



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 1GTE / pdb_00001gte
Title : DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG, BINARY COMPLEX WITH 5-IOLOURACIL
Authors : Dobritsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2002-01-15
Resolution : 1.65 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

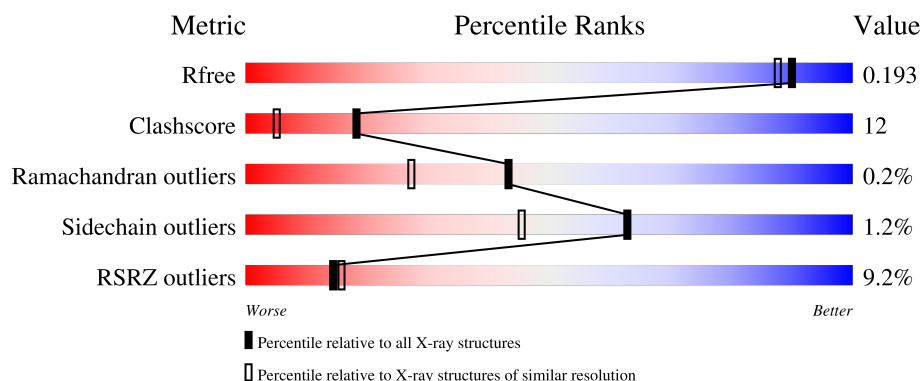
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	8% 78% 19% ..
1	B	1025	9% 78% 19% ..
1	C	1025	9% 78% 19% ..
1	D	1025	10% 79% 19% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36226 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.

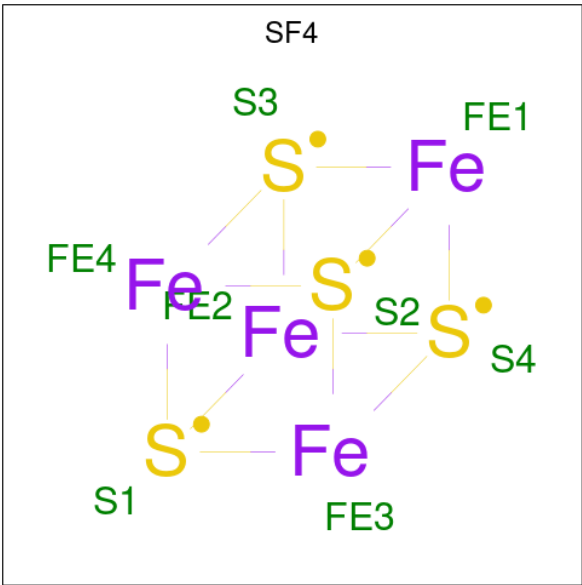
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1005	Total	C	N	O	S	0	4	0
			7683	4872	1300	1456	55			
1	B	1005	Total	C	N	O	S	0	5	0
			7693	4877	1304	1457	55			
1	C	1010	Total	C	N	O	S	0	11	0
			7748	4920	1309	1464	55			
1	D	1014	Total	C	N	O	S	0	7	0
			7754	4916	1312	1470	56			

There are 4 discrepancies between the modelled and reference sequences:

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

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



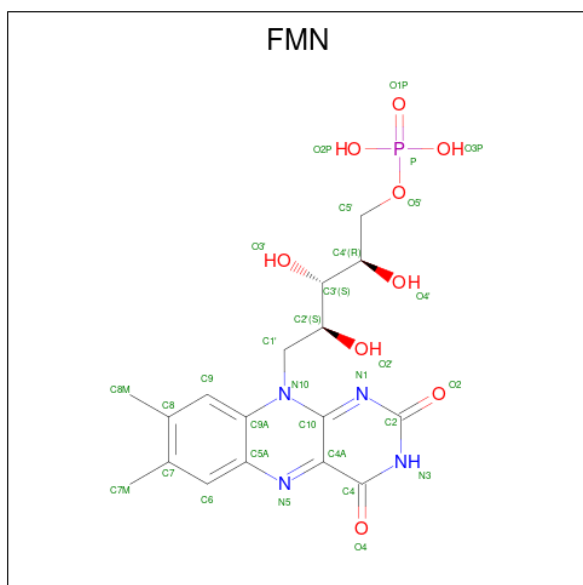
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

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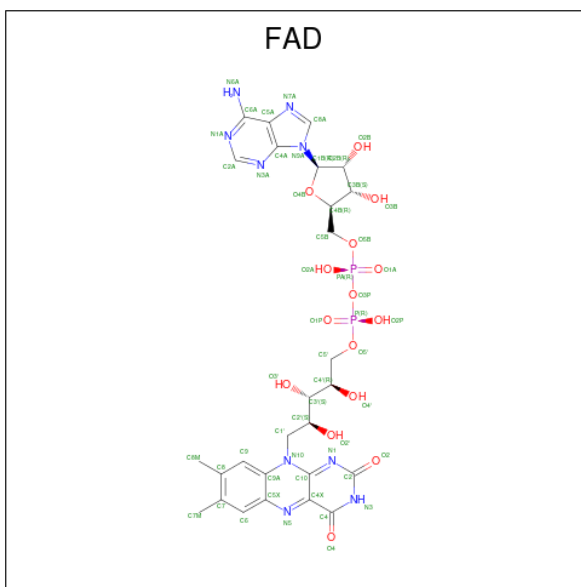
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

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



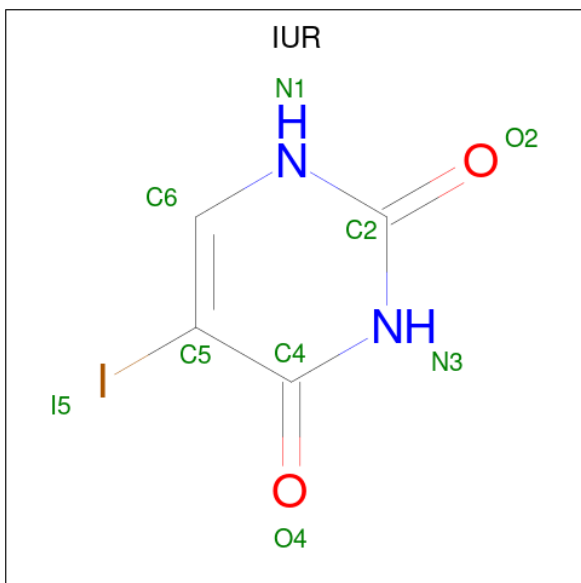
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	I	N	O	
			9	4	1	2	2	
5	B	1	Total	C	I	N	O	
			9	4	1	2	2	
5	C	1	Total	C	I	N	O	
			9	4	1	2	2	
5	D	1	Total	C	I	N	O	
			9	4	1	2	2	

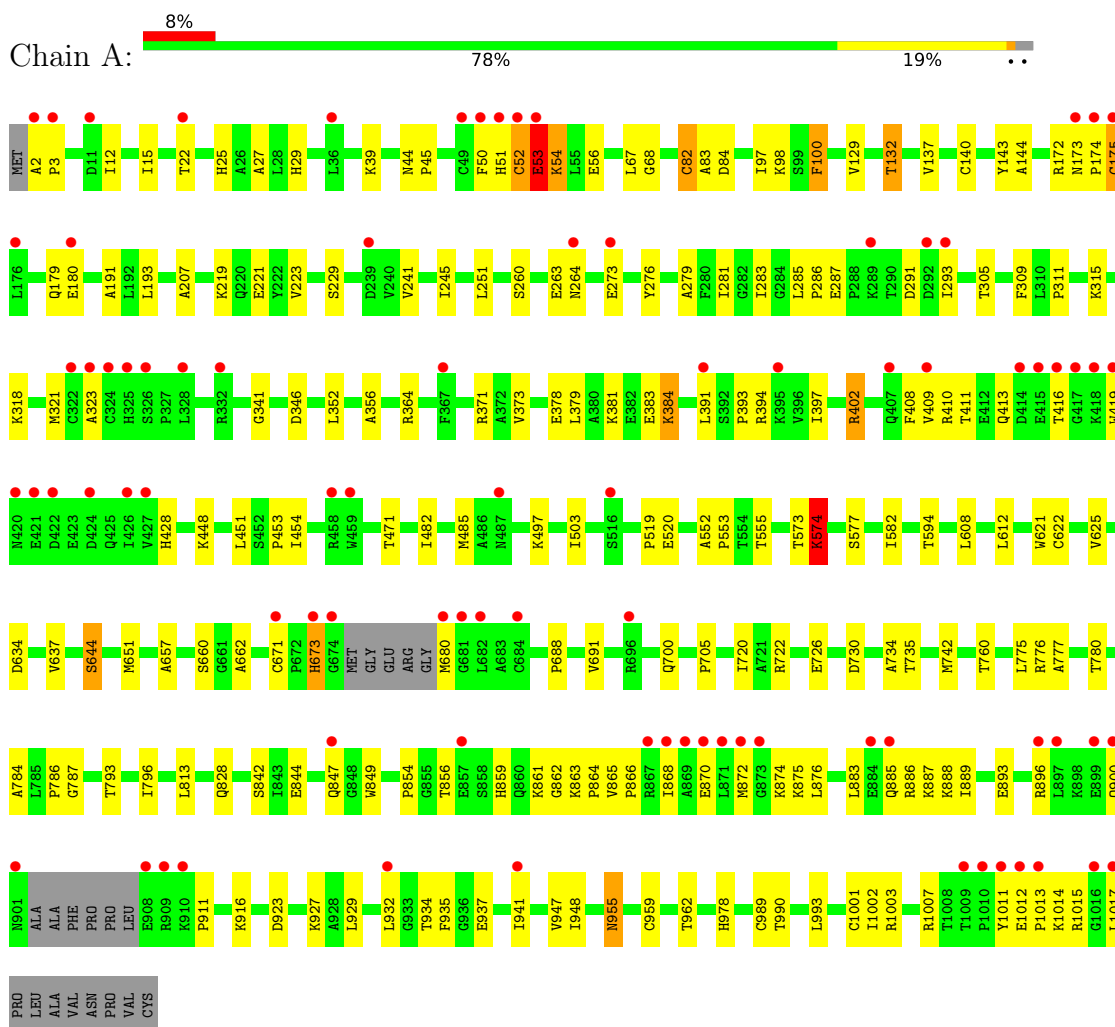
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1170	Total	O		
			1170	1170	0	0
6	B	1221	Total	O		
			1221	1221	0	0
6	C	1189	Total	O		
			1189	1189	0	0
6	D	1268	Total	O		
			1268	1268	0	0

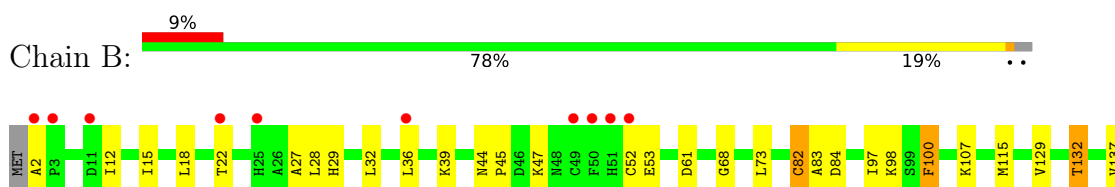
3 Residue-property plots

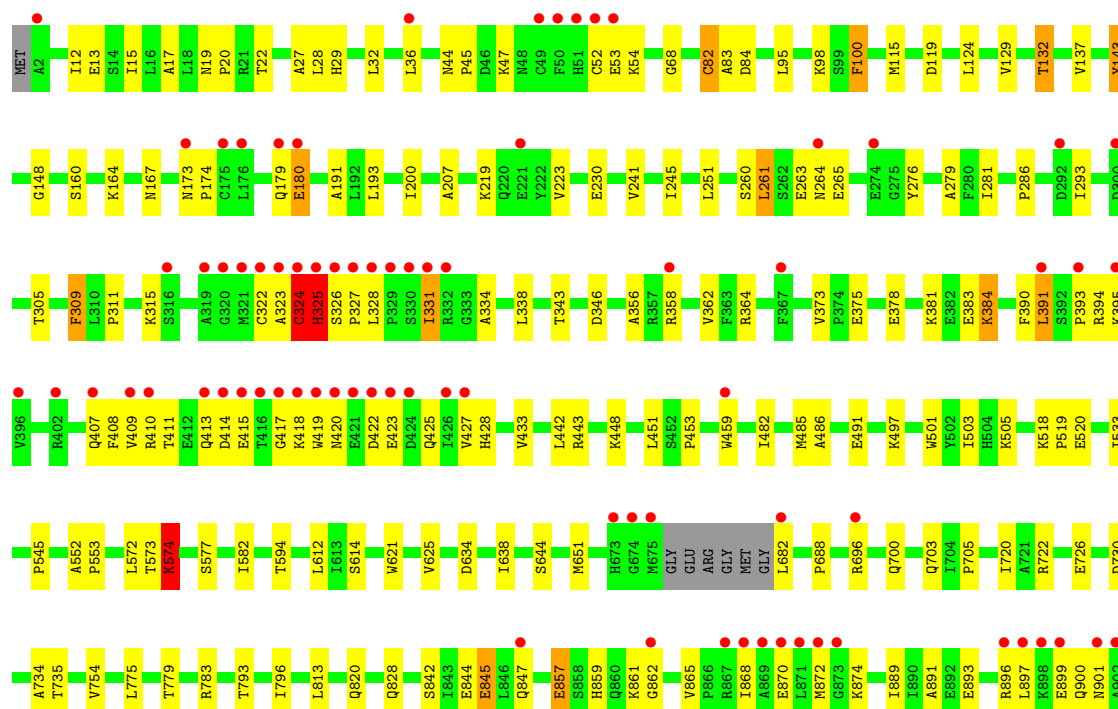
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

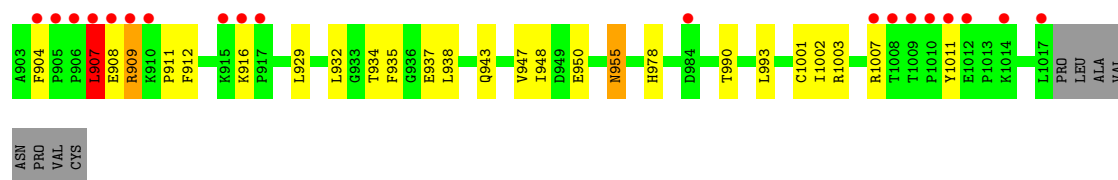
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE



