HE1	1:D:255:ILE:HD11	1.99	0.44
1:D:342:ASP:CB	5:D:1032:NDP:C5N	2.94	0.44
1:A:485:MET:HE1	1:B:32:LEU:CB	2.32	0.44
1:A:734:ALA:HB1	1:A:735:THR:CG2	2.47	0.44
1:A:905:PRO:O	1:A:906:PRO:O	2.35	0.44
1:C:56:GLU:OE2	1:C:898:LYS:NZ	2.51	0.44
1:C:747:ASP:OD2	1:C:747:ASP:C	2.60	0.44
1:D:192:LEU:N	1:D:192:LEU:HD12	2.32	0.44
1:A:97:ILE:HG22	1:A:101:ILE:HD12	2.00	0.44
1:B:560:ILE:O	1:B:563:ALA:HB3	2.17	0.44
1:D:166:MET:HE2	1:D:840:LEU:HD21	2.00	0.44
1:D:608:LEU:HD23	1:D:608:LEU:C	2.42	0.44
1:D:816:CYS:HB3	3:D:1030:FMN:O1P	2.18	0.44
1:A:390:PHE:CE1	1:B:388:LEU:HD21	2.53	0.44
1:A:646:ASN:OD1	1:A:646:ASN:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:O	1:A:889:ILE:HD13	2.17	0.44
1:B:131:PRO:HB3	1:B:373:VAL:HG11	2.00	0.44
1:C:140:CYS:HA	2:C:1027:SF4:S3	2.58	0.44
1:C:147:GLU:CD	1:D:70:ARG:HH22	2.26	0.44
1:C:954:ILE:HG23	1:C:998:ILE:HG13	2.00	0.44
1:D:90:SER:CB	1:D:136:CYS:HA	2.48	0.44
1:D:963:CYS:HA	1:D:967:GLY:HA3	1.99	0.44
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.71	0.44
1:C:578:LEU:CD2	1:C:653:LEU:HD13	2.47	0.44
1:D:533:ILE:O	1:D:545:PRO:HD3	2.18	0.44
1:D:779:THR:HG22	1:D:808:SER:HB3	1.99	0.44
1:C:309:PHE:HE1	1:C:331:ILE:HD11	1.81	0.44
1:C:313:VAL:HG13	1:C:328:LEU:HD11	1.99	0.44
1:C:547:GLY:HA3	1:C:570:PHE:CE1	2.52	0.44
1:C:631:ASP:C	1:C:633:PRO:HD3	2.43	0.44
1:D:589:ARG:HG3	1:D:590:ILE:HG13	1.99	0.44
1:D:734:ALA:HA	1:D:735:THR:HA	1.62	0.44
1:D:968:TYR:O	1:D:969:GLN:C	2.60	0.44
1:A:243:PHE:CD1	1:A:243:PHE:C	2.96	0.43
1:A:345:PHE:CE2	1:A:361:LEU:HD13	2.52	0.43
1:A:656:LYS:O	1:A:659:ALA:HB3	2.18	0.43
1:B:294:PHE:CA	1:B:297:LEU:HD12	2.45	0.43
1:B:792:ALA:HB1	1:B:805:PHE:CD2	2.53	0.43
1:C:106:ASN:O	1:C:107:LYS:HB2	2.17	0.43
1:C:184:GLU:O	1:C:185:ALA:C	2.61	0.43
1:C:568:TRP:CE2	1:C:827:ILE:HB	2.53	0.43
1:D:443:ARG:O	1:D:444:ASP:C	2.60	0.43
1:D:796:ILE:CD1	1:D:813:LEU:HB3	2.48	0.43
1:D:998:ILE:HB	1:D:1001:CYS:HB2	1.99	0.43
1:B:373:VAL:HG22	1:B:376:GLU:CB	2.47	0.43
1:B:382:GLU:C	1:B:384:LYS:H	2.26	0.43
1:B:593:GLY:HA3	1:B:606:SER:OG	2.18	0.43
1:C:291:ASP:OD1	1:C:292:ASP:N	2.51	0.43
1:C:521:LEU:O	1:D:25:HIS:HB3	2.18	0.43
1:D:172:ARG:O	1:D:173:ASN:C	2.61	0.43
1:A:55:LEU:HD13	1:A:353:ARG:NH1	2.34	0.43
1:A:331:ILE:HG23	1:A:433:VAL:HG21	2.00	0.43
1:A:865:VAL:HG11	1:A:951:GLU:OE1	2.18	0.43
1:B:363:PHE:CZ	1:B:370:ILE:HD11	2.53	0.43
1:C:62:ILE:HG21	1:C:353:ARG:HH22	1.83	0.43
1:C:589:ARG:O	1:C:609:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:ILE:HG21	1:D:991:LEU:HG	1.99	0.43
1:D:173:ASN:ND2	1:D:175:CYS:HB2	2.32	0.43
1:A:131:PRO:CB	1:A:373:VAL:HG11	2.49	0.43
1:A:342:ASP:CB	5:A:1032:NDP:C4N	2.95	0.43
1:A:598:PRO:HG2	1:B:77:MET:SD	2.57	0.43
1:A:600:TYR:CE1	1:B:999:ILE:HD11	2.53	0.43
1:B:67:LEU:HD13	1:B:72:ALA:HA	1.98	0.43
1:B:146:GLU:OE1	1:B:146:GLU:N	2.45	0.43
1:B:611:GLU:O	6:B:1035:UAA:H5	2.19	0.43
1:B:699:ARG:NE	1:B:699:ARG:CA	2.81	0.43
1:C:439:GLY:HA2	5:C:1032:NDP:O2N	2.19	0.43
1:D:309:PHE:CD2	1:D:435:ILE:HD13	2.53	0.43
1:A:52:CYS:O	1:A:53:GLU:C	2.61	0.43
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.78	0.43
1:B:750:PRO:HG3	1:B:760:THR:HG22	2.00	0.43
1:B:954:ILE:HG23	1:B:998:ILE:HG13	1.99	0.43
1:C:993:LEU:HD23	1:C:993:LEU:C	2.43	0.43
1:D:108:ASN:HD21	1:D:111:GLY:HA3	1.81	0.43
1:D:454:ILE:HG13	1:D:456:PHE:HE1	1.83	0.43
1:A:500:SER:OG	1:A:501:TRP:N	2.52	0.43
1:A:528:VAL:O	1:A:531:VAL:HG23	2.18	0.43
1:B:573:THR:O	1:B:574:LYS:C	2.61	0.43
1:C:788:PHE:HA	1:C:789:PRO:HD3	1.84	0.43
1:D:100:PHE:C	1:D:100:PHE:HD1	2.24	0.43
1:D:324:CYS:SG	1:D:325:HIS:N	2.91	0.43
1:D:845:GLU:OE2	1:D:845:GLU:N	2.47	0.43
1:A:379:LEU:O	1:A:383:GLU:HG3	2.18	0.43
1:A:879:PHE:CD1	1:A:879:PHE:C	2.97	0.43
1:D:348:ALA:HB2	1:D:361:LEU:HD21	1.99	0.43
1:D:782:ALA:HB1	1:D:929:LEU:HD11	1.99	0.43
1:A:2:ALA:C	1:A:3:PRO:O	2.61	0.43
1:A:63:LYS:HE3	1:A:128:MET:CG	2.39	0.43
1:A:63:LYS:HD3	1:A:235:ARG:O	2.19	0.43
1:A:79:CYS:SG	1:A:101:ILE:HG21	2.58	0.43
1:A:262:SER:O	1:A:264:ASN:N	2.51	0.43
1:A:410:ARG:HH22	1:B:427:VAL:HG21	1.82	0.43
1:A:920:ALA:O	1:A:921:ILE:C	2.62	0.43
1:B:46:ASP:HB3	1:B:49:CYS:CB	2.48	0.43
1:B:409:VAL:HG21	1:B:423:GLU:HA	2.00	0.43
1:B:557:SER:CB	1:B:624:SER:HB3	2.49	0.43
1:B:587:SER:HA	1:B:588:PRO:C	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:ARG:N	1:B:772:PRO:CD	2.82	0.43
1:C:217:PHE:CE2	1:C:256:ILE:HD12	2.54	0.43
1:D:218:GLU:CD	4:D:1031:FAD:H1B	2.44	0.43
1:D:935:PHE:CD1	1:D:938:LEU:HD12	2.53	0.43
1:C:375:GLU:CD	1:C:375:GLU:N	2.77	0.43
1:D:997:PRO:CD	2:D:1028:SF4:S3	3.07	0.43
1:A:108:ASN:HA	1:A:852:GLN:HE22	1.84	0.43
1:A:191:ALA:C	1:A:192:LEU:HD12	2.44	0.43
1:A:369:ASN:ND2	1:B:50:PHE:CE2	2.82	0.43
1:B:454:ILE:HD12	1:B:462:PRO:HB3	2.01	0.43
1:C:230:GLU:HG2	1:C:310:LEU:HB2	2.00	0.43
1:C:267:THR:HG22	1:C:269:ASN:H	1.83	0.43
1:C:382:GLU:C	1:C:384:LYS:H	2.26	0.43
1:C:879:PHE:CD1	1:C:879:PHE:C	2.96	0.43
1:D:401:GLY:C	1:D:402:ARG:HG3	2.44	0.43
1:D:622:CYS:SG	1:D:656:LYS:HG2	2.59	0.43
1:D:993:LEU:C	1:D:993:LEU:HD23	2.44	0.43
1:B:106:ASN:O	1:B:107:LYS:HB2	2.19	0.42
1:B:537:MET:CE	1:B:791:LEU:HD11	2.48	0.42
1:B:807:HIS:O	1:B:928:ALA:HB3	2.19	0.42
1:C:294:PHE:HZ	1:C:338:LEU:CD1	2.31	0.42
1:C:379:LEU:HD23	1:C:379:LEU:HA	1.91	0.42
1:C:440:SER:O	1:C:441:VAL:HG13	2.19	0.42
1:D:150:ILE:O	1:D:152:ILE:HG13	2.18	0.42
1:D:546:PHE:CZ	1:D:830:TYR:HB3	2.54	0.42
1:A:390:PHE:CD1	1:B:388:LEU:HD21	2.54	0.42
1:A:572:LEU:HD13	1:A:638:ILE:HB	2.01	0.42
1:B:131:PRO:HG2	1:B:135:LEU:HD11	2.00	0.42
1:B:665:LEU:HB2	1:B:706:PHE:HB2	2.01	0.42
1:C:103:SER:HA	1:C:829:ASP:OD1	2.19	0.42
1:D:305:THR:H	1:D:308:ASP:HB2	1.84	0.42
1:D:382:GLU:C	1:D:384:LYS:H	2.26	0.42
1:D:779:THR:HG22	1:D:808:SER:CB	2.49	0.42
1:B:147:GLU:CD	1:B:147:GLU:H	2.27	0.42
1:B:622:CYS:SG	1:B:656:LYS:HG2	2.59	0.42
1:B:714:VAL:HG21	1:B:720:ILE:HD11	2.00	0.42
1:B:845:GLU:HG3	1:B:912:PHE:CE1	2.55	0.42
1:C:309:PHE:CE1	1:C:331:ILE:CD1	3.02	0.42
1:A:41:TRP:CZ2	1:B:89:LYS:HD2	2.55	0.42
1:A:248:MET:HE1	1:A:255:ILE:HD11	2.01	0.42
1:A:647:LYS:O	1:A:651:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ASP:OD1	1:B:532:ASP:C	2.62	0.42
1:B:991:LEU:HD23	1:B:991:LEU:HA	1.90	0.42
1:C:905:PRO:HA	1:C:906:PRO:HD3	1.86	0.42
1:D:893:GLU:O	1:D:897:LEU:HG	2.19	0.42
1:A:443:ARG:O	1:A:444:ASP:C	2.62	0.42
1:A:801:SER:O	1:A:804:GLN:HB2	2.20	0.42
1:B:2:ALA:O	1:B:3:PRO:O	2.38	0.42
1:B:193:LEU:N	1:B:193:LEU:CD2	2.82	0.42
1:C:731:GLY:HA2	1:C:788:PHE:CZ	2.54	0.42
1:C:771:ARG:N	1:C:772:PRO:CD	2.83	0.42
1:C:969:GLN:CD	1:C:969:GLN:N	2.78	0.42
1:D:844:GLU:OE1	1:D:915:LYS:HD2	2.18	0.42
1:A:184:GLU:O	1:A:185:ALA:C	2.62	0.42
1:A:965:ASP:O	1:B:553:PRO:HA	2.19	0.42
1:C:464:VAL:HG12	1:C:471:THR:HG22	2.02	0.42
1:D:537:MET:HE3	1:D:707:PHE:CE2	2.54	0.42
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.53	0.42
1:A:382:GLU:C	1:A:384:LYS:H	2.27	0.42
1:B:554:THR:HG22	1:B:560:ILE:HG12	2.02	0.42
1:B:616:LYS:HD3	1:B:620:TYR:CE2	2.55	0.42
1:C:885:GLN:O	1:C:889:ILE:HG13	2.19	0.42
1:C:910:LYS:HA	1:C:911:PRO:HD3	1.85	0.42
1:A:43:ARG:HB2	1:B:138:GLY:O	2.19	0.42
1:A:260:SER:O	1:A:266:ILE:HB	2.19	0.42
1:B:589:ARG:HG3	1:B:590:ILE:HG13	2.02	0.42
1:B:692:ARG:HH11	1:B:692:ARG:HB3	1.85	0.42
1:B:939:SER:OG	1:B:941:ILE:HG13	2.20	0.42
1:C:968:TYR:CD1	1:C:968:TYR:N	2.87	0.42
1:A:80:LEU:HD23	1:A:602:PRO:HD3	2.00	0.42
1:A:608:LEU:C	1:A:608:LEU:HD23	2.45	0.42
1:C:140:CYS:SG	1:C:149:SER:HB3	2.60	0.42
1:C:560:ILE:H	1:C:560:ILE:HG13	1.73	0.42
1:C:606:SER:HA	1:C:767:GLY:HA3	2.02	0.42
1:D:305:THR:O	1:D:308:ASP:N	2.39	0.42
1:D:413:GLN:HA	1:D:418:LYS:O	2.20	0.42
1:D:972:GLN:O	1:D:980:PRO:HA	2.19	0.42
1:A:41:TRP:O	1:A:42:LYS:C	2.63	0.42
1:A:82:CYS:O	1:A:98:LYS:HD2	2.19	0.42
1:A:132:THR:HB	1:A:137:VAL:HG23	2.02	0.42
1:A:369:ASN:ND2	1:B:50:PHE:CD2	2.88	0.42
1:A:699:ARG:NE	1:A:699:ARG:CA	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:O	1:A:726:GLU:HG3	2.20	0.42
1:C:220:GLN:HG3	1:C:222:TYR:CZ	2.55	0.42
1:C:477:PHE:CE1	1:C:503:ILE:HA	2.55	0.42
1:C:806:LEU:O	1:C:925:ILE:HA	2.20	0.42
1:C:943:GLN:HE22	1:D:586:VAL:HA	1.84	0.42
1:D:699:ARG:NE	1:D:699:ARG:CA	2.81	0.42
1:A:192:LEU:HD12	1:A:192:LEU:N	2.35	0.41
1:B:55:LEU:HD13	1:B:353:ARG:NH1	2.35	0.41
1:B:608:LEU:HA	1:B:764:GLY:O	2.20	0.41
1:C:608:LEU:HD13	1:C:742:MET:CB	2.41	0.41
1:D:112:ALA:O	1:D:116:ILE:HG13	2.20	0.41
1:D:342:ASP:CB	5:D:1032:NDP:C4N	2.98	0.41
1:A:5:LEU:HG	1:B:623:GLN:NE2	2.36	0.41
1:A:95:LEU:O	1:A:97:ILE:HG13	2.20	0.41
1:A:152:ILE:H	1:A:152:ILE:HG13	1.65	0.41
1:A:905:PRO:HA	1:A:906:PRO:HD3	1.79	0.41
1:A:947:VAL:O	1:A:947:VAL:CG1	2.68	0.41
1:B:689:GLU:HA	1:B:692:ARG:HH12	1.86	0.41
1:B:825:THR:C	1:B:827:ILE:N	2.75	0.41
1:B:959:CYS:SG	1:B:960:TYR:N	2.93	0.41
1:C:222:TYR:CE2	1:C:321:MET:HE2	2.54	0.41
1:C:651:MET:CE	1:C:701:ALA:HB2	2.50	0.41
1:C:709:LYS:HG3	1:C:733:THR:CG2	2.49	0.41
1:A:302:GLY:C	1:A:403:ILE:HD12	2.45	0.41
1:A:449:GLU:C	1:A:451:LEU:N	2.78	0.41
1:B:50:PHE:N	1:B:50:PHE:CD1	2.89	0.41
1:C:750:PRO:HG3	1:C:760:THR:HG22	2.02	0.41
1:D:173:ASN:HD21	1:D:175:CYS:HB2	1.85	0.41
1:D:315:LYS:HG2	1:D:321:MET:CE	2.49	0.41
1:D:342:ASP:OD1	1:D:372:ALA:HA	2.19	0.41
1:D:587:SER:HA	1:D:588:PRO:C	2.44	0.41
1:D:869:ALA:C	1:D:871:LEU:H	2.28	0.41
1:B:958:LYS:HE3	1:B:958:LYS:HB3	1.88	0.41
1:C:140:CYS:HB3	1:C:149:SER:HB3	2.02	0.41
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.78	0.41
1:C:755:GLY:C	1:C:757:GLY:H	2.26	0.41
1:C:962:THR:CG2	1:C:991:LEU:HB3	2.50	0.41
1:D:97:ILE:O	1:D:98:LYS:C	2.64	0.41
1:D:589:ARG:O	1:D:609:ASN:HA	2.20	0.41
1:D:714:VAL:HG11	1:D:720:ILE:HD13	2.03	0.41
1:D:859:HIS:CA	1:D:865:VAL:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:NE2	1:A:247:LEU:O	2.53	0.41
1:A:373:VAL:HA	1:A:374:PRO:HD3	1.94	0.41
1:A:844:GLU:O	1:A:847:GLN:HG3	2.20	0.41
1:C:998:ILE:CG2	1:C:1001:CYS:HB2	2.51	0.41
1:D:90:SER:HB2	1:D:136:CYS:HA	2.03	0.41
1:D:991:LEU:HD23	1:D:991:LEU:HA	1.85	0.41
1:A:762:TYR:CZ	1:B:780:THR:HG23	2.56	0.41
1:A:783:ARG:CG	1:A:929:LEU:HD22	2.50	0.41
1:B:342:ASP:CB	5:B:1032:NDP:C4N	2.98	0.41
1:B:775:LEU:HD23	1:B:775:LEU:HA	1.91	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.01	0.41
1:C:205:PHE:CE1	1:C:497:LYS:HG3	2.55	0.41
1:C:589:ARG:NH2	1:D:989:CYS:HB3	2.36	0.41
1:C:685:GLY:O	1:C:720:ILE:HD13	2.20	0.41
1:C:849:TRP:CG	1:C:854:PRO:HA	2.55	0.41
1:D:56:GLU:HG3	1:D:355:GLY:HA2	2.03	0.41
1:D:611:GLU:HG2	1:D:612:LEU:O	2.21	0.41
1:D:803:LEU:O	1:D:803:LEU:HD12	2.21	0.41
1:A:95:LEU:HD22	1:A:116:ILE:HA	2.01	0.41
1:A:259:LYS:HB3	1:A:266:ILE:CD1	2.49	0.41
1:A:386:GLU:OE1	1:B:367:PHE:HB2	2.21	0.41
1:A:449:GLU:C	1:A:451:LEU:H	2.28	0.41
1:B:879:PHE:CD1	1:B:879:PHE:C	2.98	0.41
1:C:34:LYS:HD3	1:C:34:LYS:HA	1.77	0.41
1:C:167:ASN:HB2	1:C:912:PHE:CD1	2.56	0.41
1:C:222:TYR:CD1	1:C:222:TYR:C	2.98	0.41
1:C:265:GLU:O	1:C:266:ILE:C	2.63	0.41
1:D:18:LEU:HD21	1:D:975:PRO:HA	2.03	0.41
1:D:91:CYS:HA	1:D:92:PRO:HD3	1.92	0.41
1:D:114:LYS:NZ	1:D:524:PHE:O	2.50	0.41
1:A:28:LEU:HD23	1:B:519:PRO:HG2	2.03	0.41
1:A:681:GLY:HA3	1:A:686:GLN:NE2	2.35	0.41
1:A:943:GLN:HG3	1:A:1011:TYR:CD2	2.56	0.41
1:B:56:GLU:HG3	1:B:355:GLY:HA2	2.01	0.41
1:B:178:SER:OG	1:B:181:LYS:HG3	2.21	0.41
1:B:692:ARG:NH1	1:B:692:ARG:CB	2.84	0.41
1:C:83:ALA:O	1:C:84:ASP:C	2.63	0.41
1:C:87:CYS:SG	1:C:97:ILE:CD1	3.08	0.41
1:C:762:TYR:OH	1:D:780:THR:HG22	2.19	0.41
1:D:439:GLY:HA2	5:D:1032:NDP:O2N	2.21	0.41
1:D:815:VAL:CG1	1:D:816:CYS:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:930:GLN:HG3	1:D:931:TYR:N	2.34	0.41
1:A:642:MET:HB2	1:A:668:ASN:HB3	2.03	0.41
1:B:69:GLU:O	1:B:70:ARG:C	2.64	0.41
1:B:196:GLY:O	1:B:197:PRO:C	2.63	0.41
1:B:608:LEU:HD13	1:B:742:MET:CB	2.45	0.41
1:B:738:VAL:HG21	1:B:773:ILE:CD1	2.50	0.41
1:B:796:ILE:CD1	1:B:813:LEU:HB3	2.46	0.41
1:B:962:THR:HG21	1:B:991:LEU:HB3	2.02	0.41
1:C:62:ILE:HG21	1:C:353:ARG:NH2	2.36	0.41
1:C:63:LYS:HE3	1:C:128:MET:HG2	2.03	0.41
1:C:109:TYR:N	1:C:109:TYR:CD2	2.86	0.41
1:C:217:PHE:HE2	1:C:256:ILE:HD12	1.84	0.41
1:C:283:ILE:CG1	1:C:482:ILE:HD13	2.49	0.41
1:C:523:LEU:HB2	1:C:525:TYR:CE1	2.55	0.41
1:C:900:GLN:C	1:C:902:ALA:H	2.29	0.41
1:C:954:ILE:HG21	1:C:998:ILE:HD11	2.02	0.41
1:C:968:TYR:CD2	1:C:987:THR:HG21	2.55	0.41
1:D:97:ILE:HD11	2:D:1026:SF4:S4	2.61	0.41
1:D:218:GLU:OE2	4:D:1031:FAD:H1B	2.20	0.41
1:D:654:SER:O	1:D:702:VAL:HG11	2.21	0.41
1:D:920:ALA:O	1:D:921:ILE:C	2.63	0.41
1:A:131:PRO:HB2	1:A:373:VAL:HG11	2.03	0.41
1:A:410:ARG:NH2	1:B:410:ARG:CZ	2.84	0.41
1:A:438:PHE:HA	5:A:1032:NDP:O4B	2.21	0.41
1:A:979:LEU:HD23	1:A:979:LEU:HA	1.91	0.41
1:C:263:GLU:HB2	1:C:446:LYS:HB3	2.03	0.41
1:C:267:THR:HG22	1:C:268:LEU:N	2.36	0.41
1:C:410:ARG:NE	1:D:410:ARG:NH2	2.59	0.41
1:D:124:LEU:CD1	1:D:161:GLU:HG2	2.49	0.41
1:D:398:VAL:HG13	1:D:402:ARG:C	2.46	0.41
1:D:692:ARG:HA	1:D:723:ALA:O	2.21	0.41
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.85	0.40
1:A:124:LEU:HG	1:A:240:VAL:HG13	2.03	0.40
1:A:771:ARG:HB3	1:A:772:PRO:HD3	2.03	0.40
1:B:285:LEU:HA	1:B:286:PRO:HD2	1.83	0.40
1:B:444:ASP:OD1	1:B:446:LYS:HB2	2.21	0.40
1:B:547:GLY:HA3	1:B:570:PHE:CE2	2.56	0.40
1:B:732:VAL:HG13	1:B:788:PHE:HE2	1.86	0.40
1:B:882:TYR:CZ	1:B:977:THR:HG22	2.56	0.40
1:C:482:ILE:O	1:C:482:ILE:HG13	2.21	0.40
1:C:557:SER:CB	1:C:624:SER:HB3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LYS:HE3	1:D:128:MET:HG2	2.03	0.40
1:D:176:LEU:HA	1:D:177:PRO:HD3	1.93	0.40
1:D:294:PHE:CZ	1:D:338:LEU:HD12	2.56	0.40
1:D:340:ALA:HB2	1:D:363:PHE:HB3	2.03	0.40
1:A:913:ILE:HA	1:A:914:PRO:HD3	1.99	0.40
1:B:92:PRO:HD2	2:B:1026:SF4:S3	2.61	0.40
1:B:222:TYR:CD1	1:B:222:TYR:C	3.00	0.40
1:C:134:ASP:O	1:D:38:LYS:HD2	2.21	0.40
1:C:366:GLY:HA2	1:C:390:PHE:CE1	2.56	0.40
1:C:397:ILE:HD11	1:C:428:HIS:NE2	2.36	0.40
1:D:396:VAL:CG1	1:D:403:ILE:HD12	2.51	0.40
1:A:262:SER:C	1:A:264:ASN:N	2.79	0.40
1:A:373:VAL:HA	1:B:47:LYS:HD3	2.03	0.40
1:B:97:ILE:HD13	1:B:152:ILE:HD13	2.03	0.40
1:B:305:THR:H	1:B:308:ASP:HB2	1.86	0.40
1:B:962:THR:O	1:B:966:SER:N	2.54	0.40
1:C:373:VAL:HA	1:C:374:PRO:HD3	1.90	0.40
1:C:820:GLN:NE2	1:D:991:LEU:HD11	2.37	0.40
1:C:968:TYR:O	1:C:969:GLN:C	2.63	0.40
1:D:552:ALA:HB3	1:D:553:PRO:HD3	2.03	0.40
1:D:806:LEU:HA	1:D:810:ALA:O	2.21	0.40
1:A:777:ALA:O	1:A:780:THR:HG22	2.21	0.40
1:B:155:LEU:HD23	1:B:155:LEU:HA	1.87	0.40
1:B:298:THR:OG1	1:B:301:GLN:HG3	2.22	0.40
1:B:396:VAL:HG11	1:B:403:ILE:HD13	2.02	0.40
1:C:267:THR:O	1:C:268:LEU:C	2.64	0.40
1:C:410:ARG:NE	1:D:410:ARG:CZ	2.85	0.40
1:C:775:LEU:HD23	1:C:775:LEU:HA	1.77	0.40
1:C:896:ARG:NH1	1:C:896:ARG:HG2	2.35	0.40
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.60	0.40
1:D:142:LEU:HA	1:D:142:LEU:HD23	1.77	0.40
1:D:225:GLY:O	1:D:226:LEU:C	2.64	0.40
1:D:842:SER:HA	1:D:916:LYS:HG2	2.03	0.40
4:D:1031:FAD:H9	4:D:1031:FAD:H1'1	1.96	0.40
1:A:164:LYS:HD2	1:A:243:PHE:CG	2.57	0.40
1:A:248:MET:CE	1:A:255:ILE:HD11	2.51	0.40
1:A:673:HIS:CE1	1:A:675:MET:HB2	2.56	0.40
1:C:285:LEU:HA	1:C:286:PRO:HD2	1.87	0.40
1:C:353:ARG:HH12	1:C:383:GLU:CD	2.29	0.40
1:C:413:GLN:HG3	1:C:419:TRP:CE2	2.57	0.40
1:C:518:LYS:HA	1:C:519:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:THR:O	1:C:574:LYS:C	2.62	0.40
1:C:577:SER:HA	1:C:653:LEU:CD2	2.51	0.40
1:D:41:TRP:O	1:D:42:LYS:C	2.64	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	1013/1025 (99%)	927 (92%)	72 (7%)	14 (1%)	9	33
1	B	1004/1025 (98%)	920 (92%)	77 (8%)	7 (1%)	18	49
1	C	1006/1025 (98%)	926 (92%)	74 (7%)	6 (1%)	21	52
1	D	1006/1025 (98%)	924 (92%)	73 (7%)	9 (1%)	14	43
All	All	4029/4100 (98%)	3697 (92%)	296 (7%)	36 (1%)	14	43