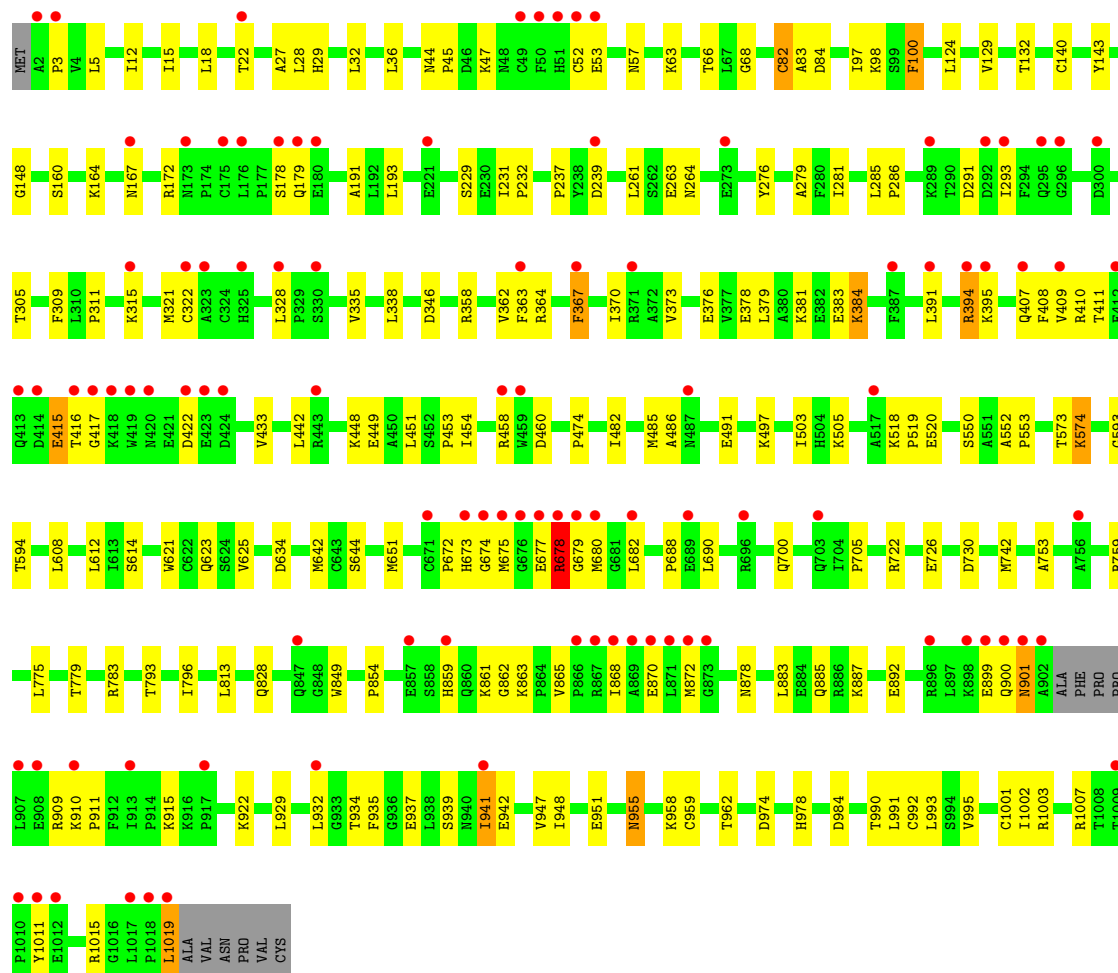
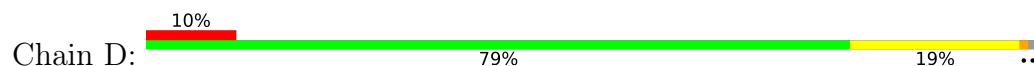
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE







● Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.71Å 158.37Å 162.33Å 90.00° 95.84° 90.00°	Depositor
Resolution (Å)	24.98 – 1.65 24.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (24.98-1.65) 98.1 (24.98-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 1.65Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.181 , 0.197 0.178 , 0.193	Depositor DCC
R_{free} test set	9508 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36226	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, SF4, IUR, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/7855	0.89	24/10643 (0.2%)
1	B	0.35	0/7870	0.88	17/10663 (0.2%)
1	C	0.35	0/7952	0.88	21/10779 (0.2%)
1	D	0.34	0/7940	0.87	22/10759 (0.2%)
All	All	0.35	0/31617	0.88	84/42844 (0.2%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ALA	CA-C-N	8.96	128.81	120.21
1	A	2	ALA	C-N-CA	8.96	128.81	120.21
1	B	305	THR	N-CA-C	-8.38	97.42	110.42
1	C	305	THR	N-CA-C	-8.29	97.57	110.42
1	D	305	THR	N-CA-C	-8.19	97.72	110.42
1	A	305	THR	N-CA-C	-8.08	97.62	110.14
1	A	3	PRO	N-CA-C	7.72	122.04	111.22
1	B	82	CYS	N-CA-C	7.68	120.80	110.35
1	A	285	LEU	CA-C-N	7.67	127.72	119.28
1	A	285	LEU	C-N-CA	7.67	127.72	119.28
1	C	82	CYS	N-CA-C	7.61	120.70	110.35
1	C	955	ASN	N-CA-C	7.55	121.91	112.24
1	A	574	LYS	N-CA-C	-7.52	100.12	110.35
1	B	309	PHE	N-CA-C	7.52	119.38	111.03
1	B	574	LYS	N-CA-C	-7.44	100.23	110.35
1	B	955	ASN	N-CA-C	7.43	121.75	112.24
1	B	285	LEU	CA-C-N	7.38	127.40	119.28
1	B	285	LEU	C-N-CA	7.38	127.40	119.28
1	C	574	LYS	N-CA-C	-7.37	100.33	110.35
1	A	309	PHE	N-CA-C	7.33	119.17	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	CYS	N-CA-C	7.33	120.32	110.35
1	D	574	LYS	N-CA-C	-7.28	100.45	110.35
1	C	907	LEU	N-CA-C	-7.22	103.41	111.28
1	D	309	PHE	N-CA-C	7.20	119.02	111.03
1	D	955	ASN	N-CA-C	7.11	121.28	111.90
1	A	82	CYS	N-CA-C	7.11	120.02	110.35
1	A	955	ASN	N-CA-C	7.03	121.23	112.24
1	C	309	PHE	N-CA-C	6.96	118.56	110.97
1	C	503	ILE	N-CA-C	-6.74	103.91	110.72
1	B	503	ILE	N-CA-C	-6.62	104.03	110.72
1	C	286	PRO	N-CA-C	6.55	122.36	113.84
1	A	503	ILE	N-CA-C	-6.46	104.20	110.72
1	B	129	VAL	N-CA-C	6.24	120.23	113.43
1	D	503	ILE	N-CA-C	-6.19	104.47	110.72
1	D	286	PRO	N-CA-C	6.18	121.87	113.84
1	C	143	TYR	N-CA-C	-6.05	105.16	112.54
1	D	573	THR	N-CA-C	-6.02	102.42	110.55
1	D	1001	CYS	N-CA-C	-5.98	104.84	111.36
1	A	129	VAL	N-CA-C	5.97	119.94	113.43
1	C	129	VAL	N-CA-C	5.93	119.90	113.43
1	D	129	VAL	N-CA-C	5.92	119.88	113.43
1	C	1001	CYS	N-CA-C	-5.91	104.92	111.36
1	A	1001	CYS	N-CA-C	-5.90	104.93	111.36
1	A	573	THR	N-CA-C	-5.89	102.59	110.55
1	B	1001	CYS	N-CA-C	-5.88	104.95	111.36
1	C	68	GLY	N-CA-C	-5.80	103.42	112.58
1	D	143	TYR	N-CA-C	-5.79	105.47	112.54
1	A	143	TYR	N-CA-C	-5.78	105.48	112.54
1	B	143	TYR	N-CA-C	-5.78	105.49	112.54
1	D	285	LEU	CA-C-N	5.76	125.44	119.56
1	D	285	LEU	C-N-CA	5.76	125.44	119.56
1	D	68	GLY	N-CA-C	-5.72	103.55	112.58
1	A	941	ILE	CB-CA-C	-5.66	105.04	111.55
1	B	573	THR	N-CA-C	-5.66	102.91	110.55
1	A	68	GLY	N-CA-C	-5.65	103.65	112.58
1	B	68	GLY	N-CA-C	-5.57	103.79	112.58
1	C	573	THR	N-CA-C	-5.55	103.06	110.55
1	A	229	SER	N-CA-C	5.45	119.19	112.54
1	D	594	THR	N-CA-C	-5.43	105.88	112.88
1	A	286	PRO	N-CA-C	5.42	120.97	113.65
1	D	261	LEU	N-CA-C	-5.41	100.29	108.67
1	B	132	THR	N-CA-C	5.39	118.66	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	HIS	N-CA-C	-5.39	99.32	110.80
1	B	286	PRO	N-CA-C	5.39	120.93	113.65
1	B	229	SER	N-CA-C	5.36	119.08	112.54
1	C	594	THR	N-CA-C	-5.33	106.01	112.88
1	D	644	SER	N-CA-C	-5.31	103.02	110.35
1	C	384	LYS	N-CA-C	5.27	118.99	112.24
1	D	229	SER	N-CA-C	5.25	118.95	112.54
1	A	323	ALA	N-CA-C	-5.24	106.89	113.28
1	C	261	LEU	N-CA-C	-5.23	100.56	108.67
1	A	132	THR	N-CA-C	5.20	118.41	111.75
1	C	148	GLY	N-CA-C	5.18	121.63	112.83
1	C	132	THR	N-CA-C	5.17	118.37	111.75
1	A	594	THR	N-CA-C	-5.16	106.22	112.88
1	B	594	THR	N-CA-C	-5.15	106.24	112.88
1	D	384	LYS	N-CA-C	5.11	118.78	112.24
1	D	550	SER	N-CA-C	-5.11	101.80	109.15
1	A	384	LYS	N-CA-C	5.09	118.75	112.24
1	D	132	THR	N-CA-C	5.08	118.26	111.75
1	D	148	GLY	N-CA-C	5.04	121.40	112.83
1	A	644	SER	N-CA-C	-5.04	103.40	110.35
1	C	230	GLU	N-CA-C	5.00	119.83	113.18
1	C	644	SER	N-CA-C	-5.00	103.45	110.35