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	GLY
1	A	676	GLY
1	A	906	PRO
1	C	613	ILE
1	A	3	PRO
1	A	550	SER
1	A	613	ILE
1	A	681	GLY
1	B	293	ILE
1	B	613	ILE
1	C	293	ILE
1	D	613	ILE

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Mol	Chain	Res	Type
1	A	53	GLU
1	A	263	GLU
1	A	901	ASN
1	B	3	PRO
1	B	53	GLU
1	C	53	GLU
1	D	405	ALA
1	A	132	THR
1	D	151	ASN
1	D	293	ILE
1	D	550	SER
1	A	794	GLY
1	B	132	THR
1	C	266	ILE
1	C	551	ALA
1	D	185	ALA
1	D	1018	PRO
1	B	474	PRO
1	C	183	PRO
1	D	674	GLY
1	D	794	GLY
1	A	293	ILE
1	B	794	GLY
1	A	404	VAL

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	847/854 (99%)	828 (98%)	19 (2%)	45	66
1	B	842/854 (99%)	813 (97%)	29 (3%)	32	59
1	C	843/854 (99%)	824 (98%)	19 (2%)	44	66
1	D	844/854 (99%)	812 (96%)	32 (4%)	29	57
All	All	3376/3416 (99%)	3277 (97%)	99 (3%)	37	62

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	100	PHE
1	A	193	LEU
1	A	197	PRO
1	A	363	PHE
1	A	367	PHE
1	A	373	VAL
1	A	426	ILE
1	A	453	PRO
1	A	519	PRO
1	A	555	THR
1	A	644	SER
1	A	720	ILE
1	A	793	THR
1	A	800	GLU
1	A	813	LEU
1	A	845	GLU
1	A	955	ASN
1	A	985	THR
1	B	15	ILE
1	B	91	CYS
1	B	95	LEU
1	B	100	PHE
1	B	193	LEU
1	B	292	ASP
1	B	331	ILE
1	B	358	ARG
1	B	367	PHE
1	B	368	VAL
1	B	371	ARG
1	B	373	VAL
1	B	409	VAL
1	B	426	ILE
1	B	453	PRO
1	B	474	PRO
1	B	487	ASN
1	B	555	THR
1	B	599	MET
1	B	644	SER
1	B	700	GLN
1	B	702	VAL
1	B	793	THR

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Mol	Chain	Res	Type
1	B	800	GLU
1	B	813	LEU
1	B	845	GLU
1	B	941	ILE
1	B	984	ASP
1	B	985	THR
1	C	15	ILE
1	C	52	CYS
1	C	100	PHE
1	C	118	SER
1	C	367	PHE
1	C	371	ARG
1	C	416	THR
1	C	555	THR
1	C	562	ARG
1	C	667	LEU
1	C	695	CYS
1	C	780	THR
1	C	793	THR
1	C	800	GLU
1	C	813	LEU
1	C	845	GLU
1	C	858	SER
1	C	941	ILE
1	C	995	VAL
1	D	15	ILE
1	D	53	GLU
1	D	100	PHE
1	D	179	GLN
1	D	197	PRO
1	D	293	ILE
1	D	322	CYS
1	D	358	ARG
1	D	367	PHE
1	D	371	ARG
1	D	373	VAL
1	D	376	GLU
1	D	410	ARG
1	D	428	HIS
1	D	436	SER
1	D	441	VAL
1	D	449	GLU

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Mol	Chain	Res	Type
1	D	453	PRO
1	D	460	ASP
1	D	500	SER
1	D	558	SER
1	D	644	SER
1	D	667	LEU
1	D	672	PRO
1	D	720	ILE
1	D	741	LEU
1	D	793	THR
1	D	800	GLU
1	D	813	LEU
1	D	845	GLU
1	D	941	ILE
1	D	985	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	170	GLN
1	A	299	GLN
1	A	470	GLN
1	A	487	ASN
1	A	494	ASN
1	A	673	HIS
1	A	686	GLN
1	A	807	HIS
1	A	900	GLN
1	A	978	HIS
1	B	51	HIS
1	B	157	GLN
1	B	167	ASN
1	B	170	GLN
1	B	299	GLN
1	B	407	GLN
1	B	470	GLN
1	B	487	ASN
1	B	498	GLN
1	B	623	GLN
1	B	807	HIS
1	B	820	GLN