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	7683	0	7711	174	0
1	B	7693	0	7719	218	0
1	C	7748	0	7785	205	0
1	D	7754	0	7785	195	0
2	A	32	0	0	2	0
2	B	32	0	0	1	0
2	C	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	32	0	0	2	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	0	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	1	0
5	A	9	0	3	1	0
5	B	9	0	3	1	0
5	C	9	0	3	0	0
5	D	9	0	3	0	0
6	A	1170	0	0	59	1
6	B	1221	0	0	81	0
6	C	1189	0	0	51	0
6	D	1268	0	0	64	0
All	All	36226	0	31212	758	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (758) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:LYS:HG3	6:B:3001:HOH:O	1.45	1.14
1:B:391:LEU:HD23	1:B:410[B]:ARG:HH22	1.10	1.12
1:D:673:HIS:CD2	1:D:675:MET:H	1.68	1.11
1:C:754:VAL:HG23	6:C:2919:HOH:O	1.53	1.06
1:D:779[B]:THR:HG21	1:D:932:LEU:HD22	1.38	1.05
1:B:413:GLN:HG2	1:B:417:GLY:O	1.56	1.05
1:A:352:LEU:HA	6:A:2542:HOH:O	1.62	0.99
1:B:634:ASP:OD1	6:B:2852:HOH:O	1.81	0.98
1:B:613:ILE:HA	6:B:3212:HOH:O	1.64	0.97
1:C:779[B]:THR:HG21	1:C:932[B]:LEU:HD22	1.44	0.97
1:D:673:HIS:HD2	1:D:675:MET:H	0.98	0.97
1:A:657:ALA:HA	6:A:2851:HOH:O	1.65	0.94
1:B:575:THR:HB	6:B:3212:HOH:O	1.68	0.91
1:C:391:LEU:HD23	1:C:410[B]:ARG:HH22	1.33	0.91
1:B:167[B]:ASN:HD22	1:B:911:PRO:HA	1.37	0.90
1:A:866:PRO:HD2	6:A:3029:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:LYS:HB3	6:C:2584:HOH:O	1.73	0.88
1:B:409:VAL:C	1:B:410[B]:ARG:HE	1.83	0.86
1:A:321:MET:HA	6:A:2388:HOH:O	1.74	0.85
1:B:408:PHE:HB3	1:B:410[B]:ARG:NH2	1.91	0.85
1:C:322:CYS:SG	1:C:324:CYS:HB3	2.17	0.85
1:B:391:LEU:HD23	1:B:410[B]:ARG:NH2	1.90	0.84
1:B:623:GLN:NE2	6:B:2841:HOH:O	2.11	0.84
1:B:612:LEU:HA	6:B:2825:HOH:O	1.76	0.84
1:C:938:LEU:HA	6:C:3080:HOH:O	1.76	0.83
1:C:634:ASP:OD1	6:C:2816:HOH:O	1.97	0.83
1:A:859:HIS:HD2	1:A:862:GLY:H	1.26	0.83
1:B:533:ILE:HD13	6:B:3001:HOH:O	1.77	0.82
1:B:954:ILE:HG23	1:B:998:ILE:HD11	1.60	0.82
1:C:859:HIS:HD2	1:C:862:GLY:H	1.27	0.81
1:B:381:LYS:HB3	6:B:2627:HOH:O	1.79	0.81
1:B:408:PHE:CB	1:B:410[B]:ARG:NH2	2.43	0.81
1:C:356:ALA:HA	6:C:2520:HOH:O	1.80	0.80
1:B:391:LEU:CD2	1:B:410[B]:ARG:HH12	1.94	0.80
1:B:410[B]:ARG:HD3	1:B:427:VAL:HG23	1.63	0.80
1:D:779[B]:THR:HG21	1:D:932:LEU:CD2	2.11	0.79
1:B:107:LYS:HE3	6:B:2192:HOH:O	1.82	0.79
1:A:929:LEU:HD12	1:D:941:ILE:HG21	1.65	0.79
1:B:73:LEU:HD11	6:B:2192:HOH:O	1.81	0.79
1:B:1014:LYS:HG3	6:B:3202:HOH:O	1.82	0.78
1:C:391:LEU:HD23	1:C:410[B]:ARG:NH2	1.97	0.78
1:D:859:HIS:HD2	1:D:862:GLY:H	1.28	0.78
1:B:394:ARG:HG3	1:B:409:VAL:HG13	1.66	0.78
1:A:844:GLU:O	1:A:847:GLN:HG3	1.84	0.77
1:B:409:VAL:N	1:B:410[B]:ARG:HH21	1.82	0.77
1:B:386:GLU:HG2	6:B:2586:HOH:O	1.84	0.77
1:D:673:HIS:HD2	1:D:675:MET:N	1.79	0.77
1:D:394:ARG:HG3	1:D:394:ARG:HH11	1.48	0.77
1:A:381:LYS:HB3	6:A:2578:HOH:O	1.84	0.77
1:C:324:CYS:SG	1:C:325:HIS:N	2.52	0.77
1:C:167[B]:ASN:ND2	1:C:911:PRO:HA	2.00	0.76
1:B:921:ILE:HG13	6:B:2754:HOH:O	1.86	0.76
1:B:167[B]:ASN:ND2	1:B:911:PRO:HA	2.00	0.75
1:C:410[A]:ARG:HG3	6:C:2607:HOH:O	1.86	0.75
1:D:634:ASP:OD1	6:D:2891:HOH:O	2.04	0.75
1:A:662:ALA:HA	6:A:2822:HOH:O	1.87	0.74
1:C:907:LEU:CD2	1:C:907:LEU:H	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:938:LEU:HD23	6:C:3080:HOH:O	1.88	0.74
1:C:378:GLU:HA	6:C:2584:HOH:O	1.88	0.74
1:D:978:HIS:HA	6:D:3200:HOH:O	1.85	0.74
1:C:950:GLU:HG2	6:C:3130:HOH:O	1.89	0.73
1:C:391:LEU:HA	1:C:410[B]:ARG:HH12	1.53	0.73
1:C:779[B]:THR:HG21	1:C:932[B]:LEU:CD2	2.19	0.72
1:D:66:THR:HG22	6:D:3105:HOH:O	1.89	0.72
1:D:677:GLU:O	1:D:678:ARG:HB2	1.90	0.72
1:B:395:LYS:HG3	1:B:407:GLN:NE2	2.05	0.71
1:D:263:GLU:OE1	1:D:449:GLU:HG2	1.90	0.71
1:A:883:LEU:HG	1:A:887:LYS:HE3	1.70	0.71
1:A:893:GLU:OE1	1:A:896:ARG:NH2	2.24	0.71
1:B:409:VAL:C	1:B:410[B]:ARG:NE	2.47	0.71
1:B:872:MET:HE3	6:B:3054:HOH:O	1.91	0.71
1:B:408:PHE:HB3	1:B:410[B]:ARG:HH22	1.54	0.71
1:C:143:TYR:O	1:D:861:LYS:HE2	1.92	0.70
1:A:22:THR:HB	6:A:2054:HOH:O	1.91	0.70
1:B:952:MET:HG2	6:B:3039:HOH:O	1.90	0.70
1:C:820:GLN:HA	6:D:3190:HOH:O	1.92	0.69
1:D:1019:LEU:N	1:D:1019:LEU:HD23	2.06	0.69
1:A:863:LYS:HA	6:A:3008:HOH:O	1.93	0.69
1:A:622:CYS:SG	6:A:2851:HOH:O	2.51	0.69
6:A:2811:HOH:O	1:B:2:ALA:HB1	1.93	0.69
1:C:251:LEU:HB3	6:C:2337:HOH:O	1.93	0.69
1:C:331:ILE:HG23	1:C:433:VAL:HG21	1.76	0.68
1:C:703:GLN:HG3	6:C:2878:HOH:O	1.92	0.68
1:C:448:LYS:HE2	6:C:2648:HOH:O	1.94	0.68
1:C:391:LEU:HG	1:C:410[B]:ARG:NH1	2.09	0.68
1:D:315:LYS:HD2	1:D:322:CYS:HB2	1.76	0.67
1:B:845:GLU:HG3	1:B:912:PHE:CE2	2.29	0.67
1:D:395:LYS:HD2	1:D:407:GLN:NE2	2.10	0.67
1:B:414:ASP:OD1	6:B:2652:HOH:O	2.12	0.67
1:A:861:LYS:HE2	1:B:143:TYR:O	1.94	0.67
1:B:391:LEU:HD21	1:B:410[B]:ARG:HH12	1.58	0.67
1:C:907:LEU:H	1:C:907:LEU:HD23	1.58	0.67
1:D:172:ARG:HB2	6:D:2333:HOH:O	1.94	0.67
1:B:410[B]:ARG:HD2	1:B:425:GLN:O	1.94	0.66
1:A:397:ILE:HD12	1:A:428:HIS:HE1	1.61	0.66
1:A:634:ASP:OD2	6:A:2819:HOH:O	2.14	0.66
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.76	0.66
1:C:164:LYS:CG	1:C:909:ARG:HH12	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:SER:HB3	6:C:2497:HOH:O	1.95	0.66
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.78	0.66
1:C:207:ALA:HB1	6:C:2337:HOH:O	1.94	0.66
1:C:164:LYS:HG3	1:C:909:ARG:HH12	1.61	0.66
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.77	0.66
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.11	0.65
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.61	0.65
1:B:518:LYS:HE3	6:B:2739:HOH:O	1.94	0.65
1:A:50:PHE:HE2	1:B:369:ASN:HA	1.60	0.65
1:A:856:THR:HG23	6:A:3001:HOH:O	1.96	0.65
1:C:410[B]:ARG:NE	1:C:427:VAL:HG23	2.11	0.65
1:A:927:LYS:HB3	6:A:3059:HOH:O	1.97	0.65
1:B:722:ARG:O	1:B:726:GLU:HG3	1.97	0.64
1:D:394:ARG:HD2	1:D:409:VAL:CG1	2.27	0.64
1:B:167[B]:ASN:ND2	1:B:910:LYS:O	2.31	0.64
1:D:36:LEU:HD23	6:D:2113:HOH:O	1.98	0.64
1:A:448:LYS:HE2	6:A:2648:HOH:O	1.97	0.64
1:D:178:SER:HB3	6:D:2340:HOH:O	1.97	0.63
1:D:376:GLU:HB2	6:D:2657:HOH:O	1.98	0.63
1:A:173:ASN:HD22	1:A:174:PRO:HD2	1.63	0.63
1:B:831:CYS:O	6:B:3001:HOH:O	2.15	0.63
1:A:378:GLU:CD	6:A:2578:HOH:O	2.42	0.62
1:D:651:MET:HE3	1:D:700:GLN:HG3	1.81	0.62
1:A:293:ILE:CD1	1:A:393:PRO:HB2	2.29	0.62
1:D:722:ARG:O	1:D:726:GLU:HG3	1.99	0.62
1:A:786:PRO:HB3	1:D:942:GLU:HA	1.82	0.62
1:B:875:LYS:HE2	6:B:3133:HOH:O	1.99	0.62
1:C:13:GLU:HB2	6:C:2018:HOH:O	1.98	0.62
1:D:379:LEU:HD23	6:D:2663:HOH:O	1.99	0.62
1:D:984:ASP:HB3	6:D:3220:HOH:O	1.99	0.62
1:C:907:LEU:CD2	1:C:907:LEU:N	2.62	0.62
1:D:901:ASN:N	1:D:901:ASN:HD22	1.96	0.62
1:C:845:GLU:HG3	1:C:912:PHE:CE2	2.34	0.61
1:B:12:ILE:O	1:B:15:ILE:HG22	2.00	0.61
1:B:414:ASP:CG	6:B:2652:HOH:O	2.43	0.61
1:C:22:THR:HB	6:C:2056:HOH:O	2.00	0.61
1:D:783:ARG:HD3	6:D:3029:HOH:O	2.00	0.61
1:B:408:PHE:HB2	1:B:410[B]:ARG:NH2	2.16	0.61
1:B:981:THR:HG23	6:B:3167:HOH:O	2.00	0.61
1:C:410[A]:ARG:HG2	1:C:411:THR:N	2.15	0.61
6:C:3080:HOH:O	1:D:759:ARG:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:VAL:HB	6:A:2822:HOH:O	1.99	0.61
1:A:722:ARG:O	1:A:726:GLU:HG3	2.00	0.61
1:B:845:GLU:HG3	1:B:912:PHE:CD2	2.35	0.61
1:D:394:ARG:NH1	1:D:409:VAL:HG21	2.15	0.61
1:B:416:THR:O	1:B:416:THR:OG1	2.18	0.60
1:C:722:ARG:O	1:C:726:GLU:HG3	2.01	0.60
1:C:408:PHE:HB2	1:C:410[B]:ARG:NH2	2.16	0.60
1:C:327:PRO:O	1:C:328:LEU:C	2.43	0.60
1:A:287:GLU:HG2	6:A:2454:HOH:O	2.02	0.60
1:A:865:VAL:HG13	6:A:3029:HOH:O	2.00	0.60
1:D:63:LYS:HB2	6:D:2172:HOH:O	2.02	0.59
1:A:410:ARG:HG2	1:A:411:THR:N	2.16	0.59
1:D:5:LEU:HD23	6:D:2001:HOH:O	2.01	0.59
1:A:173:ASN:HD22	1:A:174:PRO:CD	2.15	0.59
1:B:414:ASP:OD1	1:B:418:LYS:HB2	2.02	0.59
1:D:673:HIS:CG	1:D:675:MET:HG2	2.38	0.59
1:D:474:PRO:HG2	6:D:2345:HOH:O	2.03	0.59
1:D:995:VAL:HB	6:D:3187:HOH:O	2.03	0.59
1:A:293:ILE:HD11	1:A:393:PRO:HB2	1.85	0.58
1:B:952:MET:HE3	6:B:3039:HOH:O	2.04	0.58
6:C:3080:HOH:O	1:D:759:ARG:HD3	2.01	0.58
1:B:61:ASP:HB2	6:B:2070:HOH:O	2.03	0.58
1:C:497:LYS:HE2	1:D:27:ALA:O	2.03	0.58
1:A:273:GLU:HB3	6:A:2441:HOH:O	2.03	0.58
1:B:409:VAL:C	1:B:410[B]:ARG:HH21	2.11	0.58
1:D:958:LYS:NZ	6:D:3187:HOH:O	2.35	0.58
1:A:52:CYS:HB3	1:A:384:LYS:HG2	1.85	0.58
1:B:408:PHE:CB	1:B:410[B]:ARG:HH22	2.12	0.58
1:C:378:GLU:CD	6:C:2584:HOH:O	2.47	0.58
1:D:167:ASN:HB3	6:D:3137:HOH:O	2.04	0.58
1:B:263:GLU:OE1	1:B:449:GLU:HG2	2.03	0.58
1:B:856:THR:HG23	6:B:3033:HOH:O	2.03	0.58
1:C:845:GLU:HG3	1:C:912:PHE:CD2	2.38	0.58
1:D:328:LEU:HD12	6:D:2153:HOH:O	2.04	0.58
1:B:917:PRO:HA	6:B:3087:HOH:O	2.04	0.57
1:A:660:SER:HB3	6:A:2851:HOH:O	2.04	0.57
6:C:2909:HOH:O	1:D:775[A]:LEU:HD12	2.04	0.57
1:D:315:LYS:HD3	1:D:321:MET:HE2	1.86	0.57
1:C:52:CYS:HB2	1:C:384:LYS:HB2	1.85	0.57
1:D:363:PHE:HE1	1:D:367:PHE:HE1	1.51	0.57
1:B:681:GLY:C	1:B:682:LEU:HD12	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:LYS:HD2	1:C:407:GLN:NE2	2.18	0.57
6:C:2192:HOH:O	1:D:29:HIS:HB2	2.03	0.57
1:A:497:LYS:HE2	1:B:27:ALA:O	2.05	0.57
1:C:391:LEU:HG	1:C:410[B]:ARG:HH12	1.67	0.57
1:C:408:PHE:CB	1:C:410[B]:ARG:NH2	2.67	0.57
1:D:899:GLU:HG2	1:D:899:GLU:O	2.02	0.57
1:D:673:HIS:CD2	1:D:675:MET:HG2	2.38	0.57
1:D:900:GLN:HG2	1:D:901:ASN:H	1.69	0.57
1:B:115:MET:HE1	6:B:2996:HOH:O	2.05	0.57
1:B:173:ASN:HB3	1:B:176:LEU:HG	1.87	0.57
1:B:367:PHE:HE1	1:B:387:PHE:CB	2.17	0.57
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	1.85	0.57
1:C:651:MET:HE3	1:C:700:GLN:HG3	1.87	0.57
1:C:978:HIS:HE1	1:D:84:ASP:OD2	1.86	0.57
1:A:872:MET:HE1	6:A:2998:HOH:O	2.05	0.57
1:B:952:MET:O	1:B:998:ILE:HD13	2.05	0.57
1:D:410:ARG:HG2	1:D:411:THR:N	2.20	0.57
1:A:39:LYS:HG3	6:A:2084:HOH:O	2.04	0.56
1:C:783:ARG:HD3	6:D:3013:HOH:O	2.05	0.56
1:A:859:HIS:HD2	1:A:862:GLY:N	1.99	0.56
1:B:954:ILE:CG2	1:B:998:ILE:HD11	2.31	0.56
1:D:673:HIS:CD2	1:D:675:MET:N	2.54	0.56
1:D:959:CYS:O	1:D:962[B]:THR:HG22	2.05	0.56
1:C:908:GLU:O	1:C:909:ARG:C	2.48	0.56
1:D:36:LEU:HG	6:D:2110:HOH:O	2.05	0.56
1:B:859:HIS:HA	1:B:865:VAL:HG23	1.88	0.56
1:C:775:LEU:HD12	6:D:2990:HOH:O	2.04	0.56
1:D:1007:ARG:HG2	6:D:3247:HOH:O	2.06	0.56
1:C:907:LEU:N	1:C:907:LEU:HD22	2.21	0.56
1:A:391:LEU:HD22	1:A:408:PHE:CB	2.36	0.56
1:A:1014:LYS:HB3	6:A:3159:HOH:O	2.06	0.56
1:B:577[B]:SER:HB2	6:B:2797:HOH:O	2.06	0.56
1:C:505:LYS:HE2	6:C:2692:HOH:O	2.05	0.56
1:B:22:THR:HA	6:B:2064:HOH:O	2.05	0.56
1:B:777:ALA:HA	6:B:2956:HOH:O	2.05	0.56
1:C:407:GLN:HG2	6:C:2604:HOH:O	2.06	0.56
1:A:172:ARG:HD2	6:A:2318:HOH:O	2.04	0.55
1:B:378:GLU:CD	6:B:2627:HOH:O	2.48	0.55
1:B:409:VAL:CA	1:B:410[B]:ARG:HE	2.19	0.55
1:D:52:CYS:HB3	1:D:384:LYS:HG2	1.87	0.55
1:D:990:THR:HG22	1:D:990:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:O	1:A:15:ILE:HG22	2.06	0.55
1:B:872:MET:HA	1:B:872:MET:HE2	1.89	0.55
1:C:36:LEU:HG	6:C:2082:HOH:O	2.07	0.55
1:D:52:CYS:HB3	1:D:384:LYS:CG	2.36	0.55
1:D:363:PHE:HE1	1:D:367:PHE:CE1	2.25	0.55
1:B:651:MET:HE3	1:B:700:GLN:HG3	1.89	0.55
1:C:410[B]:ARG:HG2	1:C:425:GLN:O	2.06	0.55
1:D:677:GLU:HG2	1:D:678:ARG:H	1.72	0.55
1:D:783:ARG:NH1	6:D:3029:HOH:O	2.38	0.55
1:A:990:THR:HG22	1:A:990:THR:O	2.07	0.55
1:A:775:LEU:HD12	6:B:2932:HOH:O	2.07	0.55
1:A:777:ALA:HA	6:A:2924:HOH:O	2.06	0.55
1:B:954:ILE:HG23	1:B:998:ILE:CD1	2.33	0.55
1:B:391:LEU:CG	1:B:410[B]:ARG:HH12	2.19	0.54
1:B:787:GLY:N	6:B:2969:HOH:O	2.39	0.54
1:B:394:ARG:NH2	1:B:423:GLU:OE2	2.40	0.54
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.88	0.54
1:C:842:SER:HA	1:C:916:LYS:HG2	1.90	0.54
1:C:857:GLU:HG3	6:C:3012:HOH:O	2.06	0.54
1:D:394:ARG:HD2	1:D:409:VAL:HG11	1.88	0.54