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Mol	Chain	Res	Type
1	B	822	GLN
1	B	859	HIS
1	C	23	GLN
1	C	64	HIS
1	C	170	GLN
1	C	173	ASN
1	C	470	GLN
1	C	487	ASN
1	C	544	ASN
1	C	693	ASN
1	C	822	GLN
1	C	859	HIS
1	C	878	ASN
1	C	901	ASN
1	D	57	ASN
1	D	170	GLN
1	D	299	GLN
1	D	325	HIS
1	D	407	GLN
1	D	487	ASN
1	D	508	GLN
1	D	510	GLN
1	D	623	GLN
1	D	673	HIS
1	D	693	ASN
1	D	820	GLN
1	D	822	GLN
1	D	828	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	1029	1	0,12,12	-	-	-		
5	NDP	C	1032	-	51,52,52	1.58	8 (15%)	71,80,80	1.61	14 (19%)
2	SF4	B	1026	1	0,12,12	-	-	-		
4	FAD	C	1031	-	58,58,58	2.48	23 (39%)	85,89,89	1.65	10 (11%)
6	UAA	B	1035	-	12,12,12	0.90	0	13,16,16	1.70	5 (38%)
3	FMN	A	1030	-	33,33,33	1.87	9 (27%)	48,50,50	1.77	11 (22%)
2	SF4	B	1028	1	0,12,12	-	-	-		
3	FMN	B	1030	-	33,33,33	1.94	8 (24%)	48,50,50	1.85	12 (25%)
2	SF4	D	1028	1	0,12,12	-	-	-		
2	SF4	C	1028	1	0,12,12	-	-	-		
3	FMN	C	1030	-	33,33,33	2.00	8 (24%)	48,50,50	1.79	10 (20%)
5	NDP	B	1032	-	51,52,52	1.67	7 (13%)	71,80,80	1.53	10 (14%)
2	SF4	A	1028	1	0,12,12	-	-	-		
2	SF4	C	1027	1	0,12,12	-	-	-		
2	SF4	A	1027	-	0,12,12	-	-	-		
2	SF4	D	1027	1	0,12,12	-	-	-		
2	SF4	D	1029	1	0,12,12	-	-	-		
2	SF4	C	1029	1	0,12,12	-	-	-		
4	FAD	B	1031	-	58,58,58	2.42	20 (34%)	85,89,89	1.66	7 (8%)
5	NDP	D	1032	-	51,52,52	1.83	11 (21%)	71,80,80	1.83	19 (26%)
2	SF4	A	1029	1	0,12,12	-	-	-		
6	UAA	D	1035	-	12,12,12	1.17	2 (16%)	13,16,16	1.66	4 (30%)
2	SF4	D	1026	1	0,12,12	-	-	-		
2	SF4	C	1026	1	0,12,12	-	-	-		
2	SF4	A	1026	-	0,12,12	-	-	-		
6	UAA	A	1035	-	12,12,12	1.01	0	13,16,16	1.58	3 (23%)
4	FAD	D	1031	-	58,58,58	2.51	20 (34%)	85,89,89	1.68	9 (10%)
2	SF4	B	1027	1	0,12,12	-	-	-		
4	FAD	A	1031	-	58,58,58	2.38	19 (32%)	85,89,89	1.66	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	UAA	C	1035	-	12,12,12	0.89	0	13,16,16	1.74	4 (30%)
3	FMN	D	1030	-	33,33,33	1.89	9 (27%)	48,50,50	1.82	12 (25%)
5	NDP	A	1032	-	51,52,52	1.74	12 (23%)	71,80,80	1.89	15 (21%)

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	1029	1	-	-	0/6/5/5
5	NDP	C	1032	-	-	5/34/77/77	0/5/5/5
4	FAD	C	1031	-	-	5/34/50/50	0/6/6/6
2	SF4	B	1026	1	-	-	0/6/5/5
6	UAA	B	1035	-	-	0/4/4/4	0/1/1/1
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	B	1028	1	-	-	0/6/5/5
5	NDP	B	1032	-	-	4/34/77/77	0/5/5/5
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1028	1	-	-	0/6/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	A	1028	1	-	-	0/6/5/5
2	SF4	C	1027	1	-	-	0/6/5/5
2	SF4	A	1027	-	-	-	0/6/5/5
4	FAD	B	1031	-	-	7/34/50/50	0/6/6/6
5	NDP	D	1032	-	-	4/34/77/77	0/5/5/5
2	SF4	C	1029	1	-	-	0/6/5/5
2	SF4	D	1027	1	-	-	0/6/5/5
2	SF4	D	1029	1	-	-	0/6/5/5
2	SF4	A	1029	1	-	-	0/6/5/5
6	UAA	D	1035	-	-	0/4/4/4	0/1/1/1
2	SF4	D	1026	1	-	-	0/6/5/5
2	SF4	C	1026	1	-	-	0/6/5/5
2	SF4	A	1026	-	-	-	0/6/5/5
6	UAA	A	1035	-	-	0/4/4/4	0/1/1/1
4	FAD	D	1031	-	-	4/34/50/50	0/6/6/6
2	SF4	B	1027	1	-	-	0/6/5/5
4	FAD	A	1031	-	-	5/34/50/50	0/6/6/6
6	UAA	C	1035	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
5	NDP	A	1032	-	-	4/34/77/77	0/5/5/5

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1031	FAD	PA-O3P	10.51	1.70	1.59
4	C	1031	FAD	P-O3P	-10.23	1.48	1.59
4	D	1031	FAD	PA-O3P	10.20	1.70	1.59
4	A	1031	FAD	PA-O3P	9.29	1.69	1.59
4	A	1031	FAD	P-O3P	-8.20	1.50	1.59
4	D	1031	FAD	P-O3P	-8.11	1.50	1.59
4	C	1031	FAD	PA-O3P	8.07	1.68	1.59
4	B	1031	FAD	P-O3P	-7.36	1.51	1.59
5	A	1032	NDP	C4N-C3N	-5.49	1.39	1.50
5	B	1032	NDP	C4N-C3N	-5.36	1.39	1.50
5	C	1032	NDP	C4N-C3N	-5.08	1.40	1.50
5	D	1032	NDP	C4N-C3N	-5.00	1.40	1.50
3	C	1030	FMN	C4A-N5	4.91	1.41	1.30
3	D	1030	FMN	C7M-C7	4.76	1.59	1.51
5	D	1032	NDP	PA-O3	-4.75	1.54	1.59
5	B	1032	NDP	C4N-C5N	-4.62	1.37	1.49
3	B	1030	FMN	C7M-C7	4.57	1.59	1.51
5	A	1032	NDP	C4N-C5N	-4.54	1.37	1.49
5	D	1032	NDP	C4N-C5N	-4.50	1.37	1.49
5	C	1032	NDP	C4N-C5N	-4.46	1.37	1.49
3	B	1030	FMN	C4A-N5	4.40	1.40	1.30
3	C	1030	FMN	C7M-C7	4.28	1.59	1.51
3	A	1030	FMN	C7M-C7	4.23	1.58	1.51
4	B	1031	FAD	PA-O2A	-4.21	1.35	1.55
3	D	1030	FMN	C4A-N5	4.20	1.39	1.30
3	A	1030	FMN	C1'-N10	-4.19	1.37	1.47
4	D	1031	FAD	PA-O2A	-4.15	1.36	1.55
5	D	1032	NDP	C2N-C3N	4.14	1.46	1.35
4	A	1031	FAD	PA-O2A	-4.13	1.36	1.55
5	A	1032	NDP	PA-O3	-4.07	1.55	1.59
3	C	1030	FMN	C1'-N10	-4.06	1.38	1.47
3	A	1030	FMN	C4A-N5	4.05	1.39	1.30
3	B	1030	FMN	C1'-N10	-3.96	1.38	1.47
3	D	1030	FMN	C1'-N10	-3.95	1.38	1.47
4	C	1031	FAD	PA-O2A	-3.94	1.37	1.55
5	B	1032	NDP	C2N-C3N	3.85	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C9A-N10	3.85	1.47	1.41
5	C	1032	NDP	C2N-C3N	3.84	1.45	1.35
5	A	1032	NDP	C2N-C3N	3.54	1.44	1.35
4	D	1031	FAD	C4X-N5	3.53	1.38	1.30
4	B	1031	FAD	P-O2P	-3.47	1.39	1.55
4	C	1031	FAD	P-O2P	-3.47	1.39	1.55
5	D	1032	NDP	PN-O3	-3.46	1.55	1.59
4	C	1031	FAD	C4X-N5	3.42	1.38	1.30
4	B	1031	FAD	C4X-N5	3.42	1.38	1.30
4	D	1031	FAD	C9A-N10	3.37	1.47	1.41
4	A	1031	FAD	P-O2P	-3.35	1.39	1.55
3	B	1030	FMN	C9A-N10	3.28	1.46	1.41
4	B	1031	FAD	O5'-C5'	3.27	1.57	1.44
3	B	1030	FMN	C1'-C2'	3.23	1.57	1.52
4	C	1031	FAD	O5'-C5'	3.22	1.56	1.44
5	B	1032	NDP	C3B-C2B	-3.21	1.46	1.53
4	A	1031	FAD	O5'-C5'	3.21	1.56	1.44
3	C	1030	FMN	C9A-C5A	3.21	1.46	1.41
3	C	1030	FMN	C4'-C3'	3.18	1.59	1.53
4	D	1031	FAD	C5A-C4A	3.15	1.44	1.39
4	B	1031	FAD	C9A-N10	3.10	1.46	1.41
4	D	1031	FAD	O5'-C5'	3.08	1.56	1.44
3	D	1030	FMN	C4'-C3'	3.07	1.58	1.53
5	A	1032	NDP	P2B-O2B	-3.07	1.54	1.59
3	B	1030	FMN	C9A-C5A	3.04	1.46	1.41
3	D	1030	FMN	C9A-N10	3.03	1.46	1.41
4	A	1031	FAD	C8-C7	3.02	1.48	1.40
3	A	1030	FMN	C9A-N10	2.99	1.46	1.41
4	D	1031	FAD	C9A-C5X	2.99	1.46	1.41
3	A	1030	FMN	C9A-C5A	2.98	1.46	1.41
3	A	1030	FMN	C4'-C3'	2.95	1.58	1.53
4	C	1031	FAD	C5A-C6A	2.95	1.49	1.41
4	C	1031	FAD	C9A-N10	2.93	1.46	1.41
4	A	1031	FAD	C4X-N5	2.91	1.37	1.30
4	D	1031	FAD	P-O2P	-2.89	1.41	1.55
4	C	1031	FAD	C4A-N3A	2.86	1.39	1.34
3	B	1030	FMN	C4'-C3'	2.84	1.58	1.53
3	D	1030	FMN	C9A-C5A	2.83	1.45	1.41
4	D	1031	FAD	C6-C5X	2.82	1.44	1.40
4	A	1031	FAD	C4A-N3A	2.79	1.39	1.34
4	D	1031	FAD	C5A-C6A	2.79	1.48	1.41
3	D	1030	FMN	C1'-C2'	2.75	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	C5B-C4B	2.72	1.59	1.51
4	D	1031	FAD	C2A-N1A	2.72	1.38	1.33
4	D	1031	FAD	O4B-C4B	2.72	1.51	1.45
4	D	1031	FAD	C4A-N3A	2.71	1.39	1.34
4	C	1031	FAD	C10-N1	2.71	1.38	1.33
4	C	1031	FAD	C6-C5X	2.70	1.44	1.40
4	C	1031	FAD	O4B-C1B	2.70	1.48	1.42
5	C	1032	NDP	C5D-C4D	2.68	1.59	1.51
4	A	1031	FAD	C5A-C6A	2.67	1.48	1.41
5	D	1032	NDP	P2B-O2B	-2.64	1.54	1.59
4	B	1031	FAD	C4A-N3A	2.64	1.39	1.34
4	B	1031	FAD	O4B-C4B	2.64	1.50	1.45
4	A	1031	FAD	C9A-N10	2.62	1.45	1.41
4	A	1031	FAD	C1'-C2'	2.58	1.56	1.52
4	C	1031	FAD	O4B-C4B	2.56	1.50	1.45
4	A	1031	FAD	C10-N1	2.56	1.38	1.33
4	A	1031	FAD	O4B-C4B	2.55	1.50	1.45
4	B	1031	FAD	C9A-C5X	2.54	1.45	1.41
4	D	1031	FAD	C9-C9A	2.54	1.43	1.39
4	D	1031	FAD	C8-C7	2.53	1.47	1.40
6	D	1035	UAA	C6-N1	2.52	1.41	1.37
4	B	1031	FAD	O4B-C1B	2.51	1.47	1.42
4	B	1031	FAD	C5B-C4B	2.50	1.59	1.51
4	C	1031	FAD	C1'-C2'	2.48	1.56	1.52
4	C	1031	FAD	C8-C7	2.48	1.46	1.40
4	B	1031	FAD	C5A-C6A	2.48	1.47	1.41
4	B	1031	FAD	C10-N1	2.47	1.38	1.33
5	D	1032	NDP	C5D-C4D	2.47	1.59	1.51
3	C	1030	FMN	C10-N1	2.47	1.38	1.33
5	A	1032	NDP	C5D-C4D	2.46	1.59	1.51
4	B	1031	FAD	C5A-C4A	2.46	1.43	1.39
4	C	1031	FAD	C5A-C4A	2.45	1.43	1.39
4	C	1031	FAD	C2A-N1A	2.45	1.38	1.33
4	C	1031	FAD	C5B-C4B	2.44	1.58	1.51
4	A	1031	FAD	C9A-C5X	2.43	1.45	1.41
5	B	1032	NDP	C8A-N9A	2.43	1.41	1.37
4	B	1031	FAD	C6-C5X	2.41	1.43	1.40
5	A	1032	NDP	PN-O3	-2.39	1.56	1.59
5	B	1032	NDP	C5D-C4D	2.38	1.58	1.51
4	A	1031	FAD	C6-C5X	2.37	1.43	1.40
4	D	1031	FAD	C10-N1	2.35	1.38	1.33
5	D	1032	NDP	C4A-N3A	2.35	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1032	NDP	C3B-C2B	-2.33	1.47	1.53
5	A	1032	NDP	C8A-N9A	2.29	1.41	1.37
4	A	1031	FAD	C5A-C4A	2.28	1.43	1.39
4	C	1031	FAD	C9-C8	2.26	1.42	1.39
4	B	1031	FAD	C2-N3	2.26	1.43	1.39
5	A	1032	NDP	C3B-C2B	-2.25	1.48	1.53
4	A	1031	FAD	C2A-N1A	2.24	1.37	1.33
4	C	1031	FAD	C2-N3	2.24	1.43	1.39
4	C	1031	FAD	PA-O5B	-2.22	1.50	1.59
4	C	1031	FAD	C9A-C5X	2.21	1.44	1.41
5	D	1032	NDP	C8A-N9A	2.21	1.41	1.37
3	A	1030	FMN	C6-C7	2.20	1.42	1.39
3	D	1030	FMN	C10-N1	2.20	1.37	1.33
5	C	1032	NDP	PA-O3	-2.17	1.57	1.59
4	D	1031	FAD	C1'-C2'	2.17	1.55	1.52
4	A	1031	FAD	C2-N3	2.16	1.43	1.39
4	C	1031	FAD	C9-C9A	2.12	1.43	1.39
5	A	1032	NDP	C2B-C1B	-2.12	1.47	1.53
4	B	1031	FAD	C2A-N1A	2.11	1.37	1.33
6	D	1035	UAA	C5-C6	2.10	1.39	1.36
4	B	1031	FAD	C8-C7	2.10	1.46	1.40
3	D	1030	FMN	C6-C7	2.08	1.42	1.39
3	A	1030	FMN	C1'-C2'	2.08	1.55	1.52
5	D	1032	NDP	PA-O1A	-2.06	1.43	1.50
5	C	1032	NDP	PA-O1A	-2.06	1.43	1.50
3	A	1030	FMN	C10-N1	2.06	1.37	1.33
5	A	1032	NDP	PA-O1A	-2.06	1.43	1.50
4	A	1031	FAD	C5B-C4B	2.05	1.57	1.51
5	C	1032	NDP	C3B-C2B	-2.04	1.48	1.53
5	A	1032	NDP	C4A-N3A	2.04	1.38	1.34
3	B	1030	FMN	C6-C7	2.04	1.42	1.39
4	B	1031	FAD	P-O5'	-2.04	1.51	1.59
4	D	1031	FAD	C2-N3	2.03	1.43	1.39
5	B	1032	NDP	P2B-O2B	-2.03	1.56	1.59
3	C	1030	FMN	C8M-C8	2.01	1.54	1.51
5	C	1032	NDP	C8A-N9A	2.00	1.40	1.37