1:B:395:LYS:HG3	1:B:407:GLN:HE21	1.72	0.54
1:D:458:ARG:HG3	6:D:2716:HOH:O	2.07	0.54
1:D:900:GLN:HG2	1:D:901:ASN:N	2.22	0.54
1:A:471:THR:HG22	6:A:2651:HOH:O	2.07	0.54
1:B:391:LEU:HD23	1:B:408:PHE:CB	2.38	0.54
1:C:408:PHE:C	1:C:410[B]:ARG:HH21	2.16	0.54
1:B:364:ARG:HA	1:B:391:LEU:O	2.08	0.54
1:A:485:MET:HE3	6:A:2315:HOH:O	2.07	0.53
1:D:394:ARG:HD2	1:D:409:VAL:HG13	1.90	0.53
1:D:859:HIS:HA	1:D:865:VAL:HG23	1.90	0.53
1:D:951:GLU:CD	6:D:3181:HOH:O	2.50	0.53
1:B:367:PHE:HE1	1:B:387:PHE:HB3	1.73	0.53
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.90	0.53
1:C:943:GLN:HB3	6:D:2844:HOH:O	2.08	0.53
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.90	0.53
1:B:990:THR:HG22	1:B:990:THR:O	2.08	0.53
1:D:885:GLN:HG2	6:D:2580:HOH:O	2.09	0.53
1:A:886:ARG:NH2	6:A:3029:HOH:O	2.34	0.53
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.43	0.53
1:C:27:ALA:O	1:D:497:LYS:HE2	2.09	0.53
1:C:164:LYS:HG3	1:C:909:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LYS:HD3	1:C:420:ASN:OD1	2.07	0.53
1:D:179:GLN:HG3	6:D:2341:HOH:O	2.09	0.53
1:A:173:ASN:ND2	1:A:175:CYS:SG	2.81	0.53
1:D:364:ARG:HA	1:D:391:LEU:O	2.09	0.53
1:B:776:ARG:NH1	6:B:2956:HOH:O	2.41	0.53
1:D:391:LEU:HD22	1:D:408:PHE:CG	2.44	0.53
1:D:673:HIS:CD2	1:D:674:GLY:N	2.77	0.53
1:B:682:LEU:HD12	1:B:682:LEU:N	2.24	0.52
1:C:485:MET:HE2	1:D:32:LEU:HD13	1.91	0.52
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.89	0.52
1:D:164:LYS:HE2	6:D:3135:HOH:O	2.09	0.52
1:D:753:ALA:HB3	6:D:3003:HOH:O	2.09	0.52
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.92	0.52
1:D:680:MET:CE	1:D:688:PRO:HD2	2.39	0.52
1:D:52:CYS:HB2	6:D:2668:HOH:O	2.08	0.52
1:A:776:ARG:NH1	6:A:2924:HOH:O	2.43	0.52
1:B:577[A]:SER:HB3	6:B:2797:HOH:O	2.10	0.52
1:D:3:PRO:HD2	6:D:2001:HOH:O	2.10	0.52
1:D:394:ARG:HH11	1:D:394:ARG:CG	2.19	0.52
1:A:651:MET:HE3	1:A:700:GLN:HG3	1.90	0.52
1:B:52:CYS:HB3	6:B:2633:HOH:O	2.09	0.52
1:C:12:ILE:O	1:C:15:ILE:HG22	2.10	0.52
1:C:47:LYS:HD3	1:D:373:VAL:HG12	1.90	0.52
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.45	0.52
1:A:397:ILE:HD12	1:A:428:HIS:CE1	2.43	0.52
1:A:828:GLN:HG2	6:A:2962:HOH:O	2.09	0.52
1:C:390:PHE:O	1:C:410[B]:ARG:NH1	2.42	0.52
1:C:828:GLN:HG2	6:C:2974:HOH:O	2.09	0.52
1:A:378:GLU:HA	6:A:2578:HOH:O	2.09	0.52
1:A:520:GLU:HG2	6:A:2708:HOH:O	2.09	0.52
1:A:842:SER:HA	1:A:916:LYS:HG2	1.92	0.52
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.44	0.52
1:C:682:LEU:HD12	1:C:682:LEU:N	2.25	0.52
1:B:52:CYS:HB2	1:B:384:LYS:HB2	1.92	0.52
1:D:410:ARG:HG3	6:D:2684:HOH:O	2.10	0.52
1:D:673:HIS:CD2	1:D:673:HIS:C	2.88	0.52
1:A:552:ALA:HB3	1:A:553:PRO:HD3	1.91	0.51
1:D:859:HIS:HD2	1:D:862:GLY:N	2.03	0.51
1:A:341:GLY:HA3	1:A:371:ARG:HH21	1.75	0.51
1:B:545:PRO:HB3	6:B:2754:HOH:O	2.09	0.51
1:A:911:PRO:HB3	6:A:2301:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:ASP:OD1	1:D:937:GLU:HG2	2.10	0.51
1:A:948:ILE:HG12	1:A:1002:ILE:HG12	1.92	0.51
1:C:373:VAL:HG12	1:D:47:LYS:HD3	1.91	0.51
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.45	0.51
1:B:417:GLY:O	1:B:418:LYS:C	2.53	0.51
1:B:842:SER:HA	1:B:916:LYS:HG2	1.91	0.51
1:C:179:GLN:HG3	6:C:2302:HOH:O	2.11	0.51
1:C:859:HIS:HA	1:C:865:VAL:HG23	1.93	0.51
1:C:908:GLU:C	1:C:909:ARG:O	2.51	0.51
1:D:828:GLN:HG2	6:D:3062:HOH:O	2.10	0.51
1:D:922:LYS:HE3	6:D:3149:HOH:O	2.10	0.51
1:D:1007:ARG:CD	1:D:1011:TYR:HB2	2.40	0.51
1:B:193:LEU:HD23	1:B:281:ILE:HD13	1.92	0.51
1:B:362:VAL:HG13	1:B:391:LEU:HD13	1.93	0.51
1:C:783:ARG:NH1	6:D:3013:HOH:O	2.42	0.51
1:D:486:ALA:HB1	1:D:491:GLU:OE1	2.10	0.51
1:A:241:VAL:O	1:A:245[B]:ILE:HG12	2.11	0.51
1:C:364:ARG:HA	1:C:391:LEU:O	2.11	0.51
1:C:582:ILE:HD11	1:D:1015:ARG:CZ	2.41	0.51
1:C:990:THR:O	1:C:990:THR:HG22	2.10	0.51
1:B:409:VAL:C	1:B:410[B]:ARG:NH2	2.69	0.51
1:B:1018:PRO:HD3	6:B:3208:HOH:O	2.09	0.51
1:C:29:HIS:HB2	6:D:2231:HOH:O	2.10	0.51
1:D:12:ILE:O	1:D:15:ILE:HG22	2.10	0.51
1:D:673:HIS:HD2	1:D:674:GLY:N	2.08	0.51
1:C:324:CYS:O	1:C:325:HIS:HB2	2.11	0.51
1:A:577:SER:HB2	6:A:2765:HOH:O	2.10	0.50
1:A:859:HIS:HA	1:A:865:VAL:HG23	1.92	0.50
6:A:2200:HOH:O	1:B:29:HIS:HB2	2.11	0.50
1:B:451:LEU:O	1:B:454:ILE:HG12	2.10	0.50
1:C:893:GLU:OE2	1:C:896:ARG:NH2	2.45	0.50
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.46	0.50
1:C:53:GLU:OE1	1:C:54:LYS:N	2.44	0.50
1:C:391:LEU:HD23	1:C:408:PHE:CB	2.41	0.50
1:C:859:HIS:HD2	1:C:862:GLY:N	2.04	0.50
1:D:673:HIS:CE1	1:D:679:GLY:HA3	2.46	0.50
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.41	0.50
1:C:409:VAL:C	1:C:410[B]:ARG:NH2	2.70	0.50
1:C:874:LYS:HD3	6:C:3032:HOH:O	2.12	0.50
1:D:378:GLU:HG3	6:D:2663:HOH:O	2.10	0.50
1:C:36:LEU:HD23	6:C:2086:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:LYS:HD2	6:D:2752:HOH:O	2.10	0.50
1:D:909:ARG:NH1	6:D:3135:HOH:O	2.44	0.50
1:A:394:ARG:HG3	1:A:409:VAL:HG13	1.94	0.50
1:B:358:ARG:NH2	6:B:2586:HOH:O	2.44	0.50
1:B:954:ILE:HG12	1:B:998:ILE:HD11	1.93	0.50
1:D:901:ASN:N	1:D:901:ASN:ND2	2.60	0.50
1:B:367:PHE:CE1	1:B:387:PHE:CB	2.93	0.50
1:A:179:GLN:HG3	6:A:2319:HOH:O	2.11	0.50
1:B:828:GLN:HG3	6:B:2996:HOH:O	2.12	0.50
1:A:29:HIS:HB2	6:B:2229:HOH:O	2.12	0.50
1:B:82:CYS:O	1:B:98:LYS:HD2	2.11	0.50
1:C:409:VAL:C	1:C:410[B]:ARG:CZ	2.84	0.50
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.93	0.50
1:D:911:PRO:HG3	6:D:2157:HOH:O	2.11	0.50
1:C:22:THR:HA	6:C:2055:HOH:O	2.12	0.49
1:A:364:ARG:HA	1:A:391:LEU:O	2.11	0.49
1:A:787:GLY:HA3	1:D:942:GLU:OE2	2.12	0.49
1:A:947[A]:VAL:HG12	1:A:1003:ARG:O	2.11	0.49
1:D:263:GLU:O	1:D:264:ASN:HB2	2.11	0.49
1:C:261:LEU:HD21	1:C:451:LEU:HD21	1.95	0.49
1:D:552:ALA:HB3	1:D:553:PRO:HD3	1.93	0.49
1:D:962[A]:THR:HG21	1:D:991:LEU:HB3	1.93	0.49
1:A:859:HIS:CD2	1:A:862:GLY:H	2.17	0.49
1:B:391:LEU:CD2	1:B:410[B]:ARG:NH1	2.70	0.49
1:B:699:ARG:HA	1:B:699:ARG:NE	2.27	0.49
1:C:281[B]:ILE:HD13	1:C:451:LEU:HD22	1.93	0.49
1:C:391:LEU:CD2	1:C:410[B]:ARG:NH2	2.72	0.49
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.95	0.49
1:A:144:ALA:O	1:B:861:LYS:HG2	2.12	0.49
1:D:677:GLU:O	1:D:678:ARG:CB	2.60	0.49
1:D:678:ARG:HG3	1:D:679:GLY:N	2.28	0.49
1:B:574:LYS:HB3	1:B:614:SER:HB2	1.94	0.49
1:C:219:LYS:HG3	1:C:260:SER:OG	2.12	0.49
1:C:311:PRO:O	1:C:315:LYS:HG3	2.13	0.49
1:D:962[A]:THR:HG23	6:D:3190:HOH:O	2.12	0.49
1:D:1007:ARG:HD3	1:D:1011:TYR:HB2	1.95	0.49
1:A:612:LEU:HA	6:A:2798:HOH:O	2.12	0.49
1:B:219:LYS:HG3	1:B:260:SER:OG	2.12	0.49
1:D:678:ARG:NH1	6:D:2945:HOH:O	2.46	0.49
1:A:485:MET:HE1	1:B:32:LEU:HB2	1.94	0.49
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:MET:O	1:B:998:ILE:CD1	2.60	0.48
1:D:410:ARG:HD3	1:D:422:ASP:OD2	2.12	0.48
1:B:828:GLN:HG2	6:B:2997:HOH:O	2.11	0.48
1:D:394:ARG:C	1:D:395:LYS:HG3	2.38	0.48
1:A:861:LYS:NZ	6:A:3006:HOH:O	2.46	0.48
1:B:672:PRO:HA	1:B:682:LEU:O	2.14	0.48
1:A:82:CYS:O	1:A:98:LYS:HD2	2.13	0.48
1:C:115:MET:HE1	6:C:2976:HOH:O	2.13	0.48
1:D:939:SER:OG	1:D:941:ILE:HG12	2.13	0.48
1:C:132:THR:HB	1:C:137:VAL:HG23	1.94	0.48
1:C:241:VAL:O	1:C:245[B]:ILE:HG12	2.13	0.48
1:C:413:GLN:HG3	1:C:419:TRP:CE2	2.48	0.48
6:C:2976:HOH:O	1:D:22:THR:HG23	2.13	0.48
1:A:263:GLU:O	1:A:264:ASN:HB2	2.12	0.48
1:B:100:PHE:CD1	1:B:100:PHE:C	2.92	0.48
1:B:420:ASN:ND2	6:B:2650:HOH:O	2.47	0.48
1:D:863:LYS:HE2	6:D:2172:HOH:O	2.12	0.48
1:A:608:LEU:HB2	1:A:742:MET:HE2	1.94	0.48
1:C:916:LYS:HE3	6:C:2988:HOH:O	2.12	0.48
1:C:191:ALA:O	1:C:279:ALA:HA	2.14	0.48
1:D:608:LEU:HB2	1:D:742:MET:HE2	1.95	0.48
1:A:54:LYS:HE3	1:A:56:GLU:HB3	1.95	0.48
1:A:485:MET:HE2	1:B:32:LEU:HD13	1.96	0.48
1:A:896:ARG:O	1:A:900:GLN:HG3	2.13	0.48
1:C:486:ALA:HB1	1:C:491:GLU:OE1	2.14	0.48
1:D:346:ASP:OD2	4:D:1031:FAD:H6	2.13	0.48
1:A:875:LYS:HB3	6:A:3018:HOH:O	2.14	0.48
1:C:338:LEU:HD23	1:C:362:VAL:HB	1.94	0.48
1:C:872:MET:HE1	6:C:3016:HOH:O	2.14	0.48
1:A:734:ALA:HA	1:A:735:THR:HA	1.57	0.47
1:B:18:LEU:HD13	6:B:3156:HOH:O	2.14	0.47
1:B:410[A]:ARG:HG2	1:B:411:THR:N	2.27	0.47
1:B:887:LYS:HD2	6:B:2550:HOH:O	2.14	0.47
1:C:164:LYS:HG2	1:C:909:ARG:HH12	1.79	0.47
1:D:621:TRP:O	1:D:625:VAL:HG23	2.14	0.47
1:B:505:LYS:HE2	6:B:2722:HOH:O	2.13	0.47
1:C:978:HIS:HD2	6:D:2291:HOH:O	1.96	0.47
1:B:191:ALA:O	1:B:279:ALA:HA	2.15	0.47
1:B:656:LYS:HD2	6:B:2869:HOH:O	2.14	0.47
1:C:334:ALA:HA	6:C:2549:HOH:O	2.14	0.47
1:D:680:MET:HE3	1:D:688:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:SER:CB	6:A:2851:HOH:O	2.61	0.47
1:A:874:LYS:HG2	6:A:3015:HOH:O	2.14	0.47
1:A:959:CYS:O	1:A:962[B]:THR:HG22	2.14	0.47
1:B:394:ARG:HG3	1:B:409:VAL:CG1	2.40	0.47
1:B:448:LYS:HD3	6:B:2681:HOH:O	2.14	0.47
1:C:993:LEU:HD23	1:C:993:LEU:C	2.40	0.47
1:D:36:LEU:HB3	6:D:2117:HOH:O	2.14	0.47
1:D:779[B]:THR:CG2	1:D:932:LEU:HD22	2.27	0.47
1:D:962[A]:THR:CG2	1:D:991:LEU:HB3	2.45	0.47
1:A:356:ALA:O	6:A:2542:HOH:O	2.20	0.47
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.44	0.47
1:D:642:MET:HE2	6:D:2821:HOH:O	2.15	0.47
1:A:191:ALA:O	1:A:279:ALA:HA	2.14	0.47
1:B:409:VAL:O	1:B:410[B]:ARG:NH2	2.47	0.47
1:B:845:GLU:HG3	1:B:912:PHE:CZ	2.50	0.47
1:C:574:LYS:HB3	1:C:614:SER:HB2	1.97	0.47
1:D:82:CYS:O	1:D:98:LYS:HD2	2.14	0.47
1:D:779[B]:THR:HG23	1:D:929:LEU:CD2	2.45	0.47
1:D:947[B]:VAL:HG22	1:D:1003:ARG:O	2.15	0.47
1:D:993:LEU:C	1:D:993:LEU:HD23	2.39	0.47
1:C:52:CYS:HB2	1:C:383:GLU:O	2.15	0.47
1:C:54:LYS:HG3	6:C:2117:HOH:O	2.15	0.47
1:C:393:PRO:HD3	6:C:2594:HOH:O	2.14	0.47
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.49	0.47
1:A:318:LYS:C	6:A:2503:HOH:O	2.58	0.47
1:A:1015:ARG:CZ	1:B:582:ILE:HD11	2.45	0.47
1:B:367:PHE:CE1	1:B:387:PHE:HB2	2.49	0.47
1:B:608:LEU:HB2	1:B:742:MET:HE2	1.97	0.47
1:B:911:PRO:HG2	6:B:2436:HOH:O	2.14	0.47
1:C:32:LEU:HD13	1:D:485:MET:HE2	1.97	0.47
1:C:870:GLU:O	1:C:889:ILE:HD13	2.15	0.47
1:C:901:ASN:HD22	1:C:901:ASN:C	2.22	0.47
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.96	0.47
1:B:696:ARG:NH1	6:B:2901:HOH:O	2.29	0.46
1:B:744:LEU:HD21	6:B:2460:HOH:O	2.15	0.46
1:D:381:LYS:NZ	6:D:2662:HOH:O	2.48	0.46
1:B:193:LEU:N	1:B:193:LEU:HD22	2.30	0.46
1:B:311:PRO:O	1:B:315:LYS:HG3	2.14	0.46
1:B:486:ALA:HB1	1:B:491:GLU:OE1	2.16	0.46
1:B:340:ALA:N	6:B:2562:HOH:O	2.47	0.46
1:C:734:ALA:HA	1:C:735:THR:HA	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:892:GLU:HG3	6:D:3132:HOH:O	2.14	0.46
1:A:934:THR:OG1	1:A:937:GLU:HG3	2.15	0.46
1:B:358:ARG:NH2	6:B:2587:HOH:O	2.48	0.46
1:B:552:ALA:HB3	1:B:553:PRO:HD3	1.97	0.46
1:D:379:LEU:O	1:D:383:GLU:HG3	2.15	0.46
1:A:673:HIS:ND1	1:A:673:HIS:C	2.70	0.46
1:B:346:ASP:OD2	4:B:1031:FAD:H6	2.16	0.46
1:C:408:PHE:HB3	1:C:410[B]:ARG:HH22	1.81	0.46
1:B:693:ASN:HA	1:B:696:ARG:HD3	1.97	0.46
1:A:864:PRO:HD3	6:A:3008:HOH:O	2.14	0.46
1:C:323:ALA:O	1:C:324:CYS:C	2.58	0.46
1:C:391:LEU:CD2	1:C:408:PHE:CB	2.93	0.46
1:D:315:LYS:NZ	6:D:2572:HOH:O	2.48	0.46
1:A:413:GLN:HG3	1:A:419:TRP:CE2	2.51	0.46
1:B:572:LEU:HD13	1:B:638:ILE:HB	1.97	0.46
1:B:688:PRO:HG3	1:B:720:ILE:HD13	1.97	0.46
1:B:870:GLU:O	1:B:889:ILE:HD13	2.16	0.46
1:A:193:LEU:HD22	1:A:193:LEU:N	2.31	0.46
1:A:688:PRO:HG3	1:A:720:ILE:HD13	1.96	0.46
1:C:861:LYS:HD2	6:D:2292:HOH:O	2.15	0.46
1:D:394:ARG:NH1	1:D:394:ARG:CG	2.78	0.46
1:D:673:HIS:ND1	1:D:690:LEU:HD11	2.31	0.46
1:A:100:PHE:CD1	1:A:100:PHE:C	2.93	0.46
1:A:379:LEU:O	1:A:383:GLU:HG3	2.16	0.46
1:B:448:LYS:NZ	1:B:460:ASP:OD2	2.48	0.46
1:A:219:LYS:HG3	1:A:260:SER:OG	2.15	0.45
1:A:993:LEU:C	1:A:993:LEU:HD23	2.41	0.45
1:C:696:ARG:HG3	1:C:696:ARG:HH11	1.81	0.45
1:D:338:LEU:HD23	1:D:362:VAL:HB	1.98	0.45