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1031	FAD	O3P-PA-O1A	-8.90	83.92	110.70
4	A	1031	FAD	O3P-PA-O1A	-8.78	84.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1031	FAD	O3P-PA-O1A	-8.66	84.66	110.70
4	C	1031	FAD	O3P-PA-O1A	-8.45	85.30	110.70
4	C	1031	FAD	O2A-PA-O3P	-7.54	86.89	107.27
4	A	1031	FAD	O2A-PA-O3P	-7.53	86.92	107.27
4	B	1031	FAD	O2A-PA-O3P	-7.17	87.90	107.27
4	D	1031	FAD	O2A-PA-O3P	-7.13	88.00	107.27
5	D	1032	NDP	O3-PA-O1A	-7.02	89.58	110.70
5	A	1032	NDP	O3-PA-O1A	-6.70	90.53	110.70
5	B	1032	NDP	C3N-C2N-N1N	-4.84	116.10	123.20
5	C	1032	NDP	C3N-C2N-N1N	-4.84	116.10	123.20
5	B	1032	NDP	O3-PA-O1A	-4.80	96.28	110.70
3	B	1030	FMN	C10-N1-C2	4.74	127.11	116.85
5	D	1032	NDP	C3N-C2N-N1N	-4.73	116.26	123.20
5	A	1032	NDP	C3N-C2N-N1N	-4.68	116.34	123.20
5	C	1032	NDP	O3-PA-O1A	-4.61	96.83	110.70
3	A	1030	FMN	C10-N1-C2	4.58	126.78	116.85
3	C	1030	FMN	C10-N1-C2	4.58	126.78	116.85
3	D	1030	FMN	C10-N1-C2	4.58	126.77	116.85
5	A	1032	NDP	O2A-PA-O1A	4.28	132.34	112.44
5	A	1032	NDP	O3-PN-O1N	-4.23	97.99	110.70
5	A	1032	NDP	O5D-PN-O1N	4.22	125.67	108.94
3	D	1030	FMN	C4-C4A-C10	4.15	124.05	116.93
3	D	1030	FMN	C4A-C10-N1	-4.09	114.56	124.59
3	B	1030	FMN	C4A-C10-N1	-4.08	114.59	124.59
3	C	1030	FMN	C4A-C10-N1	-3.97	114.84	124.59
3	A	1030	FMN	C4-C4A-C10	3.88	123.59	116.93
3	A	1030	FMN	C4A-C10-N1	-3.87	115.10	124.59
3	C	1030	FMN	O4'-C4'-C3'	3.84	118.23	109.25
3	B	1030	FMN	O4'-C4'-C3'	3.83	118.21	109.25
3	C	1030	FMN	C4-C4A-C10	3.82	123.48	116.93
3	B	1030	FMN	C4-C4A-C10	3.80	123.45	116.93
3	A	1030	FMN	O4'-C4'-C3'	3.73	117.97	109.25
3	D	1030	FMN	O4'-C4'-C3'	3.71	117.92	109.25
3	A	1030	FMN	O3'-C3'-C2'	-3.65	100.63	108.93
5	D	1032	NDP	O2N-PN-O3	-3.64	97.42	107.27
4	A	1031	FAD	O2A-PA-O1A	3.59	129.15	112.44
4	D	1031	FAD	O2A-PA-O1A	3.53	128.87	112.44
5	C	1032	NDP	O3-PN-O1N	-3.53	100.09	110.70
5	B	1032	NDP	O2A-PA-O1A	3.48	128.65	112.44
5	A	1032	NDP	C1D-N1N-C2N	-3.45	115.45	121.14
4	B	1031	FAD	O2A-PA-O1A	3.45	128.50	112.44
4	C	1031	FAD	O2A-PA-O1A	3.43	128.40	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1030	FMN	O3'-C3'-C2'	-3.35	101.31	108.93
3	B	1030	FMN	O3'-C3'-C2'	-3.34	101.33	108.93
5	D	1032	NDP	O4B-C1B-N9A	3.34	114.51	108.09
5	A	1032	NDP	C2B-C1B-N9A	-3.32	108.29	113.75
3	D	1030	FMN	O3'-C3'-C2'	-3.23	101.60	108.93
5	D	1032	NDP	C2B-C1B-N9A	-3.19	108.50	113.75
5	C	1032	NDP	C1D-N1N-C2N	-3.14	115.97	121.14
5	C	1032	NDP	O5D-PN-O1N	3.13	121.34	108.94
5	D	1032	NDP	O5D-PN-O1N	3.08	121.16	108.94
3	C	1030	FMN	C5'-C4'-C3'	-3.07	106.42	112.22
5	B	1032	NDP	C1D-N1N-C2N	-3.00	116.20	121.14
6	C	1035	UAA	O4-C4-N3	2.98	123.59	119.27
5	D	1032	NDP	O2A-PA-O1A	2.97	126.28	112.44
6	D	1035	UAA	C4-N3-C2	2.96	128.41	125.55
5	A	1032	NDP	O2N-PN-O3	2.90	115.12	107.27
6	D	1035	UAA	O4-C4-N3	2.90	123.48	119.27
6	A	1035	UAA	C4-N3-C2	2.90	128.36	125.55
3	B	1030	FMN	C5'-C4'-C3'	-2.89	106.77	112.22
3	B	1030	FMN	O3'-C3'-C4'	2.87	115.46	108.93
5	A	1032	NDP	O4B-C1B-N9A	2.87	113.61	108.09
5	C	1032	NDP	C2B-C1B-N9A	-2.85	109.06	113.75
5	D	1032	NDP	O7N-C7N-N7N	-2.83	116.54	122.89
5	C	1032	NDP	O4B-C1B-N9A	2.83	113.52	108.09
5	D	1032	NDP	C1D-N1N-C2N	-2.83	116.48	121.14
4	D	1031	FAD	O4B-C1B-N9A	-2.80	102.70	108.09
5	C	1032	NDP	O7N-C7N-N7N	-2.80	116.62	122.89
3	B	1030	FMN	C4A-C10-N10	2.80	120.48	116.48
3	D	1030	FMN	C5'-C4'-C3'	-2.79	106.95	112.22
4	D	1031	FAD	C5'-C4'-C3'	-2.74	107.04	112.22
6	B	1035	UAA	C4-N3-C2	2.73	128.19	125.55
4	B	1031	FAD	C2A-N1A-C6A	2.71	123.18	118.73
3	C	1030	FMN	O3'-C3'-C4'	2.68	115.03	108.93
4	B	1031	FAD	O4B-C1B-N9A	-2.65	102.99	108.09
5	A	1032	NDP	O5B-PA-O1A	-2.65	98.43	108.94
5	C	1032	NDP	C6N-N1N-C2N	2.65	122.15	119.32
3	D	1030	FMN	O3'-C3'-C4'	2.64	114.93	108.93
3	A	1030	FMN	C5'-C4'-C3'	-2.64	107.24	112.22
4	D	1031	FAD	C2A-N1A-C6A	2.63	123.05	118.73
5	A	1032	NDP	O2B-C2B-C3B	2.62	121.09	111.68
5	B	1032	NDP	O7N-C7N-N7N	-2.62	117.02	122.89
6	A	1035	UAA	O4-C4-N3	2.60	123.04	119.27
5	A	1032	NDP	C6N-N1N-C2N	2.59	122.09	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1032	NDP	O7N-C7N-N7N	-2.59	117.09	122.89
5	D	1032	NDP	O3-PN-O1N	-2.56	103.02	110.70
6	C	1035	UAA	O4-C4-C5	-2.53	121.97	125.46
3	A	1030	FMN	C4A-C10-N10	2.49	120.05	116.48
4	C	1031	FAD	C5'-C4'-C3'	-2.49	107.52	112.22
4	C	1031	FAD	O4B-C1B-N9A	-2.48	103.32	108.09
3	D	1030	FMN	C4A-C10-N10	2.48	120.03	116.48
6	B	1035	UAA	O4-C4-N3	2.48	122.86	119.27
4	A	1031	FAD	C2A-N1A-C6A	2.47	122.79	118.73
6	C	1035	UAA	C5-C6-N1	2.46	121.57	119.54
6	D	1035	UAA	O4-C4-C5	-2.43	122.10	125.46
5	D	1032	NDP	O2B-C2B-C3B	2.42	120.37	111.68
3	A	1030	FMN	O3'-C3'-C4'	2.41	114.40	108.93
6	C	1035	UAA	C4-N3-C2	2.40	127.87	125.55
3	C	1030	FMN	C4A-C10-N10	2.36	119.86	116.48
4	B	1031	FAD	C5'-C4'-C3'	-2.35	107.78	112.22
6	B	1035	UAA	C5-C6-N1	2.35	121.48	119.54
3	D	1030	FMN	N10-C10-N1	2.34	125.40	118.51
5	B	1032	NDP	C6N-N1N-C2N	2.34	121.82	119.32
5	A	1032	NDP	N9A-C8A-N7A	-2.34	110.62	113.94
4	A	1031	FAD	O4B-C1B-N9A	-2.33	103.62	108.09
5	C	1032	NDP	O2B-C2B-C3B	2.32	120.00	111.68
5	B	1032	NDP	C4B-O4B-C1B	-2.32	104.35	109.47
3	C	1030	FMN	N10-C10-N1	2.30	125.29	118.51
4	C	1031	FAD	C5X-C9A-N10	-2.28	115.91	117.97
4	D	1031	FAD	C5X-C9A-N10	-2.27	115.92	117.97
4	C	1031	FAD	C2A-N1A-C6A	2.27	122.45	118.73
5	A	1032	NDP	N3A-C2A-N1A	-2.26	125.16	128.58
6	B	1035	UAA	C4-C5-C6	-2.25	118.79	120.56
3	B	1030	FMN	C6-C5A-C9A	2.25	122.13	119.05
6	B	1035	UAA	O4-C4-C5	-2.24	122.36	125.46
3	B	1030	FMN	C9A-C5A-N5	-2.24	120.08	122.45
3	D	1030	FMN	C4-C4A-N5	-2.23	115.13	118.21
5	D	1032	NDP	C4B-O4B-C1B	-2.22	104.56	109.47
5	C	1032	NDP	N9A-C8A-N7A	-2.22	110.79	113.94
4	A	1031	FAD	C5'-C4'-C3'	-2.22	108.04	112.22
5	D	1032	NDP	C6N-N1N-C2N	2.21	121.69	119.32
5	C	1032	NDP	N3A-C2A-N1A	-2.21	125.24	128.58
4	C	1031	FAD	C4-N3-C2	-2.21	121.72	125.64
6	D	1035	UAA	C6-N1-C2	-2.20	120.90	123.15
5	B	1032	NDP	N9A-C8A-N7A	-2.19	110.83	113.94
5	D	1032	NDP	N3A-C2A-N1A	-2.19	125.27	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1032	NDP	O2N-PN-O1N	2.19	122.62	112.44
5	D	1032	NDP	O4B-C1B-C2B	2.18	110.34	106.59
3	B	1030	FMN	N10-C10-N1	2.18	124.92	118.51
4	D	1031	FAD	C4-C4X-N5	2.16	121.19	118.21
5	C	1032	NDP	C4B-O4B-C1B	-2.16	104.71	109.47
5	B	1032	NDP	O5B-C5B-C4B	-2.15	101.67	108.99
3	A	1030	FMN	N10-C10-N1	2.15	124.83	118.51
4	C	1031	FAD	C10-N1-C2	2.13	121.47	116.85
4	A	1031	FAD	C5X-C9A-N10	-2.13	116.04	117.97
3	D	1030	FMN	C6-C5A-C9A	2.13	121.97	119.05
3	A	1030	FMN	C4-C4A-N5	-2.13	115.27	118.21
5	D	1032	NDP	N9A-C8A-N7A	-2.09	110.97	113.94
3	B	1030	FMN	N3-C2-N1	-2.09	115.06	119.50
5	B	1032	NDP	N3A-C2A-N1A	-2.08	125.43	128.58
3	C	1030	FMN	C6-C5A-C9A	2.06	121.88	119.05
3	A	1030	FMN	N3-C2-N1	-2.06	115.12	119.50
5	C	1032	NDP	O2B-P2B-O1X	-2.06	102.00	109.33
4	B	1031	FAD	C4-N3-C2	-2.06	121.99	125.64
5	D	1032	NDP	O5B-C5B-C4B	-2.05	102.01	108.99
5	D	1032	NDP	O5B-PA-O1A	-2.04	100.86	108.94
3	D	1030	FMN	O2'-C2'-C1'	2.03	118.55	110.20
4	C	1031	FAD	O2A-PA-O5B	2.03	116.77	107.57
4	D	1031	FAD	C10-N1-C2	2.03	121.24	116.85
6	A	1035	UAA	O4-C4-C5	-2.00	122.69	125.46

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	C5B-O5B-PA-O3P
4	B	1031	FAD	C5B-O5B-PA-O3P
4	C	1031	FAD	C5B-O5B-PA-O3P
4	D	1031	FAD	C5B-O5B-PA-O3P
5	A	1032	NDP	O4D-C1D-N1N-C2N
5	B	1032	NDP	O4D-C1D-N1N-C2N
5	C	1032	NDP	O4D-C1D-N1N-C2N
5	D	1032	NDP	C3B-C2B-O2B-P2B
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	A	1032	NDP	C1B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
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	D	1031	FAD	C3B-C4B-C5B-O5B
4	A	1031	FAD	C3B-C4B-C5B-O5B
4	B	1031	FAD	C3B-C4B-C5B-O5B
4	C	1031	FAD	O4B-C4B-C5B-O5B
4	C	1031	FAD	C3B-C4B-C5B-O5B
4	A	1031	FAD	O4B-C4B-C5B-O5B
4	B	1031	FAD	O4B-C4B-C5B-O5B
4	D	1031	FAD	O4B-C4B-C5B-O5B
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
4	B	1031	FAD	PA-O3P-P-O5'
5	A	1032	NDP	PN-O3-PA-O5B
5	B	1032	NDP	PN-O3-PA-O5B
5	C	1032	NDP	PN-O3-PA-O5B
5	D	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
4	B	1031	FAD	P-O3P-PA-O1A
4	B	1031	FAD	P-O3P-PA-O2A
4	A	1031	FAD	PA-O3P-P-O5'
5	C	1032	NDP	PN-O3-PA-O1A
4	C	1031	FAD	O4B-C1B-N9A-C8A

There are no ring outliers.

28 monomers are involved in 64 short contacts:

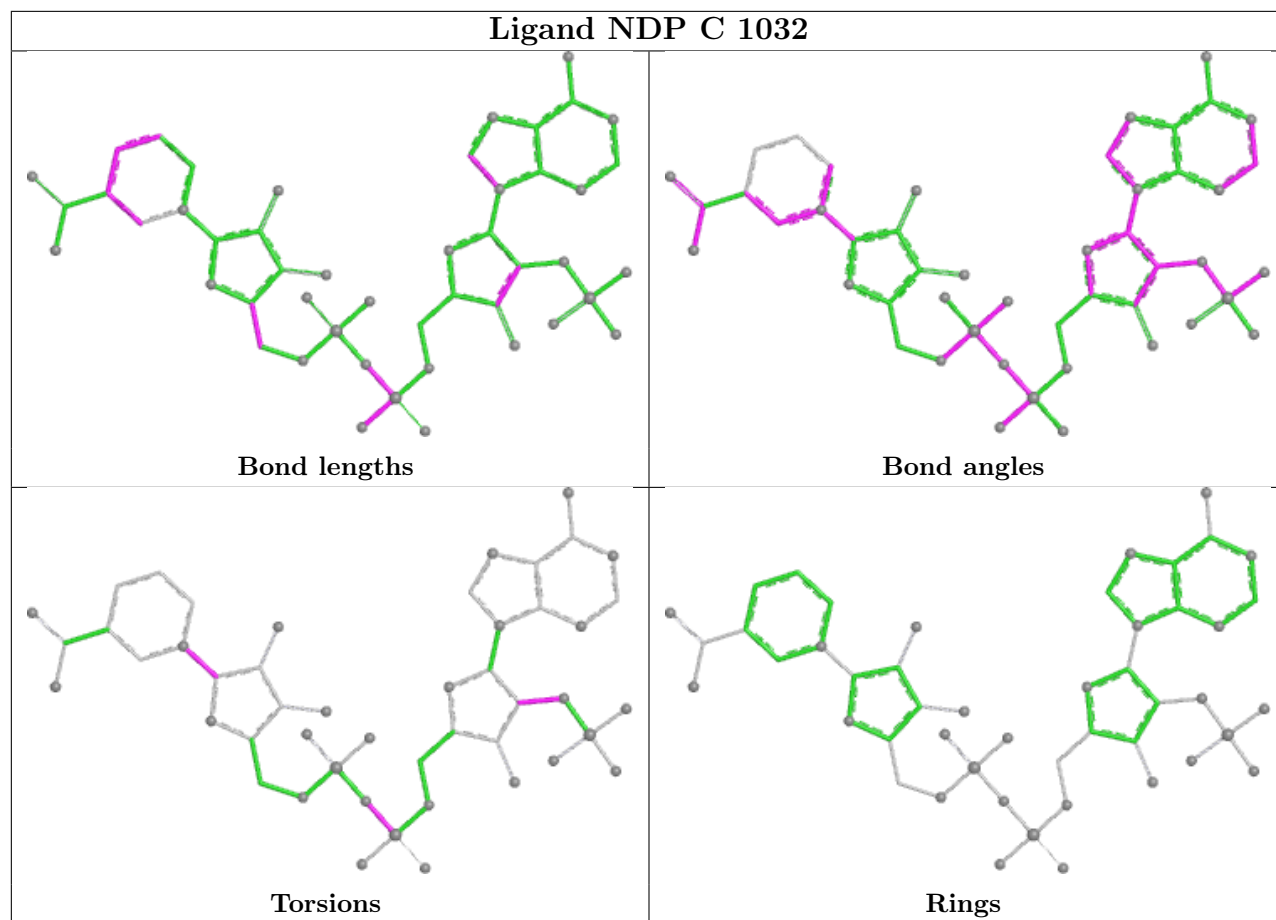
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1029	SF4	2	0
5	C	1032	NDP	6	0
2	B	1026	SF4	2	0
4	C	1031	FAD	2	0
6	B	1035	UAA	1	0
2	B	1028	SF4	2	0
2	D	1028	SF4	4	0
2	C	1028	SF4	2	0

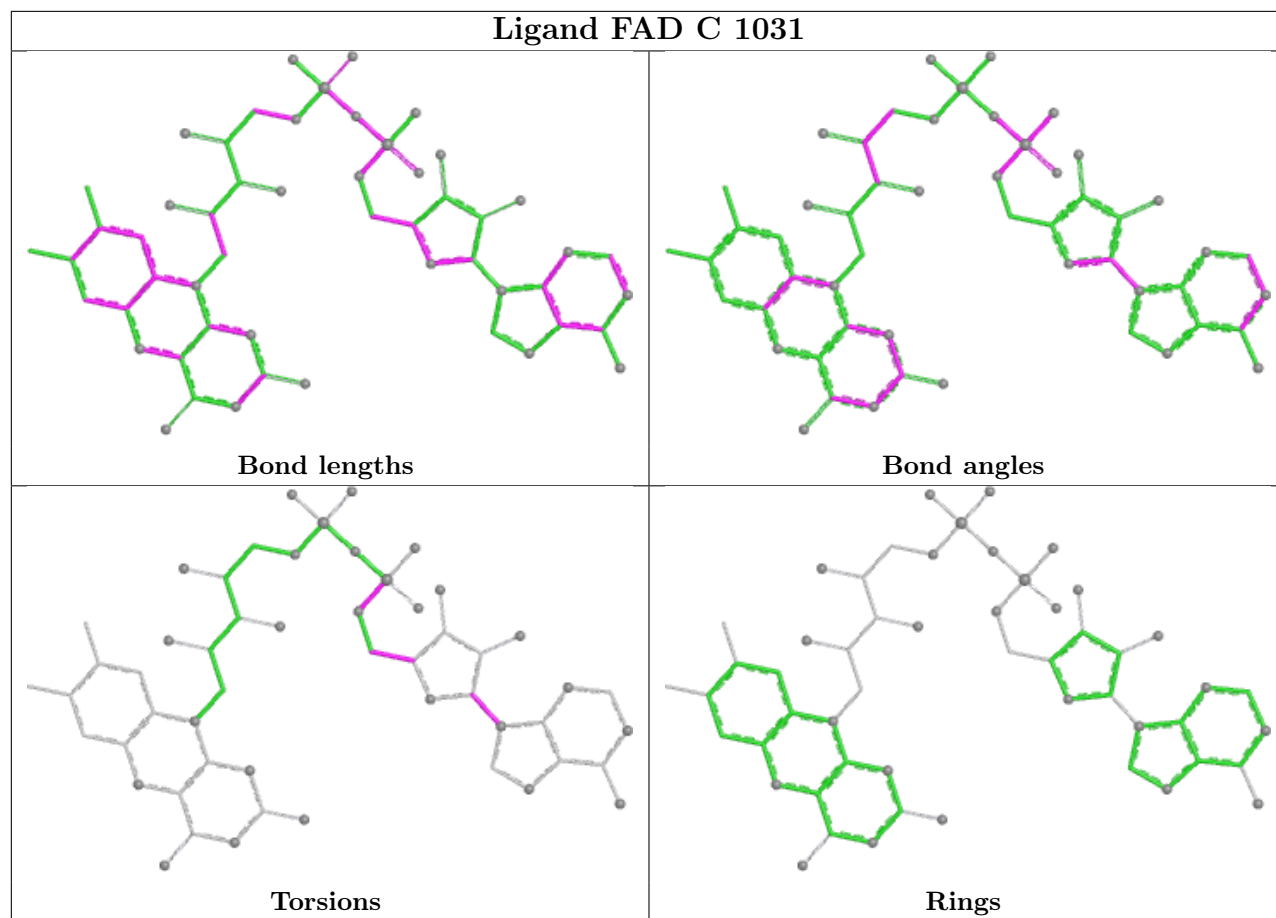
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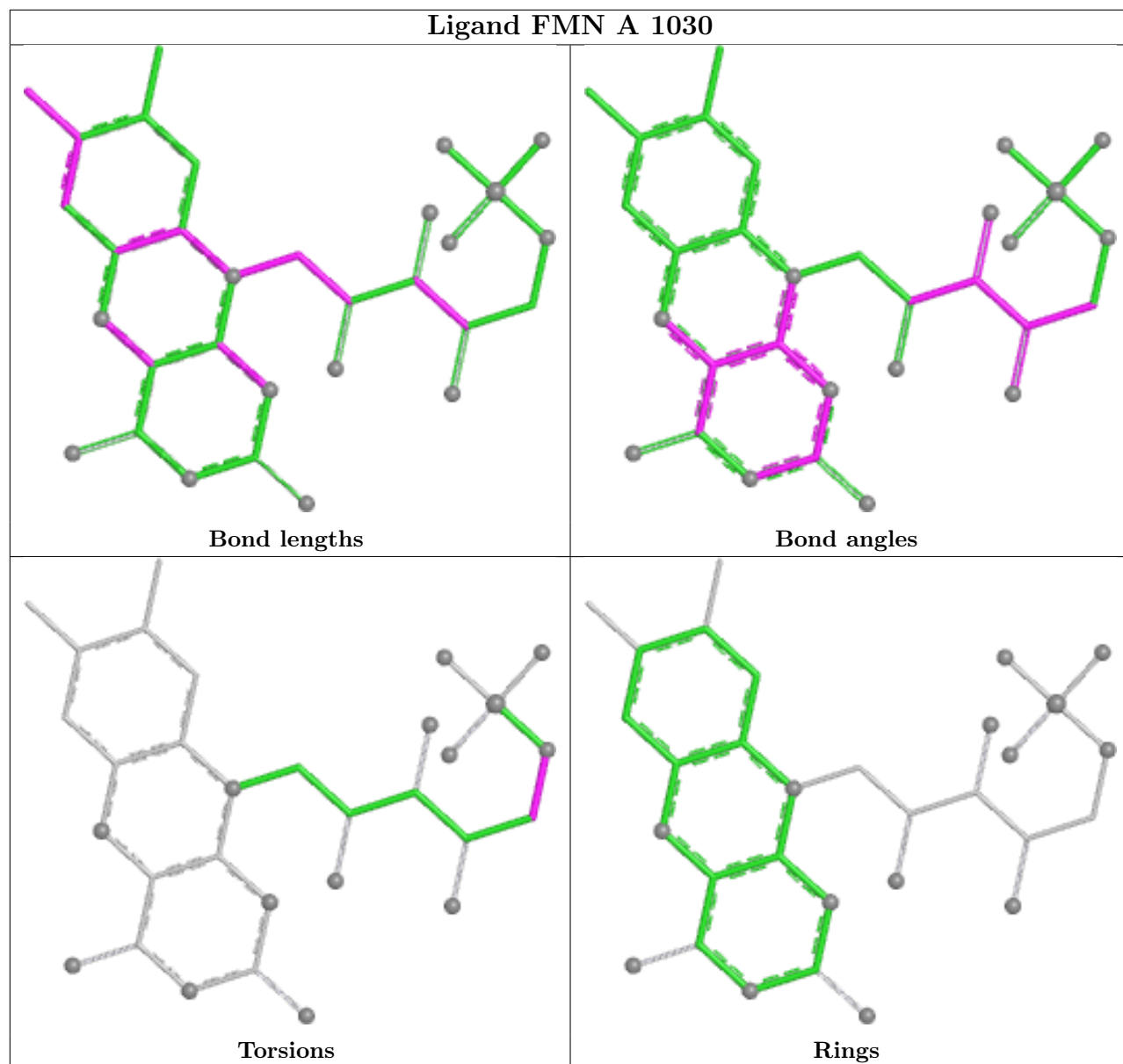
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1032	NDP	5	0
2	A	1028	SF4	2	0
2	C	1027	SF4	2	0
2	A	1027	SF4	2	0
2	D	1027	SF4	2	0
2	D	1029	SF4	1	0
2	C	1029	SF4	1	0
4	B	1031	FAD	1	0
5	D	1032	NDP	6	0
2	A	1029	SF4	1	0
2	D	1026	SF4	1	0
2	C	1026	SF4	1	0
2	A	1026	SF4	1	0
6	A	1035	UAA	1	0
4	D	1031	FAD	5	0
2	B	1027	SF4	2	0
4	A	1031	FAD	1	0
6	C	1035	UAA	1	0
3	D	1030	FMN	1	0
5	A	1032	NDP	6	0