1:B:36:LEU:HD23	6:B:2105:HOH:O	2.15	0.45
1:D:191:ALA:O	1:D:279:ALA:HA	2.16	0.45
1:A:346:ASP:OD2	4:A:1031:FAD:H6	2.15	0.45
1:D:872:MET:CE	6:D:3181:HOH:O	2.64	0.45
1:A:844:GLU:HA	1:A:847:GLN:HE21	1.82	0.45
6:A:2805:HOH:O	1:B:1014:LYS:HD3	2.16	0.45
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.97	0.45
1:C:124:LEU:HD13	1:C:160:SER:HB2	1.98	0.45
1:C:621:TRP:O	1:C:625:VAL:HG23	2.17	0.45
1:D:941:ILE:N	1:D:941:ILE:HD13	2.31	0.45
1:C:947[B]:VAL:HG12	1:C:1003:ARG:O	2.17	0.45
1:A:1007:ARG:HD3	1:A:1011:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:THR:N	6:B:2652:HOH:O	2.41	0.45
1:C:1007:ARG:HD3	1:C:1011:TYR:HB2	1.99	0.45
1:D:193:LEU:N	1:D:193:LEU:HD22	2.32	0.45
1:A:760:THR:HG23	1:B:932[A]:LEU:HD23	1.99	0.45
1:D:83:ALA:O	1:D:84:ASP:C	2.60	0.45
1:B:167[B]:ASN:ND2	6:B:2320:HOH:O	2.50	0.45
1:C:167[B]:ASN:HD22	1:C:911:PRO:HA	1.76	0.45
1:C:897:LEU:HD23	1:C:900:GLN:OE1	2.17	0.45
1:A:53:GLU:O	1:A:53:GLU:HG2	2.16	0.45
1:A:393:PRO:HD3	6:A:2590:HOH:O	2.15	0.45
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.47	0.45
1:C:696:ARG:HD2	6:C:2868:HOH:O	2.16	0.45
1:D:100:PHE:CD1	1:D:100:PHE:C	2.95	0.45
1:D:191:ALA:HB2	1:D:276:TYR:CD2	2.52	0.45
1:A:223:VAL:HG23	6:A:2389:HOH:O	2.17	0.45
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.17	0.45
1:C:410[B]:ARG:HE	1:C:427:VAL:HG23	1.81	0.45
1:C:859:HIS:CD2	1:C:862:GLY:H	2.19	0.45
1:A:27:ALA:O	1:B:497:LYS:HE2	2.17	0.44
1:B:391:LEU:HG	1:B:410[B]:ARG:HH12	1.81	0.44
1:B:394:ARG:C	1:B:395:LYS:HG2	2.42	0.44
1:B:691:VAL:HG21	1:B:720:ILE:HG23	2.00	0.44
1:C:193:LEU:N	1:C:193:LEU:HD22	2.32	0.44
1:A:223:VAL:HG23	1:A:245[A]:ILE:CD1	2.47	0.44
1:A:318:LYS:HB3	6:A:2503:HOH:O	2.17	0.44
1:B:39:LYS:HG3	6:B:2108:HOH:O	2.17	0.44
1:D:451:LEU:O	1:D:454:ILE:HG12	2.17	0.44
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.52	0.44
1:B:409:VAL:N	1:B:410[B]:ARG:NH2	2.59	0.44
1:B:893:GLU:O	1:B:897:LEU:HG	2.17	0.44
1:C:394:ARG:HA	1:C:394:ARG:HD3	1.75	0.44
1:C:688:PRO:HG3	1:C:720:ILE:HD13	1.99	0.44
1:C:893:GLU:OE2	1:C:896:ARG:CZ	2.65	0.44
1:B:417:GLY:O	1:B:418:LYS:O	2.36	0.44
1:B:734:ALA:HA	1:B:735:THR:HA	1.56	0.44
1:C:328:LEU:HB2	6:C:2517:HOH:O	2.17	0.44
1:C:577[B]:SER:HB2	6:C:2763:HOH:O	2.16	0.44
1:D:239:ASP:HB2	6:D:2317:HOH:O	2.17	0.44
1:A:22:THR:HG23	6:B:2996:HOH:O	2.17	0.44
1:A:51:HIS:CE1	1:A:52:CYS:O	2.71	0.44
1:B:132:THR:HB	1:B:137:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LYS:NZ	6:B:2630:HOH:O	2.51	0.44
1:B:901:ASN:C	1:B:901:ASN:HD22	2.26	0.44
1:C:260:SER:HB2	1:C:265:GLU:OE1	2.18	0.44
1:D:1019:LEU:N	1:D:1019:LEU:CD2	2.78	0.44
1:A:83:ALA:O	1:A:84:ASP:C	2.61	0.44
1:A:644:SER:HA	1:A:671:CYS:SG	2.58	0.44
1:A:849:TRP:CH2	1:A:854:PRO:HG3	2.52	0.44
1:A:1007:ARG:CD	1:A:1011:TYR:HB2	2.47	0.44
1:B:300:ASP:HB3	6:B:2295:HOH:O	2.16	0.44
1:B:1007:ARG:CD	1:B:1011:TYR:HB2	2.47	0.44
1:C:83:ALA:O	1:C:84:ASP:C	2.61	0.44
1:C:200:ILE:CD1	1:C:245[B]:ILE:HD11	2.47	0.44
1:C:459:TRP:HD1	6:C:2674:HOH:O	2.01	0.44
1:C:519:PRO:HB3	1:D:28:LEU:HD22	1.99	0.44
1:A:932:LEU:HD11	1:B:741:LEU:HD21	2.00	0.44
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.17	0.44
1:C:779[B]:THR:HG23	1:C:929:LEU:CD2	2.47	0.44
1:D:57:ASN:HB2	6:D:2153:HOH:O	2.18	0.44
1:D:911:PRO:HG2	6:D:2470:HOH:O	2.17	0.44
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.18	0.44
1:A:876:LEU:HD21	1:A:885:GLN:NE2	2.33	0.44
1:B:83:ALA:O	1:B:84:ASP:C	2.60	0.44
1:B:399:LYS:HE2	6:B:2291:HOH:O	2.17	0.44
1:C:100:PHE:CD1	1:C:100:PHE:C	2.95	0.44
1:A:868:ILE:HG22	1:A:870:GLU:H	1.83	0.44
1:B:261:LEU:HD21	1:B:451:LEU:HD21	2.00	0.44
1:B:360:PHE:HE2	6:B:2586:HOH:O	2.01	0.44
1:C:324:CYS:SG	6:C:2515:HOH:O	2.56	0.44
1:D:394:ARG:HG3	1:D:394:ARG:NH1	2.23	0.44
1:D:486:ALA:HA	6:D:2742:HOH:O	2.17	0.44
1:A:173:ASN:HD22	1:A:174:PRO:N	2.15	0.43
1:A:410:ARG:HG3	6:A:2603:HOH:O	2.17	0.43
1:C:200:ILE:HD13	1:C:245[B]:ILE:HD11	2.00	0.43
1:D:415:GLU:O	1:D:417:GLY:N	2.50	0.43
1:A:373:VAL:HG12	1:B:47:LYS:HD3	2.00	0.43
1:B:939:SER:OG	1:B:941:ILE:HG22	2.18	0.43
1:C:82:CYS:O	1:C:98:LYS:HD2	2.18	0.43
1:C:381:LYS:NZ	6:C:2585:HOH:O	2.51	0.43
1:D:915:LYS:HG3	6:D:3141:HOH:O	2.17	0.43
1:A:223:VAL:CG2	1:A:245[A]:ILE:HD13	2.47	0.43
1:A:283:ILE:CG1	1:A:482:ILE:HD12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.18	0.43
1:A:391:LEU:HD22	1:A:408:PHE:CG	2.53	0.43
1:A:859:HIS:HE1	6:A:3133:HOH:O	2.01	0.43
1:A:888:LYS:HD3	6:A:3027:HOH:O	2.17	0.43
1:A:893:GLU:CD	1:A:896:ARG:NH2	2.76	0.43
1:D:44:ASN:HB2	1:D:45:PRO:CD	2.47	0.43
1:D:358:ARG:NH2	6:D:2621:HOH:O	2.51	0.43
1:B:934:THR:OG1	1:B:937:GLU:HG3	2.17	0.43
1:D:974:ASP:N	6:D:3200:HOH:O	2.51	0.43
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.53	0.43
1:B:863:LYS:HA	1:B:864:PRO:HD3	1.92	0.43
1:C:428:HIS:O	1:D:410:ARG:NH1	2.49	0.43
1:A:680:MET:HE1	6:A:2428:HOH:O	2.19	0.43
1:B:172:ARG:HG3	6:B:2329:HOH:O	2.17	0.43
1:B:378:GLU:HA	6:B:2627:HOH:O	2.19	0.43
1:A:132:THR:HB	1:A:137:VAL:HG23	2.00	0.43
1:B:409:VAL:C	1:B:410[B]:ARG:CZ	2.92	0.43
1:C:423:GLU:OE1	1:C:423:GLU:HA	2.19	0.43
1:C:897:LEU:C	1:C:899:GLU:H	2.26	0.43
1:D:574:LYS:HB3	1:D:614:SER:HB2	2.01	0.43
1:A:311:PRO:O	1:A:315:LYS:HG3	2.19	0.43
1:D:593:GLY:HA2	1:D:742:MET:HE3	2.01	0.43
1:D:859:HIS:CD2	1:D:862:GLY:H	2.20	0.43
1:A:25:HIS:CE1	6:B:2740:HOH:O	2.72	0.43
1:B:53:GLU:HB3	6:B:3072:HOH:O	2.17	0.43
1:B:859:HIS:ND1	1:B:859:HIS:C	2.77	0.43
1:C:17:ALA:HB3	6:C:2038:HOH:O	2.19	0.43
1:C:358:ARG:NH2	6:C:2548:HOH:O	2.52	0.43
1:C:1007:ARG:CD	1:C:1011:TYR:HB2	2.49	0.43
1:D:391:LEU:HD22	1:D:408:PHE:CB	2.49	0.43
1:A:777:ALA:O	1:A:780:THR:HG22	2.19	0.42
1:A:932:LEU:HD21	6:B:2460:HOH:O	2.18	0.42
1:B:1007:ARG:HD3	1:B:1011:TYR:HB2	2.00	0.42
1:C:132:THR:HB	1:C:137:VAL:CG2	2.49	0.42
1:D:623:GLN:HG3	6:D:2880:HOH:O	2.18	0.42
1:A:67:LEU:HD23	1:B:146:GLU:HG2	2.00	0.42
1:D:672:PRO:HA	1:D:682:LEU:O	2.20	0.42
1:D:878:ASN:ND2	6:D:3117:HOH:O	2.52	0.42
1:C:54:LYS:HD3	1:C:891:ALA:HB1	2.01	0.42
1:C:32:LEU:HB2	1:D:485:MET:HE1	2.01	0.42
1:C:391:LEU:CG	1:C:410[B]:ARG:HH12	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:828:GLN:HG3	6:C:2976:HOH:O	2.19	0.42
1:C:410[A]:ARG:HD3	1:C:422:ASP:OD2	2.20	0.42
1:A:397:ILE:CD1	1:A:428:HIS:HE1	2.31	0.42
1:B:872:MET:HE1	1:B:951:GLU:HG3	1.99	0.42
1:C:572:LEU:HD13	1:C:638:ILE:HB	2.00	0.42
1:D:193:LEU:HD23	1:D:281:ILE:HD13	2.01	0.42
1:D:362:VAL:HG13	1:D:391:LEU:HD13	2.02	0.42
1:B:167[B]:ASN:HD21	1:B:910:LYS:C	2.28	0.42
1:B:621:TRP:O	1:B:625:VAL:HG23	2.19	0.42
1:C:844:GLU:O	1:C:847:GLN:HG3	2.20	0.42
1:D:335:VAL:HG22	1:D:433:VAL:HB	2.02	0.42
1:D:910:LYS:HA	1:D:911:PRO:HD3	1.90	0.42
1:A:519:PRO:HB3	1:B:28:LEU:HD22	2.01	0.42
1:A:864:PRO:CD	6:A:3008:HOH:O	2.68	0.42
1:B:364:ARG:NH1	6:B:2639:HOH:O	2.53	0.42
1:B:993:LEU:C	1:B:993:LEU:HD23	2.44	0.42
1:C:394:ARG:NH2	1:C:423:GLU:OE2	2.40	0.42
1:A:582:ILE:HD11	1:B:1015:ARG:CZ	2.50	0.42
1:A:784:ALA:C	1:A:786:PRO:HD3	2.45	0.42
1:B:36:LEU:HG	6:B:2098:HOH:O	2.19	0.42
1:B:53:GLU:HB2	6:B:2150:HOH:O	2.20	0.42
1:B:364:ARG:HG3	1:B:364:ARG:HH11	1.85	0.42
1:B:381:LYS:HD3	6:B:2628:HOH:O	2.19	0.42
1:B:1007:ARG:NH1	6:B:3174:HOH:O	2.51	0.42
1:C:577[A]:SER:HB3	6:C:2763:HOH:O	2.18	0.42
1:A:402:ARG:HH11	1:A:402:ARG:CG	2.26	0.42
1:B:189:LYS:HG2	6:B:2386:HOH:O	2.20	0.42
1:B:263:GLU:HG2	1:B:449:GLU:OE1	2.20	0.42
1:C:19:ASN:OD1	1:C:20:PRO:HD2	2.20	0.42
1:A:870:GLU:O	1:A:889:ILE:HD13	2.20	0.41
1:A:893:GLU:OE2	1:A:896:ARG:CZ	2.68	0.41
1:B:611:GLU:O	5:B:1034:IUR:H6	2.20	0.41
1:C:28:LEU:HD22	1:D:519:PRO:HB3	2.02	0.41
1:C:346:ASP:OD2	4:C:1031:FAD:H6	2.20	0.41
1:C:409:VAL:N	1:C:410[B]:ARG:NH2	2.68	0.41
1:C:443:ARG:C	1:C:448:LYS:HE3	2.45	0.41
1:D:18:LEU:HD13	6:D:3199:HOH:O	2.19	0.41
1:D:934:THR:OG1	1:D:937:GLU:HG3	2.20	0.41
1:A:22:THR:CG2	6:B:2996:HOH:O	2.69	0.41
1:A:191:ALA:HB2	1:A:276:TYR:CD2	2.56	0.41
1:A:223:VAL:HG23	1:A:245[A]:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:PRO:HA	6:B:3210:HOH:O	2.20	0.41
1:C:533:ILE:O	1:C:545:PRO:HD3	2.20	0.41
1:D:291:ASP:OD1	1:D:293:ILE:HG12	2.20	0.41
1:D:673:HIS:ND1	1:D:690:LEU:CD1	2.84	0.41
1:A:54:LYS:HG3	6:A:2120:HOH:O	2.21	0.41
1:A:989:CYS:O	1:A:990:THR:HB	2.20	0.41
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.61	0.41
1:D:677:GLU:HG2	1:D:678:ARG:N	2.35	0.41
1:A:625:VAL:HG13	6:A:2822:HOH:O	2.20	0.41
1:A:1017:LEU:HD12	1:B:620:TYR:N	2.35	0.41
1:B:273:GLU:HG3	6:B:2458:HOH:O	2.21	0.41
1:A:555:THR:HA	1:A:574:LYS:HG3	2.01	0.41
1:B:52:CYS:HB2	1:B:384:LYS:CG	2.51	0.41
1:B:237:PRO:HB2	1:B:239:ASP:OD1	2.20	0.41
1:B:391:LEU:HD23	1:B:408:PHE:HB3	2.02	0.41
1:D:124:LEU:HD13	1:D:160:SER:HB2	2.03	0.41
1:A:691:VAL:HG21	1:A:720:ILE:HG23	2.03	0.41
1:A:1012:GLU:HA	1:A:1013:PRO:HD2	1.95	0.41
1:B:291:ASP:OD1	1:B:293:ILE:HG12	2.21	0.41
1:C:343:THR:HA	4:C:1031:FAD:HM73	2.02	0.41
1:B:410[B]:ARG:HD2	1:B:425:GLN:C	2.44	0.41
1:B:828:GLN:NE2	6:B:2998:HOH:O	2.51	0.41
1:C:358:ARG:N	6:C:2549:HOH:O	2.54	0.41
1:C:845:GLU:CD	1:C:845:GLU:H	2.27	0.41
6:C:2976:HOH:O	1:D:22:THR:CG2	2.69	0.41
1:A:193:LEU:HD23	1:A:281:ILE:HD13	2.03	0.41
1:A:221:GLU:HG3	6:A:2174:HOH:O	2.20	0.41
1:B:27:ALA:HB2	6:B:2039:HOH:O	2.21	0.41
1:B:874:LYS:HE2	6:B:3057:HOH:O	2.21	0.41
1:C:173:ASN:HA	1:C:174:PRO:HD3	1.90	0.41
1:C:315:LYS:NZ	6:C:2501:HOH:O	2.51	0.41
1:C:391:LEU:HD22	1:C:408:PHE:CG	2.56	0.41
1:C:413:GLN:HG2	1:C:417:GLY:O	2.19	0.41
1:D:53:GLU:HG3	1:D:887:LYS:HD3	2.02	0.41
1:D:237:PRO:HB2	1:D:239:ASP:OD1	2.20	0.41
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.20	0.41
1:A:371:ARG:HE	1:A:371:ARG:HB2	1.43	0.41
1:C:95:LEU:HD23	1:C:119:ASP:HB2	2.01	0.41
1:C:191:ALA:HB2	1:C:276:TYR:CD2	2.56	0.41
1:C:375:GLU:CD	1:C:375:GLU:H	2.29	0.41
1:C:414:ASP:O	1:C:415:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.61	0.40
1:A:519:PRO:HD2	6:A:2707:HOH:O	2.20	0.40
1:A:621:TRP:O	1:A:625:VAL:HG23	2.21	0.40
1:B:629:LYS:HA	1:B:629:LYS:CE	2.51	0.40
1:C:323:ALA:HB1	1:C:904:PHE:CE2	2.56	0.40
1:D:5:LEU:CD2	6:D:2001:HOH:O	2.64	0.40
1:D:311:PRO:O	1:D:315:LYS:CG	2.68	0.40
1:D:883:LEU:HG	1:D:887:LYS:HE3	2.04	0.40
5:A:1034:IUR:I5	6:A:2798:HOH:O	2.93	0.40
1:B:863:LYS:NZ	6:B:3051:HOH:O	2.54	0.40
1:C:263:GLU:O	1:C:264:ASN:HB2	2.21	0.40
1:C:391:LEU:HD23	1:C:408:PHE:HB3	2.03	0.40
1:C:394:ARG:HG3	1:C:409:VAL:HG13	2.04	0.40
1:C:934:THR:OG1	1:C:937:GLU:HG3	2.21	0.40
1:D:391:LEU:CD2	1:D:408:PHE:CB	2.99	0.40
1:A:451:LEU:O	1:A:454:ILE:HG12	2.22	0.40
1:B:97:ILE:HD11	2:B:1026:SF4:S4	2.62	0.40
1:B:859:HIS:CD2	6:B:3039:HOH:O	2.74	0.40
1:C:180:GLU:H	1:C:180:GLU:CD	2.29	0.40
1:C:223:VAL:HG23	6:C:2388:HOH:O	2.21	0.40
1:C:552:ALA:HB3	1:C:553:PRO:HD3	2.02	0.40
1:C:868:ILE:HG22	1:C:870:GLU:H	1.85	0.40
1:D:962[B]:THR:HG21	1:D:992:CYS:HA	2.03	0.40
1:A:97:ILE:HD11	2:A:1026:SF4:S4	2.61	0.40
1:A:173:ASN:HB2	6:A:2352:HOH:O	2.21	0.40
1:A:207:ALA:HB1	1:A:251:LEU:HB3	2.04	0.40
1:B:871:LEU:HB3	6:B:3054:HOH:O	2.21	0.40
1:C:391:LEU:CD2	1:C:408:PHE:HB2	2.52	0.40
1:C:518:LYS:O	1:C:520:GLU:HG3	2.21	0.40
1:D:231:ILE:HA	1:D:232:PRO:HD3	1.96	0.40
1:D:518:LYS:O	1:D:520:GLU:HG3	2.22	0.40
1:D:868:ILE:HG22	1:D:870:GLU:H	1.86	0.40
1:C:409:VAL:N	1:C:410[B]:ARG:HH21	2.20	0.40
1:C:423:GLU:OE1	1:C:423:GLU:CA	2.68	0.40
1:C:501:TRP:CZ2	1:C:519:PRO:HA	2.57	0.40
1:D:97:ILE:HD11	2:D:1026:SF4:S4	2.61	0.40
1:D:367:PHE:CD1	1:D:370:ILE:HD11	2.57	0.40
1:D:448:LYS:NZ	1:D:460:ASP:OD2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2001:HOH:O	6:A:2818:HOH:O[1_655]	1.98	0.22

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1003/1025 (98%)	972 (97%)	29 (3%)	2 (0%)	43	27
1	B	1004/1025 (98%)	974 (97%)	29 (3%)	1 (0%)	48	30
1	C	1017/1025 (99%)	984 (97%)	30 (3%)	3 (0%)	36	21
1	D	1017/1025 (99%)	983 (97%)	31 (3%)	3 (0%)	36	21
All	All	4041/4100 (99%)	3913 (97%)	119 (3%)	9 (0%)	43	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	418	LYS
1	C	324	CYS
1	C	325	HIS
1	D	678	ARG
1	A	53	GLU
1	C	909	ARG
1	D	416	THR
1	D	415	GLU
1	A	416	THR

5.3.2 Protein sidechains [i](#)

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	843/854 (99%)	832 (99%)	11 (1%)	61	42
1	B	845/854 (99%)	836 (99%)	9 (1%)	65	48
1	C	854/854 (100%)	842 (99%)	12 (1%)	59	39
1	D	852/854 (100%)	843 (99%)	9 (1%)	65	48
All	All	3394/3416 (99%)	3353 (99%)	41 (1%)	63	45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	CYS
1	A	53	GLU
1	A	54	LYS
1	A	100	PHE
1	A	175	CYS
1	A	180	GLU
1	A	402	ARG
1	A	453	PRO
1	A	574	LYS
1	A	673	HIS
1	A	793	THR
1	B	100	PHE
1	B	367	PHE
1	B	391	LEU
1	B	416	THR
1	B	453	PRO
1	B	574	LYS
1	B	793	THR
1	B	845	GLU
1	B	870	GLU
1	C	100	PHE
1	C	180	GLU
1	C	293	ILE
1	C	324	CYS
1	C	331	ILE
1	C	391	LEU
1	C	453	PRO
1	C	574	LYS
1	C	793	THR
1	C	845	GLU
1	C	857	GLU
1	C	907	LEU
1	D	100	PHE

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Mol	Chain	Res	Type
1	D	367	PHE
1	D	394	ARG
1	D	453	PRO
1	D	678	ARG
1	D	793	THR
1	D	901	ASN
1	D	941	ILE
1	D	1019	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	57	ASN
1	A	173	ASN
1	A	242	ASN
1	A	295	GLN
1	A	413	GLN
1	A	428	HIS
1	A	487	ASN
1	A	498	GLN
1	A	508	GLN
1	A	693	ASN
1	A	703	GLN
1	A	859	HIS
1	A	878	ASN
1	A	885	GLN
1	A	972	GLN
1	B	170	GLN
1	B	242	ASN
1	B	295	GLN
1	B	299	GLN
1	B	369	ASN
1	B	407	GLN
1	B	413	GLN
1	B	494	ASN
1	B	693	ASN
1	B	828	GLN
1	B	847	GLN
1	B	878	ASN
1	B	901	ASN
1	C	57	ASN