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

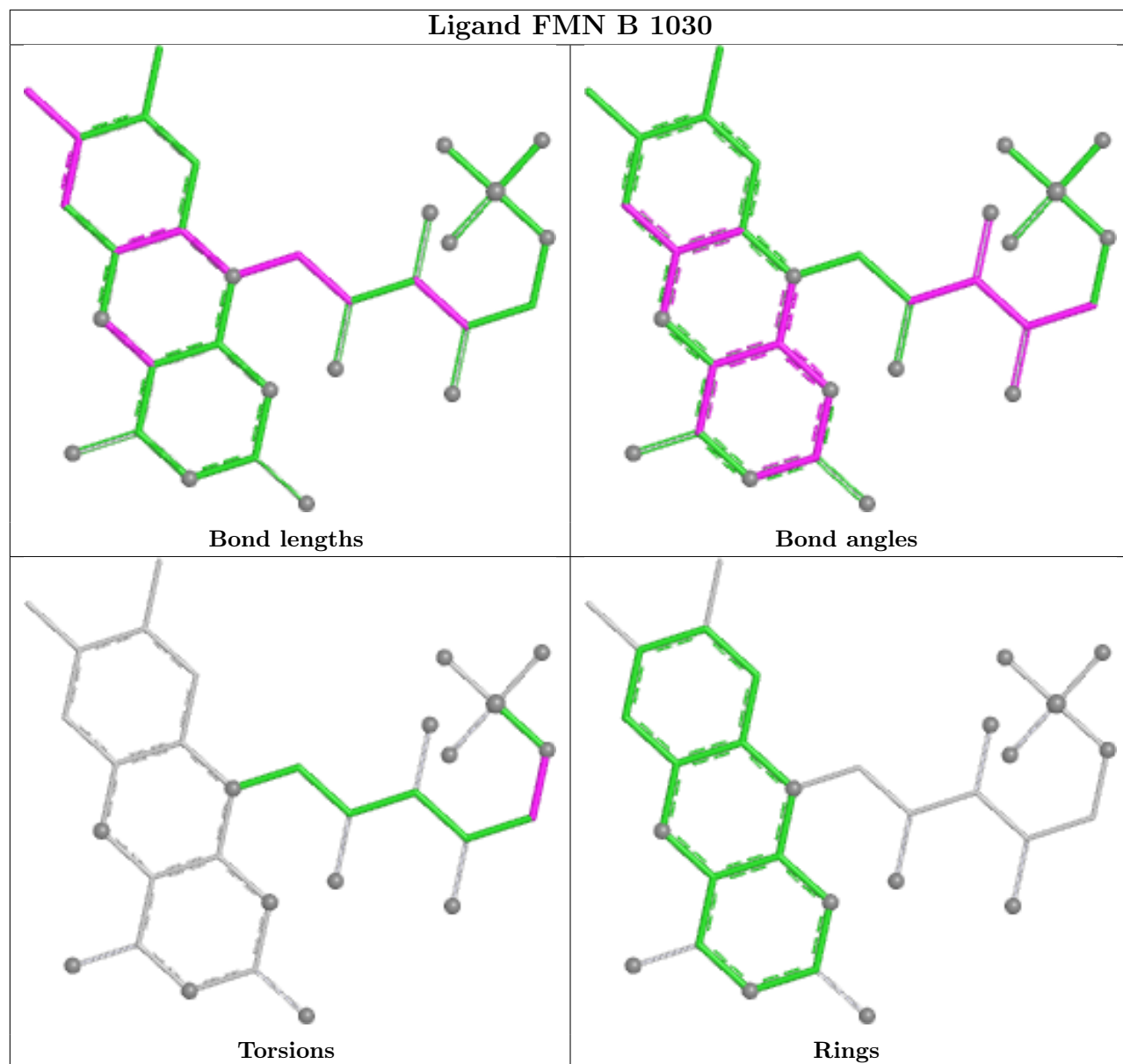




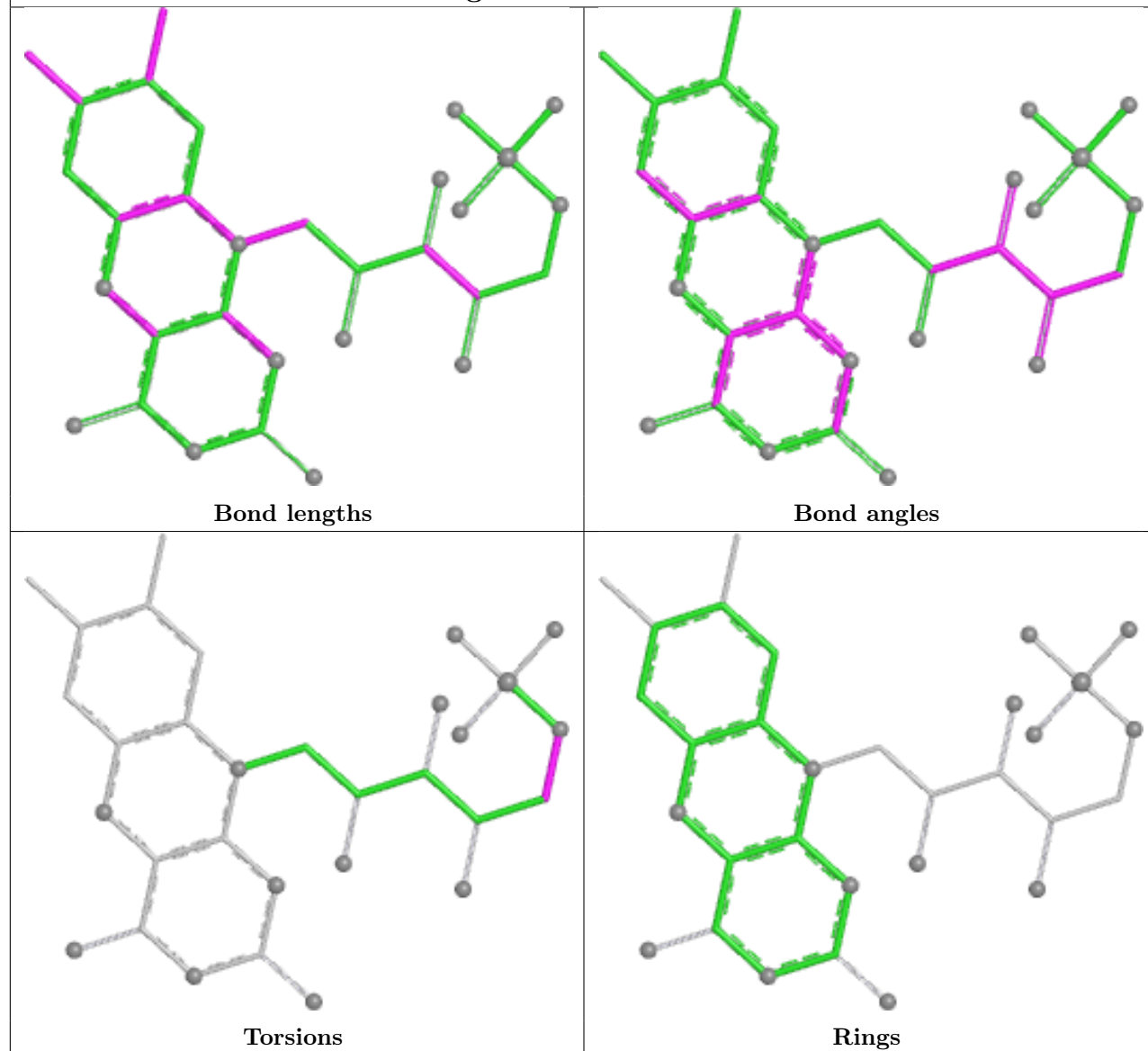
Ligand FMN A 1030

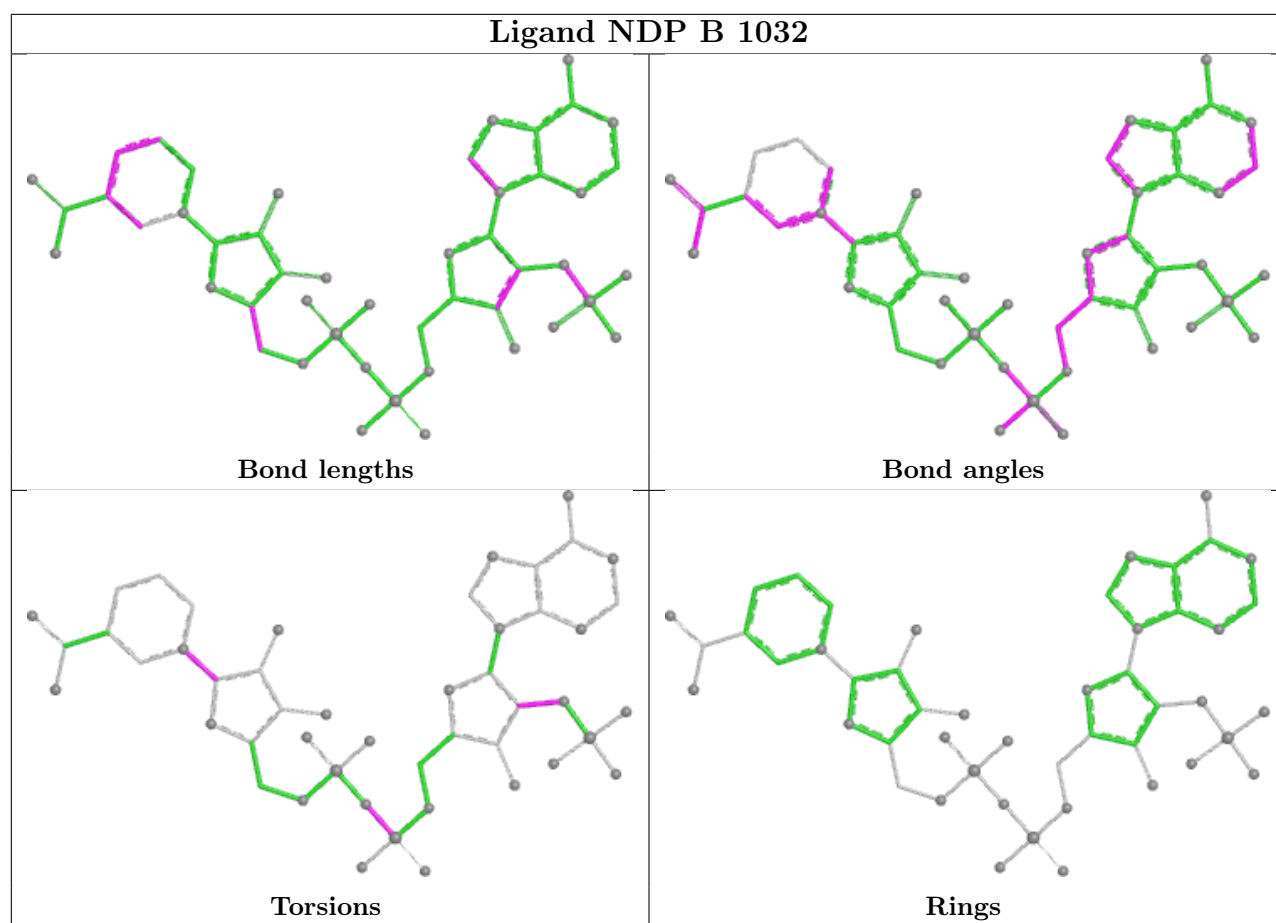


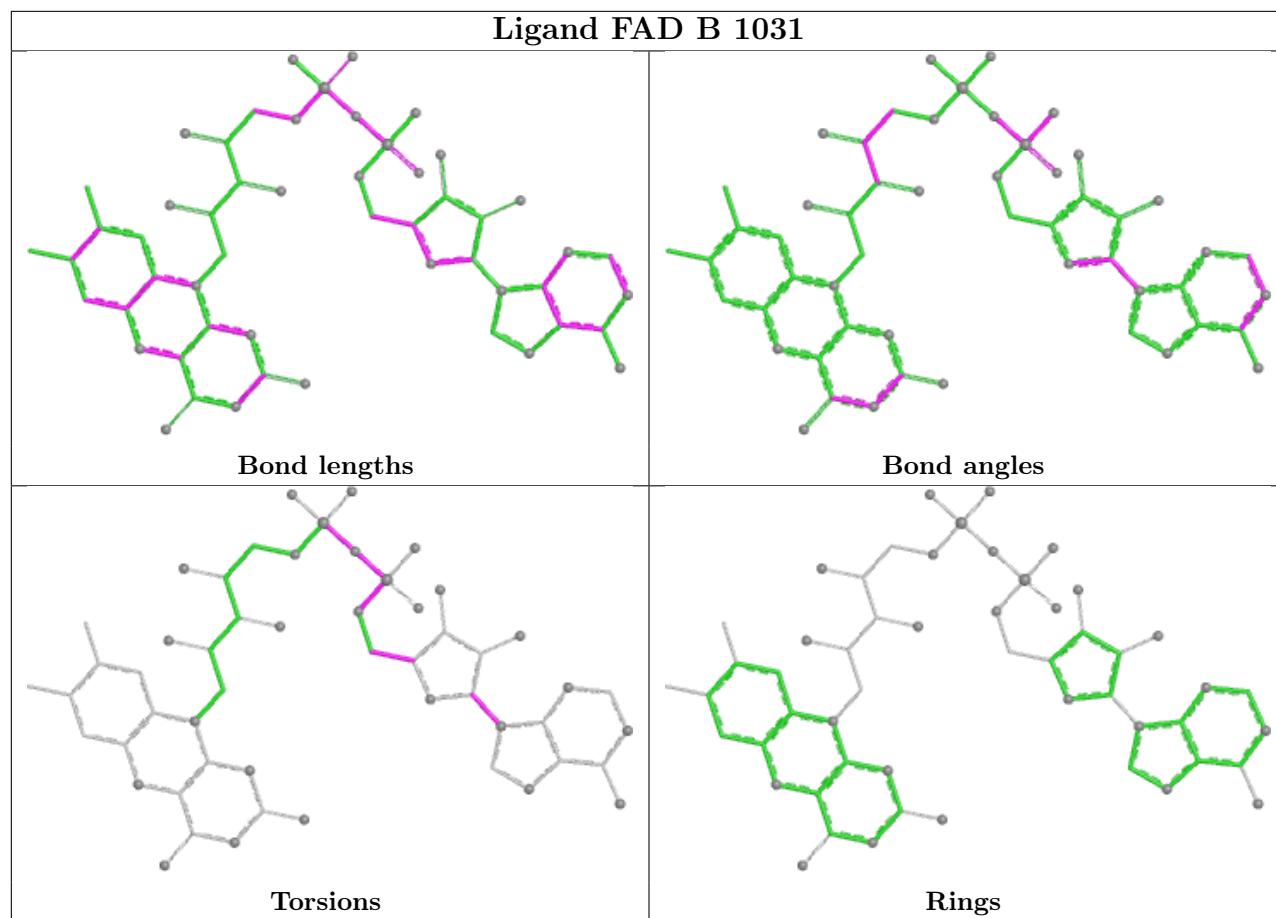
Ligand FMN B 1030

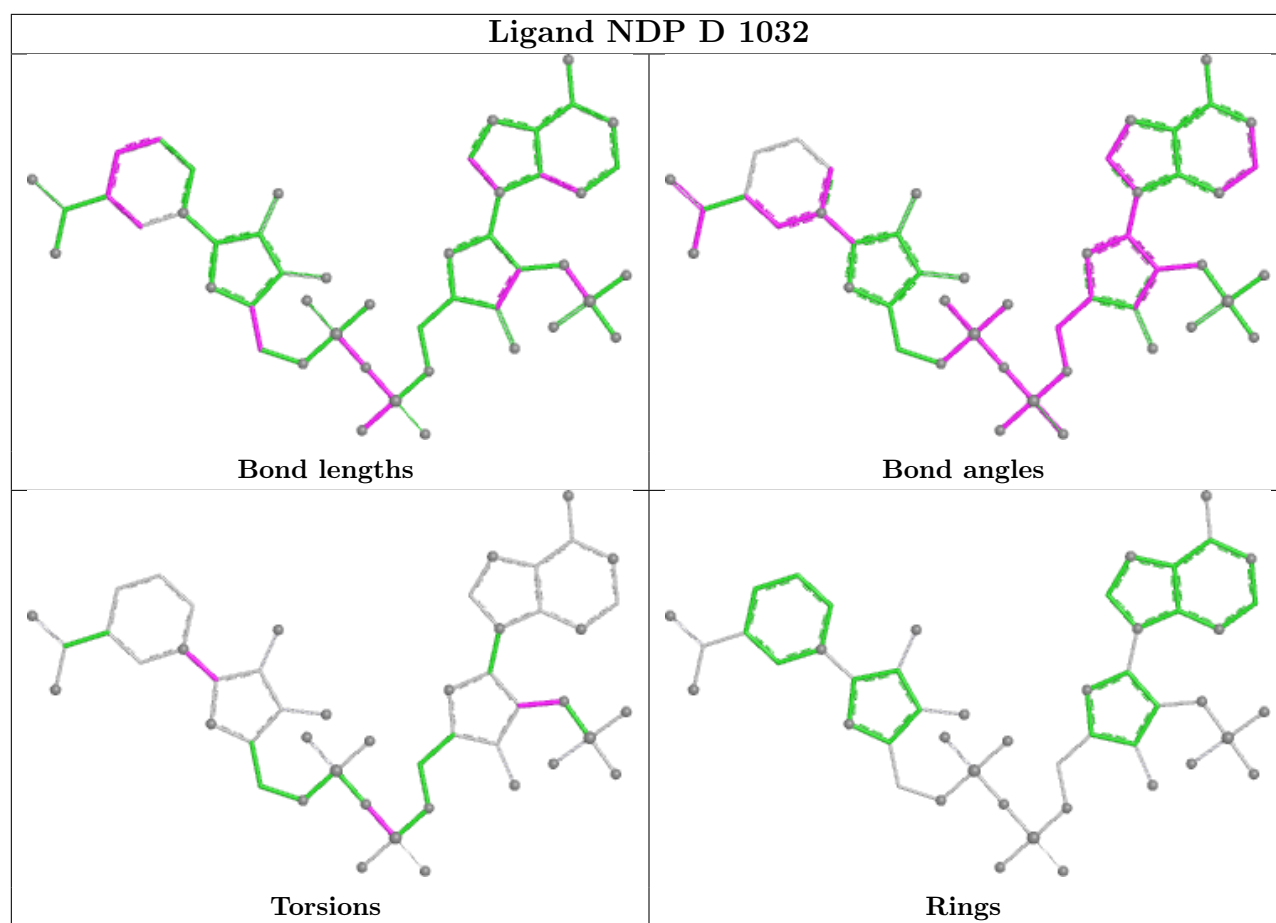


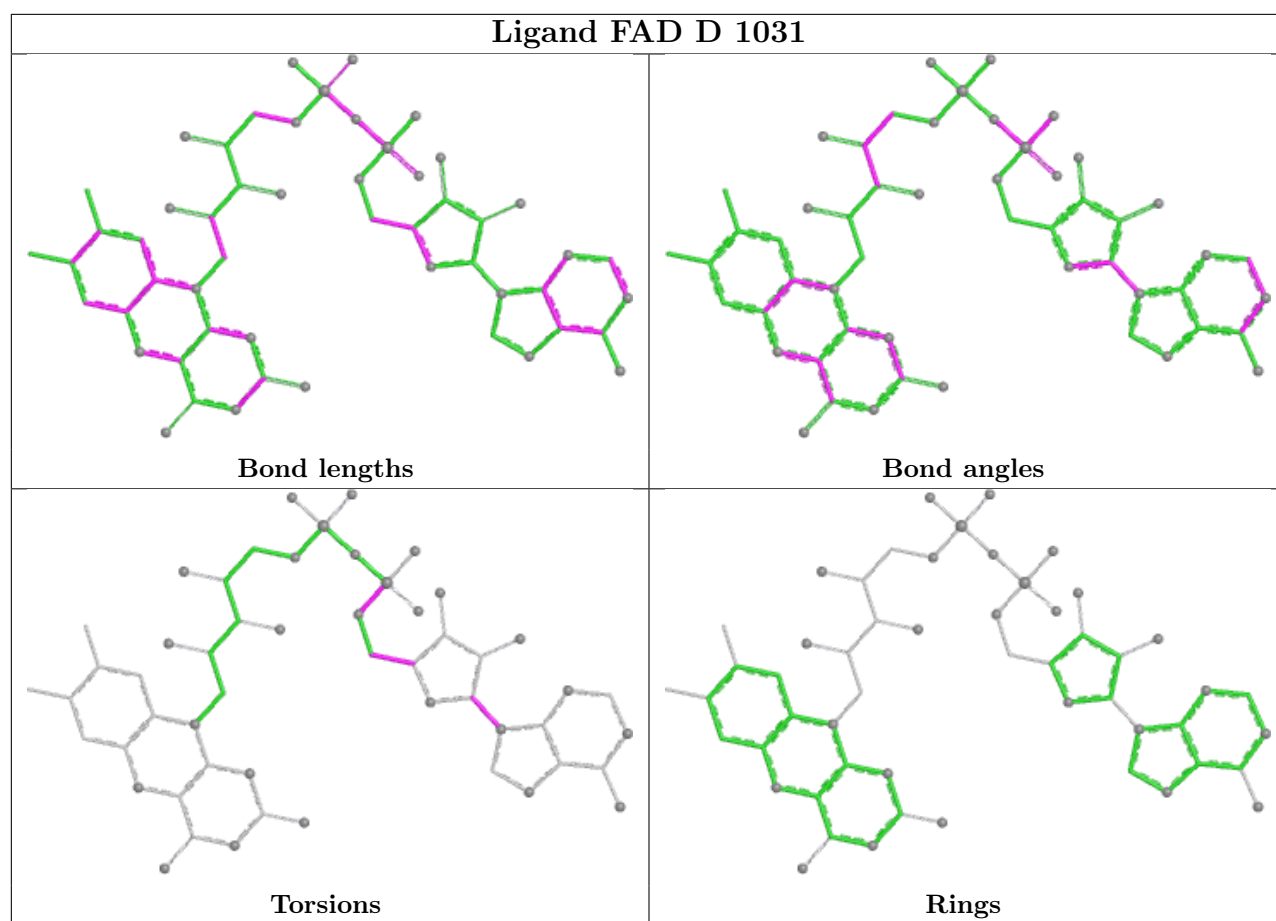
Ligand FMN C 1030

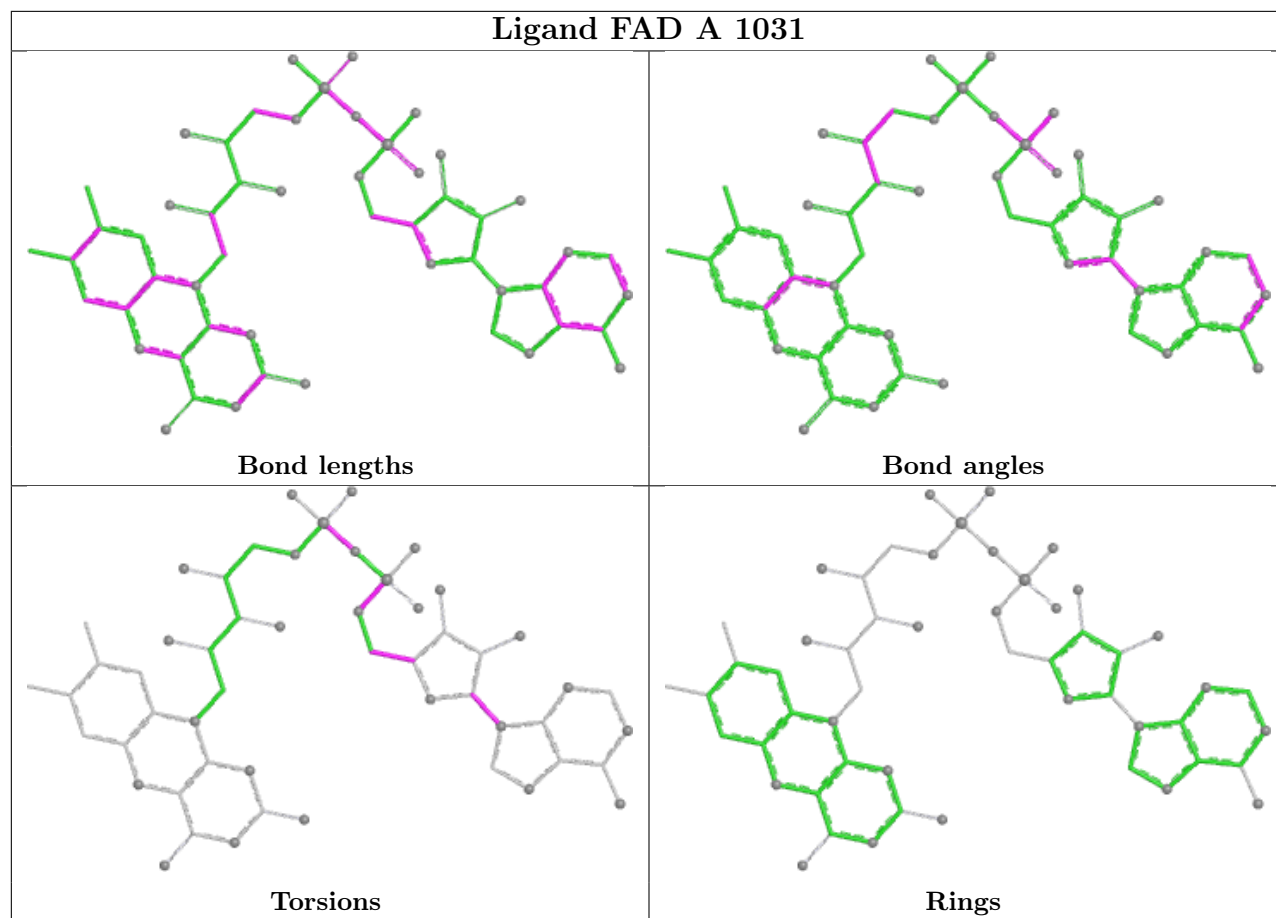


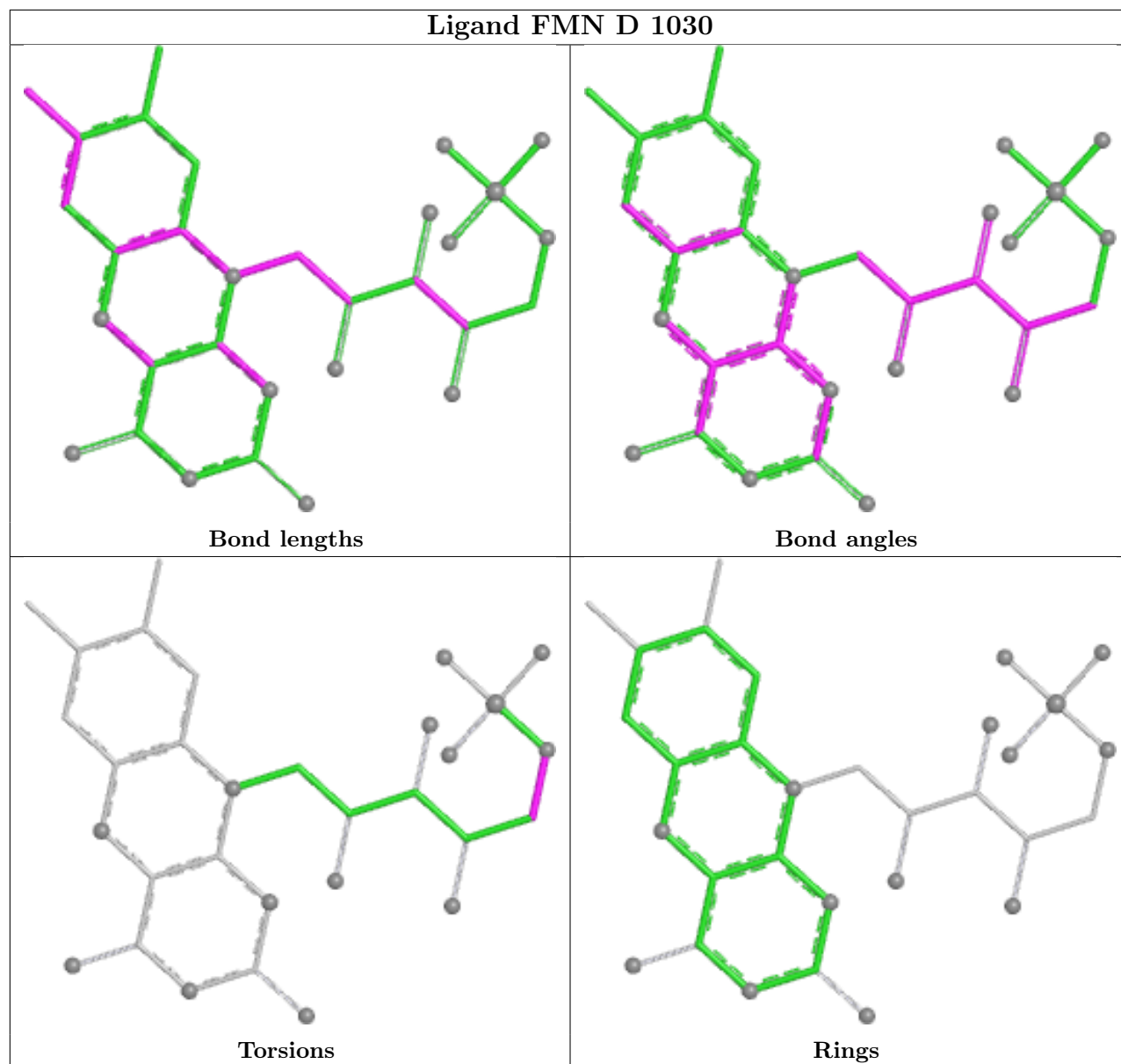


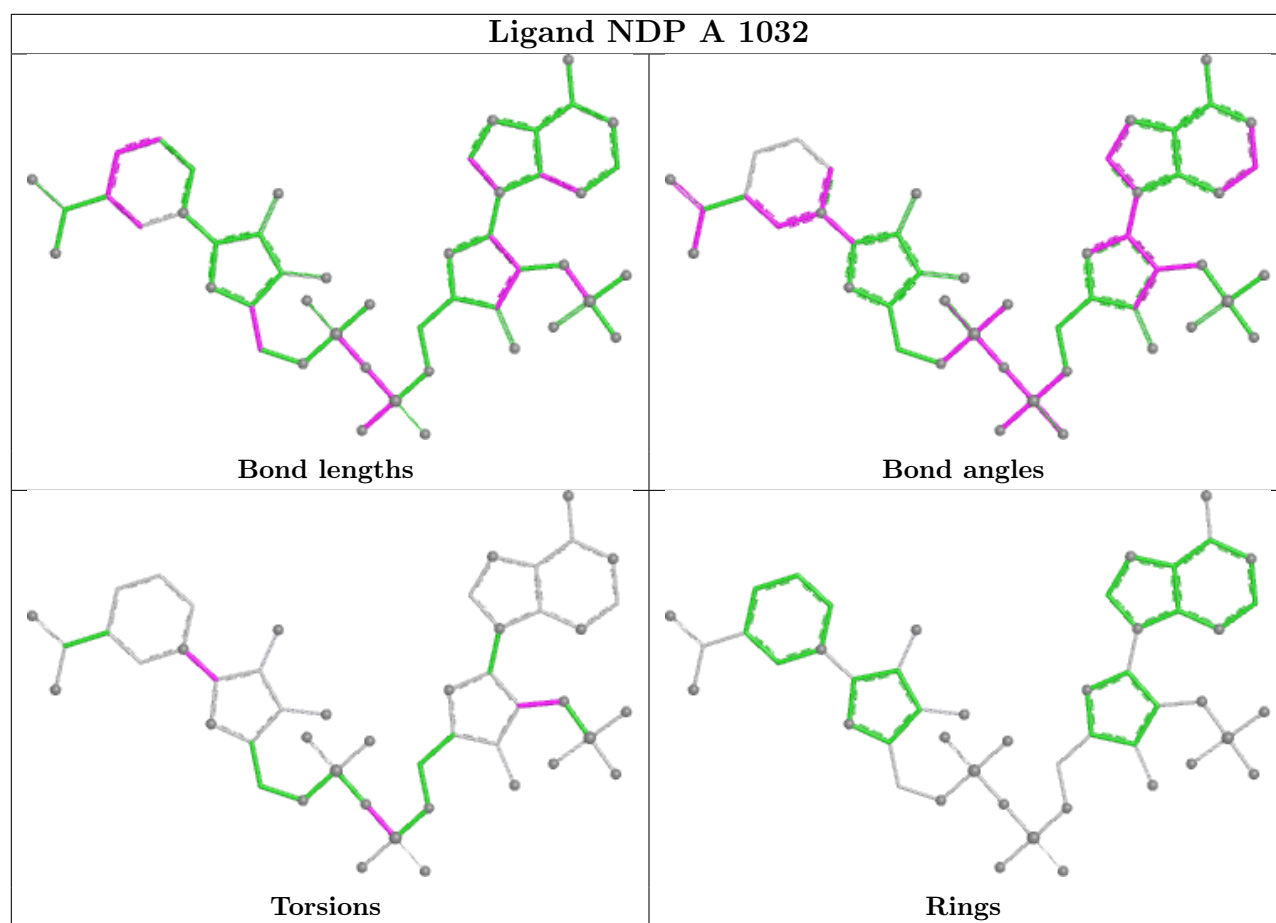












5.7 Other polymers [i](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1017/1025 (99%)	-0.64	0 100 100	7, 39, 93, 147	0
1	B	1010/1025 (98%)	-0.61	1 (0%) 92 90	7, 40, 96, 141	0
1	C	1010/1025 (98%)	-0.52	2 (0%) 91 86	14, 54, 106, 140	0
1	D	1012/1025 (98%)	-0.47	1 (0%) 92 90	14, 57, 107, 162	0
All	All	4049/4100 (98%)	-0.56	4 (0%) 92 90	7, 47, 102, 162	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	676	GLY	2.5
1	C	1014	LYS	2.4
1	C	657	ALA	2.4
1	D	17	ALA	2.3

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](#)

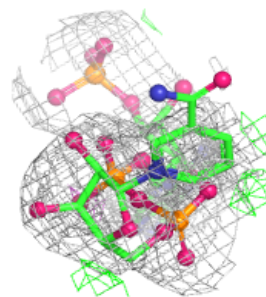
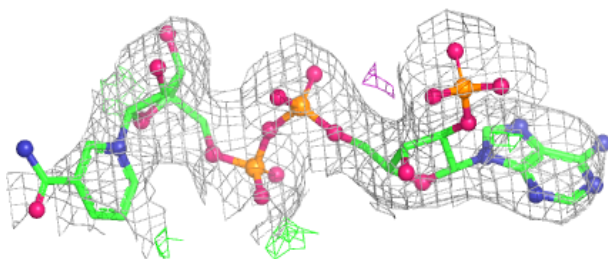
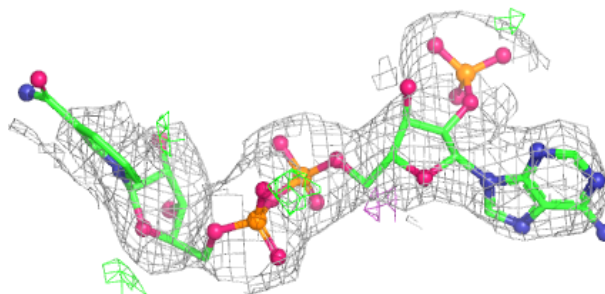
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
6	UAA	C	1035	12/12	0.70	0.11	138,140,144,144	0
6	UAA	D	1035	12/12	0.81	0.13	107,108,108,109	0
6	UAA	B	1035	12/12	0.85	0.16	146,147,148,148	0
6	UAA	A	1035	12/12	0.88	0.09	111,112,113,113	0