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Mol	Chain	Res	Type
1	C	295	GLN
1	C	407	GLN
1	C	498	GLN
1	C	508	GLN
1	C	510	GLN
1	C	623	GLN
1	C	828	GLN
1	C	859	HIS
1	C	885	GLN
1	C	901	ASN
1	C	930	GLN
1	C	978	HIS
1	D	57	ASN
1	D	157	GLN
1	D	167	ASN
1	D	295	GLN
1	D	299	GLN
1	D	407	GLN
1	D	498	GLN
1	D	510	GLN
1	D	623	GLN
1	D	673	HIS
1	D	859	HIS
1	D	901	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	FAD	B	1031	-	58,58,58	2.26	22 (37%)	85,89,89	1.62	9 (10%)
5	IUR	C	1034	-	9,9,9	1.44	1 (11%)	11,12,12	2.03	4 (36%)
2	SF4	C	1028	1	0,12,12	-	-	-	-	-
5	IUR	B	1034	-	9,9,9	1.49	2 (22%)	11,12,12	1.98	3 (27%)
4	FAD	D	1031	-	58,58,58	2.27	24 (41%)	85,89,89	1.63	8 (9%)
2	SF4	C	1027	1	0,12,12	-	-	-	-	-
5	IUR	A	1034	-	9,9,9	1.53	2 (22%)	11,12,12	1.96	3 (27%)
2	SF4	C	1029	1	0,12,12	-	-	-	-	-
2	SF4	B	1027	-	0,12,12	-	-	-	-	-
2	SF4	B	1029	-	0,12,12	-	-	-	-	-
2	SF4	B	1028	-	0,12,12	-	-	-	-	-
2	SF4	A	1028	-	0,12,12	-	-	-	-	-
2	SF4	A	1029	-	0,12,12	-	-	-	-	-
2	SF4	C	1026	-	0,12,12	-	-	-	-	-
2	SF4	A	1027	-	0,12,12	-	-	-	-	-
2	SF4	D	1028	1	0,12,12	-	-	-	-	-
2	SF4	A	1026	-	0,12,12	-	-	-	-	-
3	FMN	B	1030	-	33,33,33	1.83	8 (24%)	48,50,50	1.85	12 (25%)
3	FMN	A	1030	-	33,33,33	1.79	7 (21%)	48,50,50	1.84	11 (22%)
2	SF4	D	1027	1	0,12,12	-	-	-	-	-
2	SF4	D	1026	1	0,12,12	-	-	-	-	-
3	FMN	C	1030	-	33,33,33	1.86	7 (21%)	48,50,50	1.83	10 (20%)
3	FMN	D	1030	-	33,33,33	1.83	7 (21%)	48,50,50	1.84	14 (29%)
4	FAD	A	1031	-	58,58,58	2.28	22 (37%)	85,89,89	1.63	9 (10%)
5	IUR	D	1034	-	9,9,9	1.43	1 (11%)	11,12,12	2.06	4 (36%)
4	FAD	C	1031	-	58,58,58	2.31	23 (39%)	85,89,89	1.63	9 (10%)
2	SF4	D	1029	1	0,12,12	-	-	-	-	-
2	SF4	B	1026	-	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	B	1031	-	-	4/34/50/50	0/6/6/6
5	IUR	C	1034	-	-	-	0/1/1/1
2	SF4	C	1028	1	-	-	0/6/5/5
5	IUR	B	1034	-	-	-	0/1/1/1
4	FAD	D	1031	-	-	3/34/50/50	0/6/6/6
2	SF4	C	1027	1	-	-	0/6/5/5
5	IUR	A	1034	-	-	-	0/1/1/1
2	SF4	C	1029	1	-	-	0/6/5/5
2	SF4	B	1027	-	-	-	0/6/5/5
2	SF4	B	1029	-	-	-	0/6/5/5
2	SF4	B	1028	-	-	-	0/6/5/5
2	SF4	A	1028	-	-	-	0/6/5/5
2	SF4	A	1029	-	-	-	0/6/5/5
2	SF4	C	1026	-	-	-	0/6/5/5
2	SF4	A	1027	-	-	-	0/6/5/5
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	A	1026	-	-	-	0/6/5/5
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	D	1027	1	-	-	0/6/5/5
2	SF4	D	1026	1	-	-	0/6/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
4	FAD	A	1031	-	-	4/34/50/50	0/6/6/6
5	IUR	D	1034	-	-	-	0/1/1/1
4	FAD	C	1031	-	-	3/34/50/50	0/6/6/6
2	SF4	D	1029	1	-	-	0/6/5/5
2	SF4	B	1026	-	-	-	0/6/5/5

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1031	FAD	PA-O3P	9.38	1.69	1.59
4	A	1031	FAD	PA-O3P	9.24	1.69	1.59
4	D	1031	FAD	PA-O3P	8.95	1.69	1.59
4	B	1031	FAD	PA-O3P	8.86	1.69	1.59
4	C	1031	FAD	P-O3P	-6.76	1.52	1.59
4	D	1031	FAD	P-O3P	-6.45	1.52	1.59
4	B	1031	FAD	P-O3P	-6.22	1.52	1.59
4	A	1031	FAD	P-O3P	-6.13	1.52	1.59
3	D	1030	FMN	C4A-N5	4.31	1.40	1.30
3	C	1030	FMN	C4A-N5	4.26	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C7M-C7	4.24	1.58	1.51
4	C	1031	FAD	PA-O2A	-4.21	1.35	1.55
3	B	1030	FMN	C4A-N5	4.20	1.39	1.30
4	A	1031	FAD	PA-O2A	-4.19	1.35	1.55
4	D	1031	FAD	PA-O2A	-4.17	1.36	1.55
4	B	1031	FAD	PA-O2A	-4.15	1.36	1.55
3	D	1030	FMN	C7M-C7	4.14	1.58	1.51
3	A	1030	FMN	C4A-N5	4.12	1.39	1.30
3	B	1030	FMN	C7M-C7	4.00	1.58	1.51
3	A	1030	FMN	C7M-C7	3.96	1.58	1.51
3	C	1030	FMN	C1'-N10	-3.74	1.38	1.47
3	D	1030	FMN	C1'-N10	-3.67	1.39	1.47
3	B	1030	FMN	C1'-N10	-3.65	1.39	1.47
3	A	1030	FMN	C1'-N10	-3.55	1.39	1.47
4	D	1031	FAD	P-O2P	-3.53	1.39	1.55
4	A	1031	FAD	P-O2P	-3.46	1.39	1.55
4	B	1031	FAD	P-O2P	-3.41	1.39	1.55
4	D	1031	FAD	C4X-N5	3.40	1.38	1.30
4	C	1031	FAD	P-O2P	-3.37	1.39	1.55
4	C	1031	FAD	C4X-N5	3.35	1.38	1.30
3	B	1030	FMN	C4'-C3'	3.26	1.59	1.53
4	C	1031	FAD	C9A-N10	3.20	1.46	1.41
4	A	1031	FAD	C4X-N5	3.17	1.37	1.30
4	B	1031	FAD	C9A-N10	3.15	1.46	1.41
3	C	1030	FMN	C4'-C3'	3.15	1.58	1.53
4	B	1031	FAD	C4X-N5	3.13	1.37	1.30
3	A	1030	FMN	C4'-C3'	3.13	1.58	1.53
4	A	1031	FAD	C9A-N10	3.11	1.46	1.41
3	C	1030	FMN	C1'-C2'	3.07	1.56	1.52
4	D	1031	FAD	C9A-C5X	3.03	1.46	1.41
4	B	1031	FAD	C8-C7	3.02	1.48	1.40
3	D	1030	FMN	C4'-C3'	3.01	1.58	1.53
4	B	1031	FAD	C9A-C5X	3.00	1.46	1.41
4	A	1031	FAD	C8-C7	2.98	1.48	1.40
3	C	1030	FMN	C9A-C5A	2.98	1.46	1.41
3	D	1030	FMN	C9A-C5A	2.98	1.46	1.41
4	C	1031	FAD	C8-C7	2.96	1.48	1.40
4	A	1031	FAD	C9A-C5X	2.96	1.46	1.41
3	B	1030	FMN	C9A-C5A	2.93	1.45	1.41
3	A	1030	FMN	C9A-C5A	2.91	1.45	1.41
4	B	1031	FAD	O5'-C5'	2.86	1.55	1.44
4	D	1031	FAD	O5'-C5'	2.83	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1031	FAD	C9A-C5X	2.83	1.45	1.41
4	D	1031	FAD	C8-C7	2.81	1.47	1.40
4	A	1031	FAD	O5'-C5'	2.79	1.55	1.44
4	D	1031	FAD	C9A-N10	2.78	1.46	1.41
3	B	1030	FMN	C1'-C2'	2.71	1.56	1.52
5	C	1034	IUR	C2-N1	2.70	1.40	1.36
4	C	1031	FAD	O5'-C5'	2.69	1.54	1.44
3	D	1030	FMN	C9A-N10	2.66	1.45	1.41
3	B	1030	FMN	C9A-N10	2.66	1.45	1.41
5	A	1034	IUR	C2-N1	2.64	1.40	1.36
3	A	1030	FMN	C1'-C2'	2.64	1.56	1.52
3	C	1030	FMN	C9A-N10	2.61	1.45	1.41
5	A	1034	IUR	C6-C5	2.59	1.38	1.35
5	B	1034	IUR	C6-C5	2.59	1.38	1.35
4	A	1031	FAD	C4A-N3A	2.56	1.39	1.34
4	B	1031	FAD	C4A-N3A	2.55	1.39	1.34
4	C	1031	FAD	C5A-C6A	2.54	1.48	1.41
5	B	1034	IUR	C2-N1	2.54	1.40	1.36
5	D	1034	IUR	C2-N1	2.52	1.40	1.36
4	D	1031	FAD	C5A-C6A	2.51	1.48	1.41
4	D	1031	FAD	C4A-N3A	2.50	1.39	1.34
4	B	1031	FAD	C6-C5X	2.47	1.43	1.40
4	A	1031	FAD	C5A-C6A	2.46	1.47	1.41
4	B	1031	FAD	O4B-C4B	2.45	1.50	1.45
4	A	1031	FAD	C2-N3	2.44	1.44	1.39
4	A	1031	FAD	C2A-N1A	2.44	1.38	1.33
4	B	1031	FAD	C5A-C6A	2.43	1.47	1.41
4	C	1031	FAD	C6-C5X	2.42	1.43	1.40
4	A	1031	FAD	C6-C5X	2.42	1.43	1.40
3	A	1030	FMN	C9A-N10	2.41	1.45	1.41
4	B	1031	FAD	C9-C9A	2.40	1.43	1.39
4	B	1031	FAD	C5A-C4A	2.39	1.43	1.39
4	C	1031	FAD	C4A-N3A	2.38	1.38	1.34
4	D	1031	FAD	O4B-C4B	2.36	1.50	1.45
4	C	1031	FAD	C5A-C4A	2.36	1.43	1.39
4	D	1031	FAD	C2A-N1A	2.35	1.38	1.33
3	D	1030	FMN	C1'-C2'	2.35	1.55	1.52
4	A	1031	FAD	O4B-C4B	2.31	1.50	1.45
4	D	1031	FAD	C2-N3	2.30	1.44	1.39
4	C	1031	FAD	C2-N3	2.30	1.44	1.39
4	D	1031	FAD	C5A-C4A	2.29	1.43	1.39
4	D	1031	FAD	C9-C8	2.27	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1031	FAD	C2A-N1A	2.26	1.37	1.33
4	A	1031	FAD	C5A-C4A	2.24	1.43	1.39
4	B	1031	FAD	C10-N1	2.23	1.37	1.33
4	D	1031	FAD	C5B-C4B	2.23	1.58	1.51
4	A	1031	FAD	C5B-C4B	2.23	1.58	1.51
4	B	1031	FAD	C2A-N1A	2.22	1.37	1.33
4	C	1031	FAD	C10-N1	2.22	1.37	1.33
4	D	1031	FAD	C6-C5X	2.21	1.43	1.40
4	C	1031	FAD	C9-C9A	2.21	1.43	1.39
4	B	1031	FAD	C2-N3	2.20	1.43	1.39
4	C	1031	FAD	C5B-C4B	2.16	1.58	1.51
4	C	1031	FAD	O4B-C1B	2.15	1.47	1.42
4	A	1031	FAD	PA-O5B	-2.14	1.51	1.59
4	B	1031	FAD	PA-O5B	-2.14	1.51	1.59
4	C	1031	FAD	PA-O5B	-2.14	1.51	1.59
3	B	1030	FMN	C10-N1	2.14	1.37	1.33
4	D	1031	FAD	PA-O5B	-2.13	1.51	1.59
4	A	1031	FAD	C1'-C2'	2.12	1.55	1.52
4	C	1031	FAD	O4B-C4B	2.12	1.49	1.45
4	D	1031	FAD	C1'-C2'	2.11	1.55	1.52
4	D	1031	FAD	C3B-C4B	2.10	1.58	1.53
4	B	1031	FAD	C5B-C4B	2.10	1.57	1.51
4	D	1031	FAD	C9-C9A	2.09	1.43	1.39
4	B	1031	FAD	C1'-C2'	2.08	1.55	1.52
4	A	1031	FAD	C10-N1	2.07	1.37	1.33
4	A	1031	FAD	C3B-C4B	2.07	1.58	1.53
4	D	1031	FAD	O4B-C1B	2.06	1.46	1.42
4	C	1031	FAD	P-O5'	-2.04	1.51	1.59
4	C	1031	FAD	C3B-C4B	2.03	1.58	1.53
4	B	1031	FAD	P-O5'	-2.03	1.51	1.59
4	D	1031	FAD	C10-N1	2.02	1.37	1.33
4	A	1031	FAD	C9-C9A	2.01	1.42	1.39