5	NDP	C	1032	48/48	0.92	0.09	53,57,86,88	0
5	NDP	D	1032	48/48	0.92	0.08	57,60,89,92	0
4	FAD	D	1031	53/53	0.92	0.07	40,46,60,60	0
3	FMN	D	1030	31/31	0.94	0.07	48,52,56,59	0
3	FMN	C	1030	31/31	0.94	0.07	45,48,52,55	0
5	NDP	B	1032	48/48	0.94	0.08	42,46,77,81	0
4	FAD	C	1031	53/53	0.95	0.07	29,36,49,50	0
3	FMN	A	1030	31/31	0.95	0.07	31,37,42,45	0
5	NDP	A	1032	48/48	0.95	0.07	42,47,76,78	0
4	FAD	A	1031	53/53	0.95	0.08	20,23,37,38	0
4	FAD	B	1031	53/53	0.95	0.07	19,25,35,37	0
3	FMN	B	1030	31/31	0.96	0.07	28,33,34,38	0
2	SF4	D	1029	8/8	0.98	0.06	39,40,41,42	0
2	SF4	A	1028	8/8	0.99	0.03	9,11,13,14	0
2	SF4	A	1029	8/8	0.99	0.05	18,21,23,24	0
2	SF4	B	1026	8/8	0.99	0.05	7,10,10,12	0
2	SF4	B	1027	8/8	0.99	0.05	4,4,4,4	0
2	SF4	B	1028	8/8	0.99	0.04	21,23,24,25	0
2	SF4	B	1029	8/8	0.99	0.03	13,15,16,18	0
2	SF4	C	1026	8/8	0.99	0.04	22,24,26,27	0
2	SF4	C	1027	8/8	0.99	0.04	25,26,27,28	0
2	SF4	C	1028	8/8	0.99	0.05	29,31,33,33	0
2	SF4	C	1029	8/8	0.99	0.07	34,35,37,37	0
2	SF4	D	1026	8/8	0.99	0.04	26,27,28,28	0
2	SF4	D	1027	8/8	0.99	0.05	28,30,32,32	0
2	SF4	D	1028	8/8	0.99	0.04	34,35,37,38	0
2	SF4	A	1026	8/8	0.99	0.05	18,21,24,24	0
2	SF4	A	1027	8/8	0.99	0.04	6,10,11,12	0

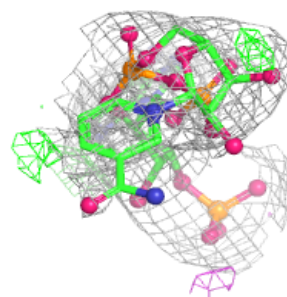
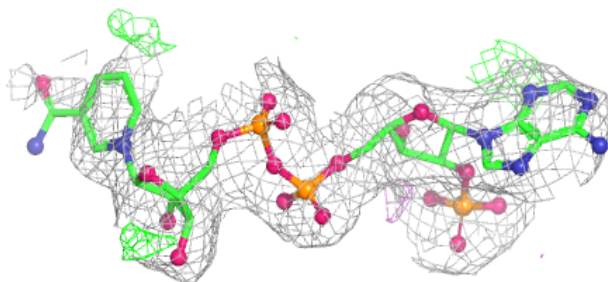
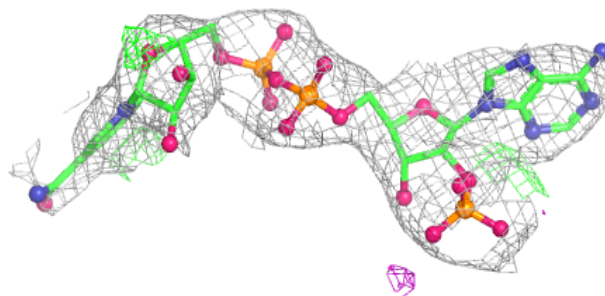
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP 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)

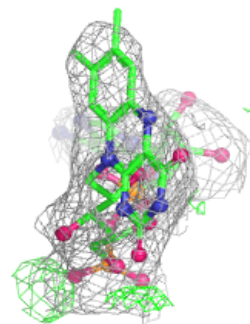
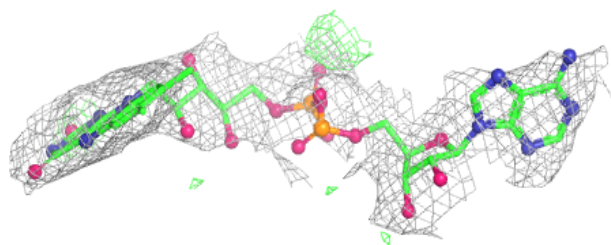
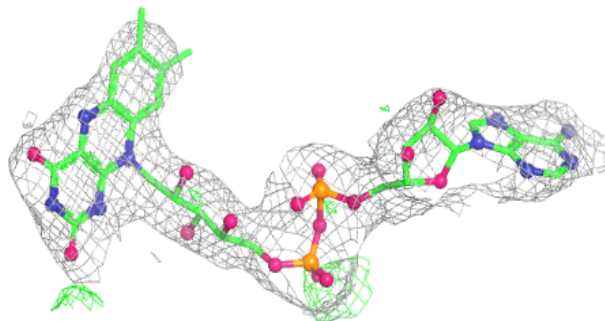
**Electron density around NDP D 1032:**

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



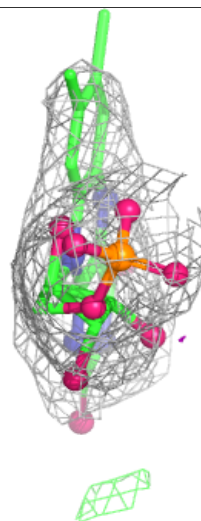
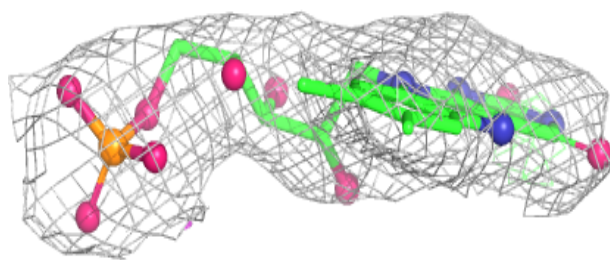
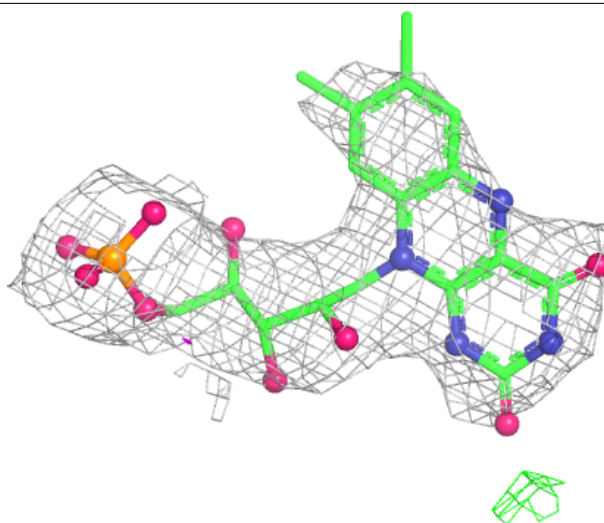
Electron density around FAD D 1031:

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



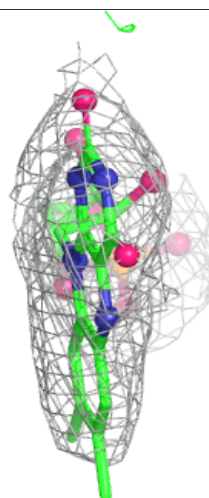
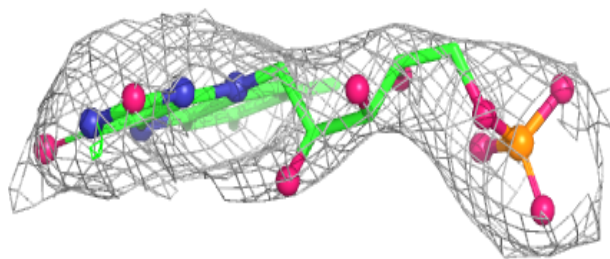
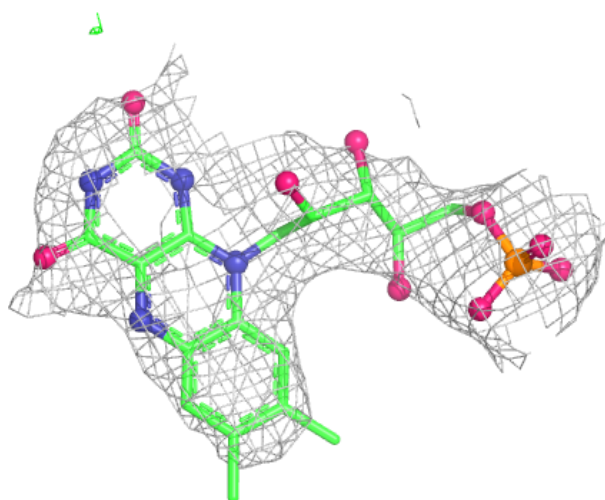
Electron density around FMN D 1030:

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



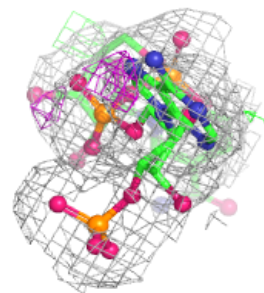
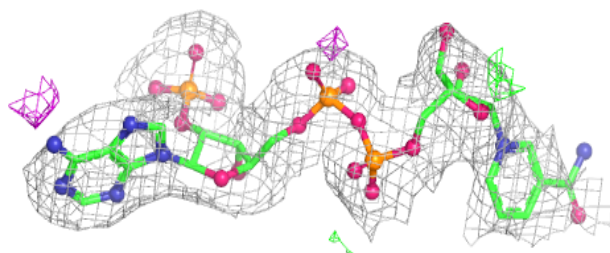
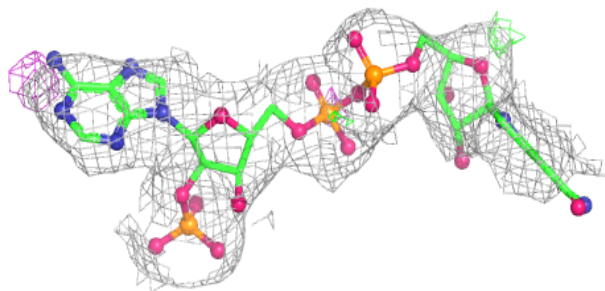
Electron density around FMN C 1030:

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

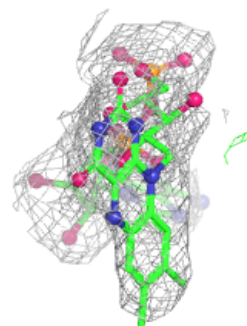
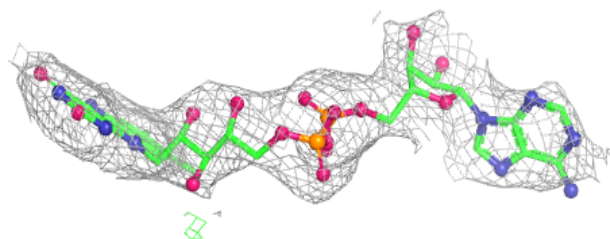
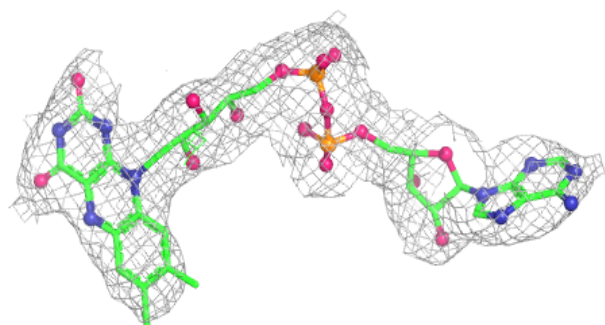


Electron density around NDP B 1032:

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

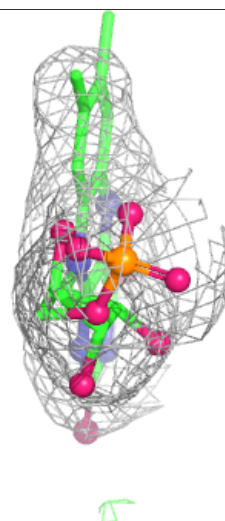
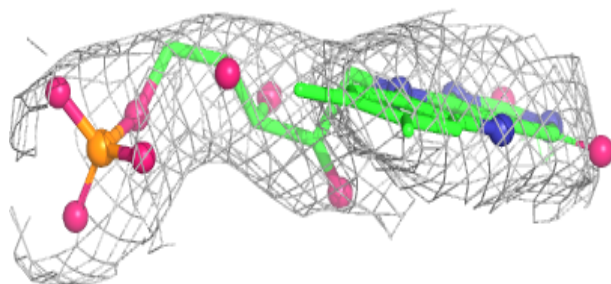
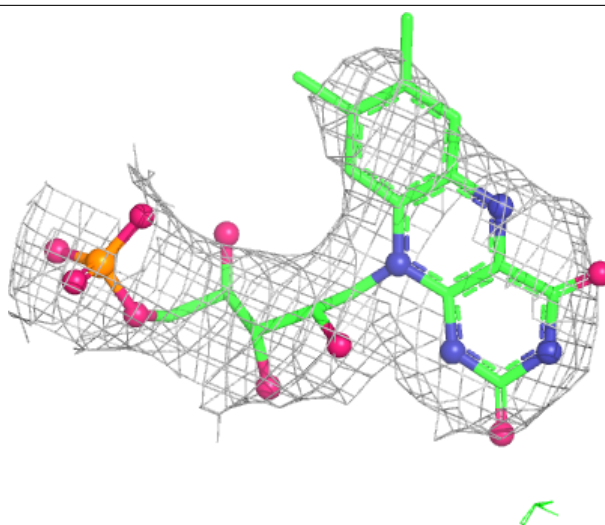
**Electron density around FAD C 1031:**

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



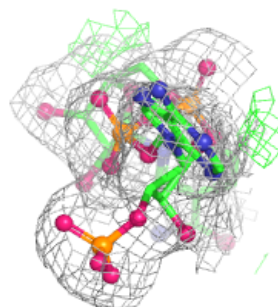
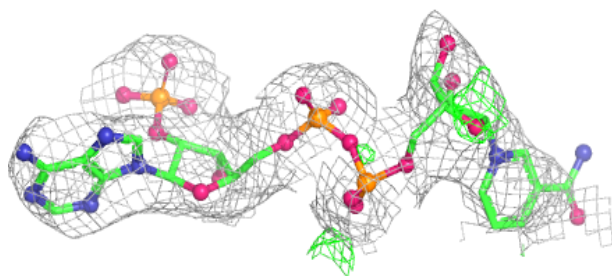
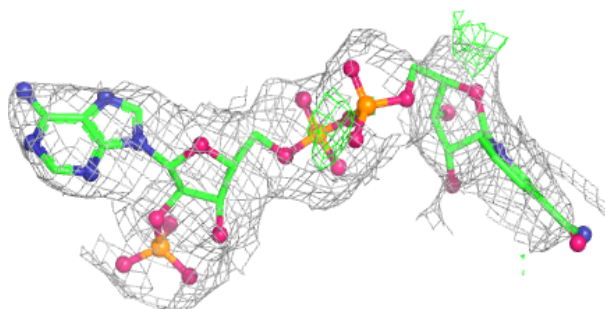
Electron density around FMN A 1030:

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

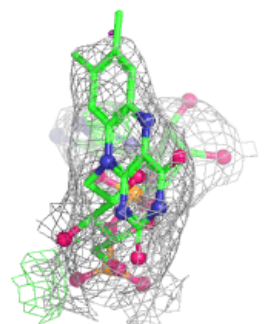
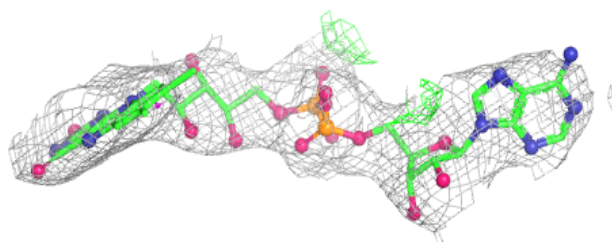
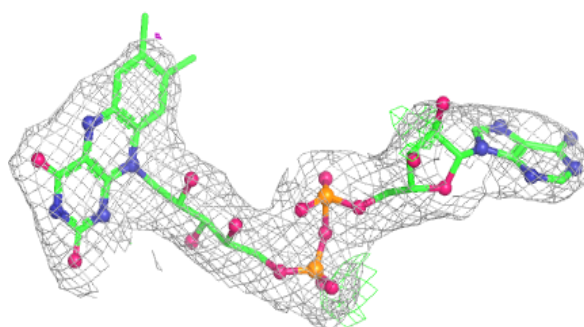


Electron density around NDP A 1032:

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

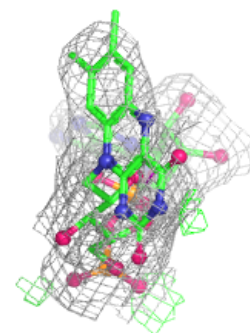
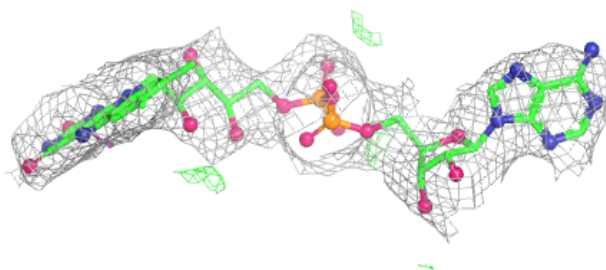
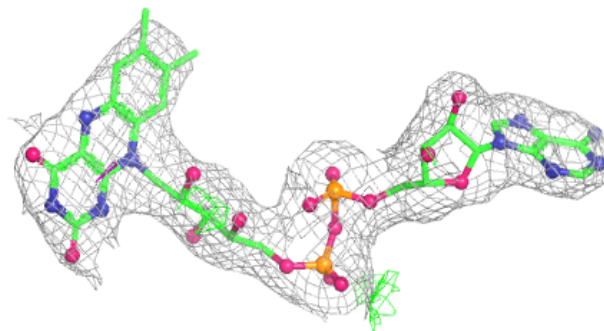
**Electron density around FAD A 1031:**

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



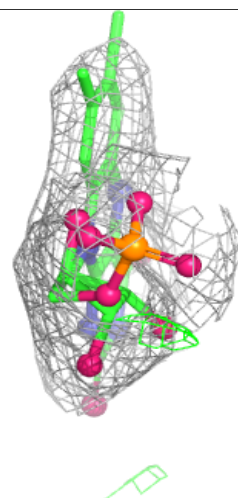
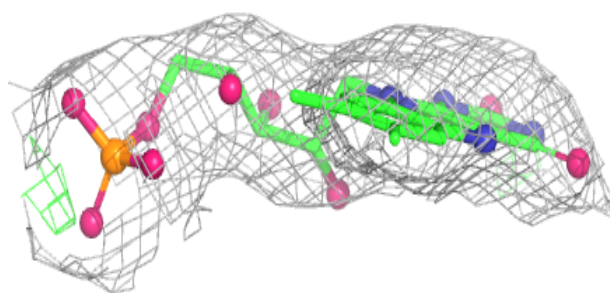
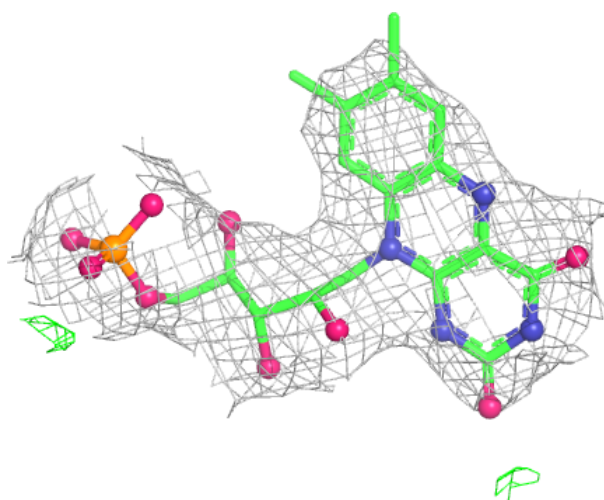
Electron density around FAD B 1031:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.