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1031	FAD	O3P-PA-O1A	-8.24	85.91	110.70
4	B	1031	FAD	O3P-PA-O1A	-8.23	85.96	110.70
4	D	1031	FAD	O3P-PA-O1A	-8.21	86.00	110.70
4	C	1031	FAD	O3P-PA-O1A	-8.15	86.17	110.70
4	C	1031	FAD	O2A-PA-O3P	-6.91	88.60	107.27
4	D	1031	FAD	O2A-PA-O3P	-6.83	88.81	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1031	FAD	O2A-PA-O3P	-6.79	88.91	107.27
4	A	1031	FAD	O2A-PA-O3P	-6.75	89.04	107.27
3	A	1030	FMN	C10-N1-C2	4.73	127.09	116.85
3	C	1030	FMN	C10-N1-C2	4.72	127.08	116.85
3	B	1030	FMN	C10-N1-C2	4.68	126.98	116.85
3	D	1030	FMN	C10-N1-C2	4.64	126.90	116.85
5	C	1034	IUR	O2-C2-N1	4.29	127.20	122.79
5	B	1034	IUR	O2-C2-N1	4.28	127.19	122.79
5	D	1034	IUR	O2-C2-N1	4.23	127.15	122.79
5	A	1034	IUR	O2-C2-N1	4.20	127.11	122.79
3	B	1030	FMN	O4'-C4'-C3'	4.06	118.76	109.25
3	B	1030	FMN	C4-C4A-C10	3.98	123.77	116.93
3	D	1030	FMN	C4-C4A-C10	3.97	123.74	116.93
3	B	1030	FMN	C4A-C10-N1	-3.96	114.88	124.59
3	B	1030	FMN	O3'-C3'-C2'	-3.92	100.02	108.93
3	A	1030	FMN	C4-C4A-C10	3.92	123.65	116.93
3	A	1030	FMN	C4A-C10-N1	-3.91	115.00	124.59
3	D	1030	FMN	O4'-C4'-C3'	3.89	118.35	109.25
3	C	1030	FMN	C4A-C10-N1	-3.88	115.07	124.59
3	D	1030	FMN	C4A-C10-N1	-3.88	115.08	124.59
3	A	1030	FMN	O3'-C3'-C2'	-3.87	100.13	108.93
4	D	1031	FAD	O2A-PA-O1A	3.87	130.45	112.44
3	A	1030	FMN	O4'-C4'-C3'	3.85	118.27	109.25
3	C	1030	FMN	O3'-C3'-C2'	-3.85	100.18	108.93
3	C	1030	FMN	C4-C4A-C10	3.85	123.53	116.93
3	C	1030	FMN	O4'-C4'-C3'	3.84	118.23	109.25
4	A	1031	FAD	O2A-PA-O1A	3.80	130.10	112.44
4	B	1031	FAD	O2A-PA-O1A	3.76	129.94	112.44
4	C	1031	FAD	O2A-PA-O1A	3.73	129.79	112.44
3	D	1030	FMN	O3'-C3'-C2'	-3.73	100.46	108.93
5	C	1034	IUR	C6-N1-C2	-3.33	119.60	122.69
5	D	1034	IUR	C6-N1-C2	-3.27	119.65	122.69
3	D	1030	FMN	C5'-C4'-C3'	-3.21	106.16	112.22
5	A	1034	IUR	C6-N1-C2	-3.19	119.73	122.69
3	C	1030	FMN	C5'-C4'-C3'	-3.14	106.30	112.22
3	B	1030	FMN	C5'-C4'-C3'	-3.11	106.35	112.22
4	C	1031	FAD	C5'-C4'-C3'	-3.07	106.43	112.22
4	C	1031	FAD	O4B-C1B-N9A	-3.05	102.24	108.09
5	B	1034	IUR	C6-N1-C2	-3.04	119.87	122.69
3	A	1030	FMN	C5'-C4'-C3'	-3.03	106.50	112.22
4	A	1031	FAD	O4B-C1B-N9A	-2.99	102.35	108.09
4	D	1031	FAD	O4B-C1B-N9A	-2.91	102.50	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1031	FAD	C5'-C4'-C3'	-2.90	106.75	112.22
4	B	1031	FAD	O4B-C1B-N9A	-2.82	102.67	108.09
4	A	1031	FAD	C5'-C4'-C3'	-2.79	106.95	112.22
4	D	1031	FAD	C5'-C4'-C3'	-2.78	106.98	112.22
3	A	1030	FMN	C4A-C10-N10	2.72	120.38	116.48
3	C	1030	FMN	C4A-C10-N10	2.68	120.32	116.48
3	A	1030	FMN	O3'-C3'-C4'	2.67	114.99	108.93
3	D	1030	FMN	C4A-C10-N10	2.62	120.23	116.48
5	D	1034	IUR	C5-C6-N1	2.62	123.39	121.33
5	B	1034	IUR	C4-N3-C2	2.60	129.95	126.37
4	B	1031	FAD	C2A-N1A-C6A	2.57	122.96	118.73
5	A	1034	IUR	C4-N3-C2	2.55	129.88	126.37
3	B	1030	FMN	C4A-C10-N10	2.51	120.08	116.48
3	B	1030	FMN	O3'-C3'-C4'	2.49	114.59	108.93
4	A	1031	FAD	C2A-N1A-C6A	2.49	122.81	118.73
4	C	1031	FAD	C2A-N1A-C6A	2.47	122.78	118.73
4	D	1031	FAD	C2A-N1A-C6A	2.46	122.77	118.73
3	C	1030	FMN	O3'-C3'-C4'	2.41	114.41	108.93
5	D	1034	IUR	C4-N3-C2	2.38	129.64	126.37
3	D	1030	FMN	O3'-C3'-C4'	2.34	114.25	108.93
4	B	1031	FAD	C5X-C9A-N10	-2.30	115.89	117.97
4	A	1031	FAD	C5X-C9A-N10	-2.26	115.92	117.97
4	D	1031	FAD	C5X-C9A-N10	-2.24	115.94	117.97
4	A	1031	FAD	C4-N3-C2	-2.24	121.67	125.64
5	C	1034	IUR	C4-N3-C2	2.23	129.43	126.37
3	B	1030	FMN	N10-C10-N1	2.22	125.04	118.51
5	C	1034	IUR	C5-C6-N1	2.19	123.05	121.33
4	D	1031	FAD	C4-N3-C2	-2.18	121.77	125.64
4	C	1031	FAD	C5X-C9A-N10	-2.18	116.00	117.97
3	B	1030	FMN	C4-C4A-N5	-2.18	115.20	118.21
3	D	1030	FMN	N3-C2-N1	-2.16	114.90	119.50
3	B	1030	FMN	N3-C2-N1	-2.14	114.95	119.50
3	A	1030	FMN	N3-C2-N1	-2.12	114.99	119.50
4	C	1031	FAD	O2A-PA-O5B	2.11	117.15	107.57
3	B	1030	FMN	C6-C5A-C9A	2.10	121.94	119.05
3	D	1030	FMN	C4-C4A-N5	-2.10	115.31	118.21
3	D	1030	FMN	N10-C10-N1	2.10	124.68	118.51
4	C	1031	FAD	C4-N3-C2	-2.09	121.93	125.64
3	C	1030	FMN	N3-C2-N1	-2.09	115.06	119.50
4	B	1031	FAD	C4-N3-C2	-2.08	121.94	125.64
3	A	1030	FMN	N10-C10-N1	2.07	124.61	118.51
3	A	1030	FMN	C4-C4A-N5	-2.07	115.35	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1031	FAD	O2A-PA-O5B	2.06	116.91	107.57
3	C	1030	FMN	N10-C10-N1	2.06	124.56	118.51
3	D	1030	FMN	C6-C5A-C9A	2.03	121.84	119.05
3	D	1030	FMN	O4'-C4'-C5'	2.02	114.44	109.99
4	B	1031	FAD	O2A-PA-O5B	2.02	116.70	107.57
3	D	1030	FMN	C9A-C5A-N5	-2.01	120.32	122.45

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	C5B-O5B-PA-O1A
4	A	1031	FAD	PA-O3P-P-O5'
4	B	1031	FAD	C5B-O5B-PA-O1A
4	B	1031	FAD	PA-O3P-P-O5'
4	C	1031	FAD	C5B-O5B-PA-O1A
4	C	1031	FAD	PA-O3P-P-O5'
4	D	1031	FAD	C5B-O5B-PA-O1A
4	D	1031	FAD	PA-O3P-P-O5'
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
3	C	1030	FMN	C4'-C5'-O5'-P
3	D	1030	FMN	C4'-C5'-O5'-P
3	A	1030	FMN	C4'-C5'-O5'-P
3	B	1030	FMN	C4'-C5'-O5'-P
4	B	1031	FAD	P-O3P-PA-O2A
4	A	1031	FAD	P-O3P-PA-O2A

There are no ring outliers.

11 monomers are involved in 12 short contacts:

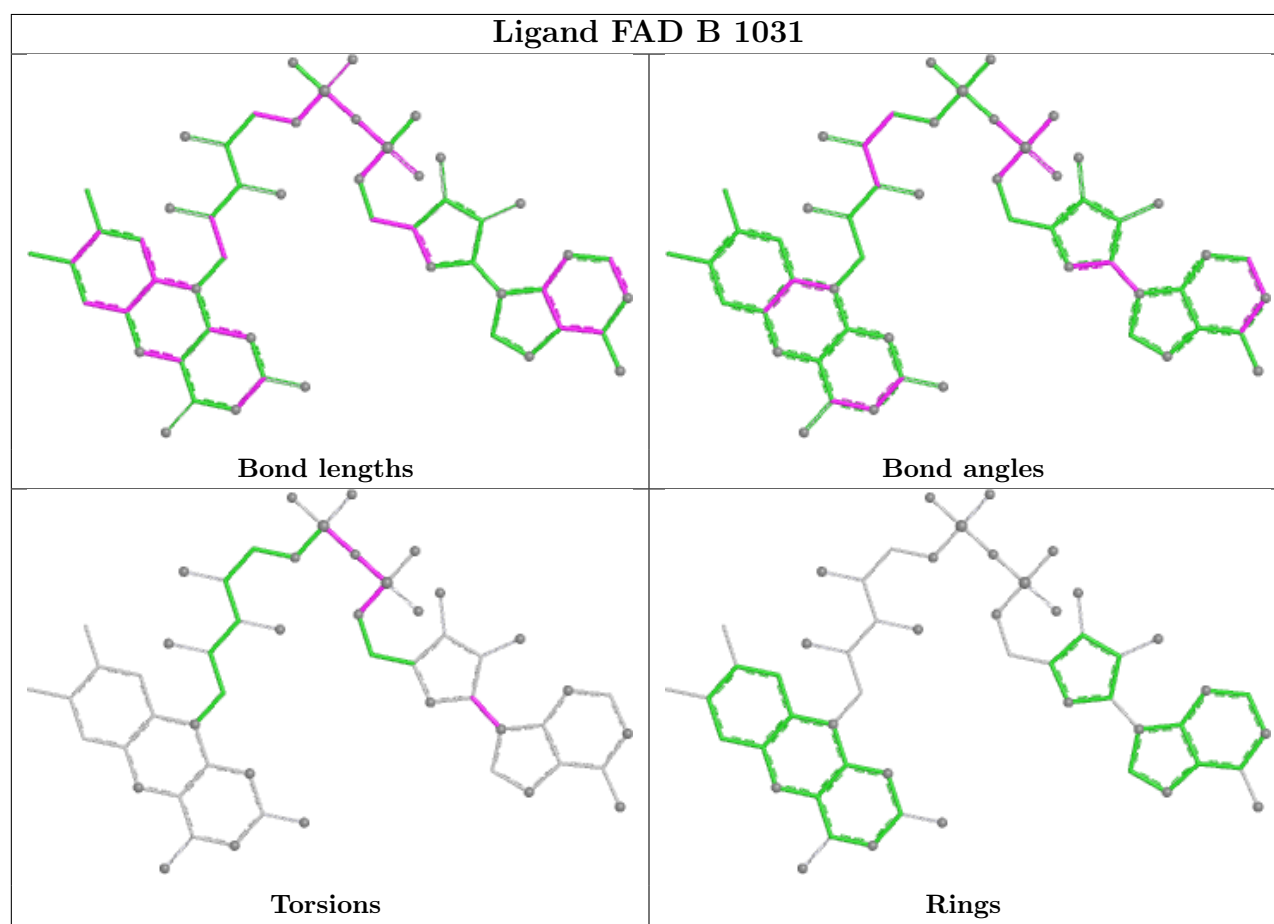
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1031	FAD	1	0
5	B	1034	IUR	1	0
4	D	1031	FAD	1	0
5	A	1034	IUR	1	0
2	A	1027	SF4	1	0
2	A	1026	SF4	1	0
2	D	1027	SF4	1	0

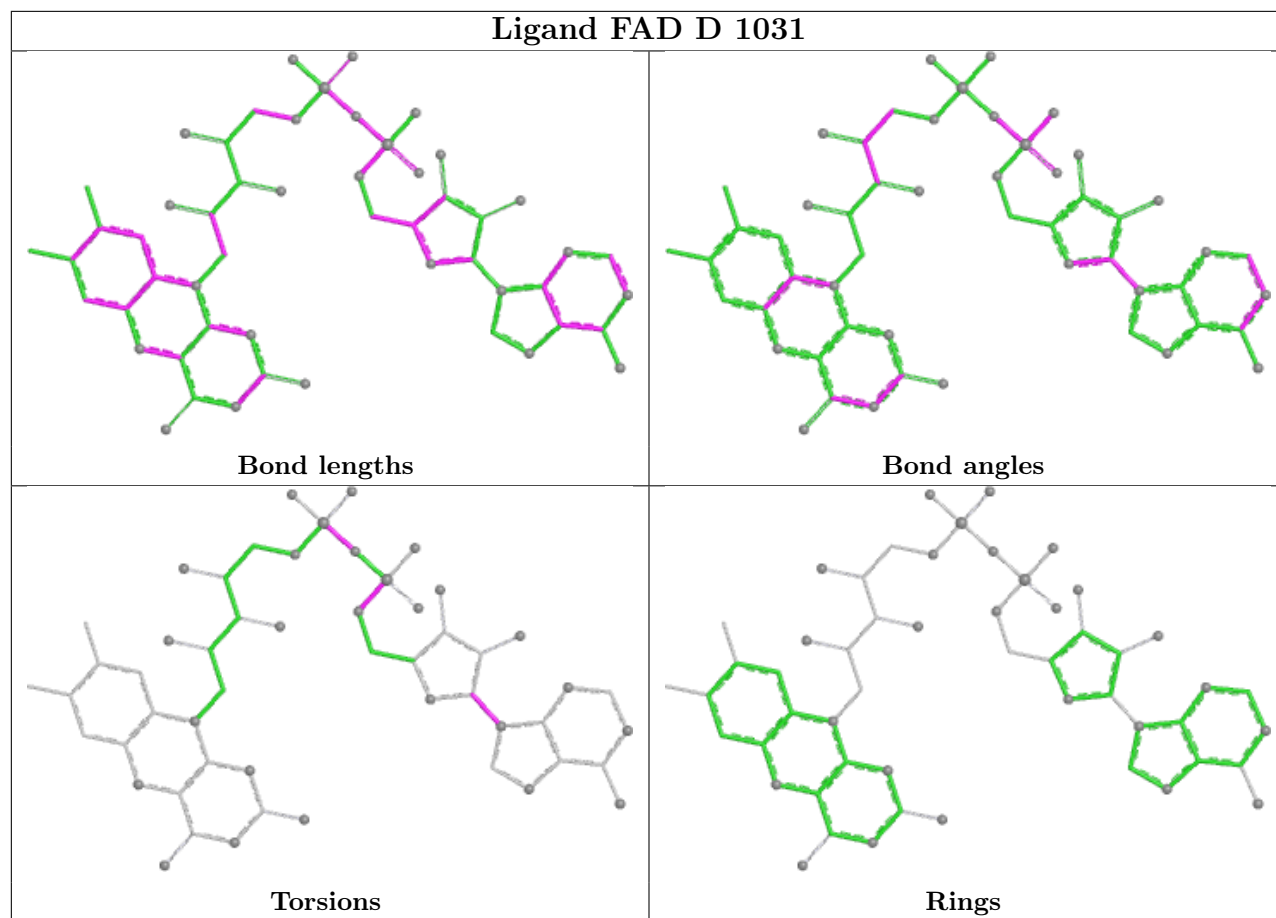
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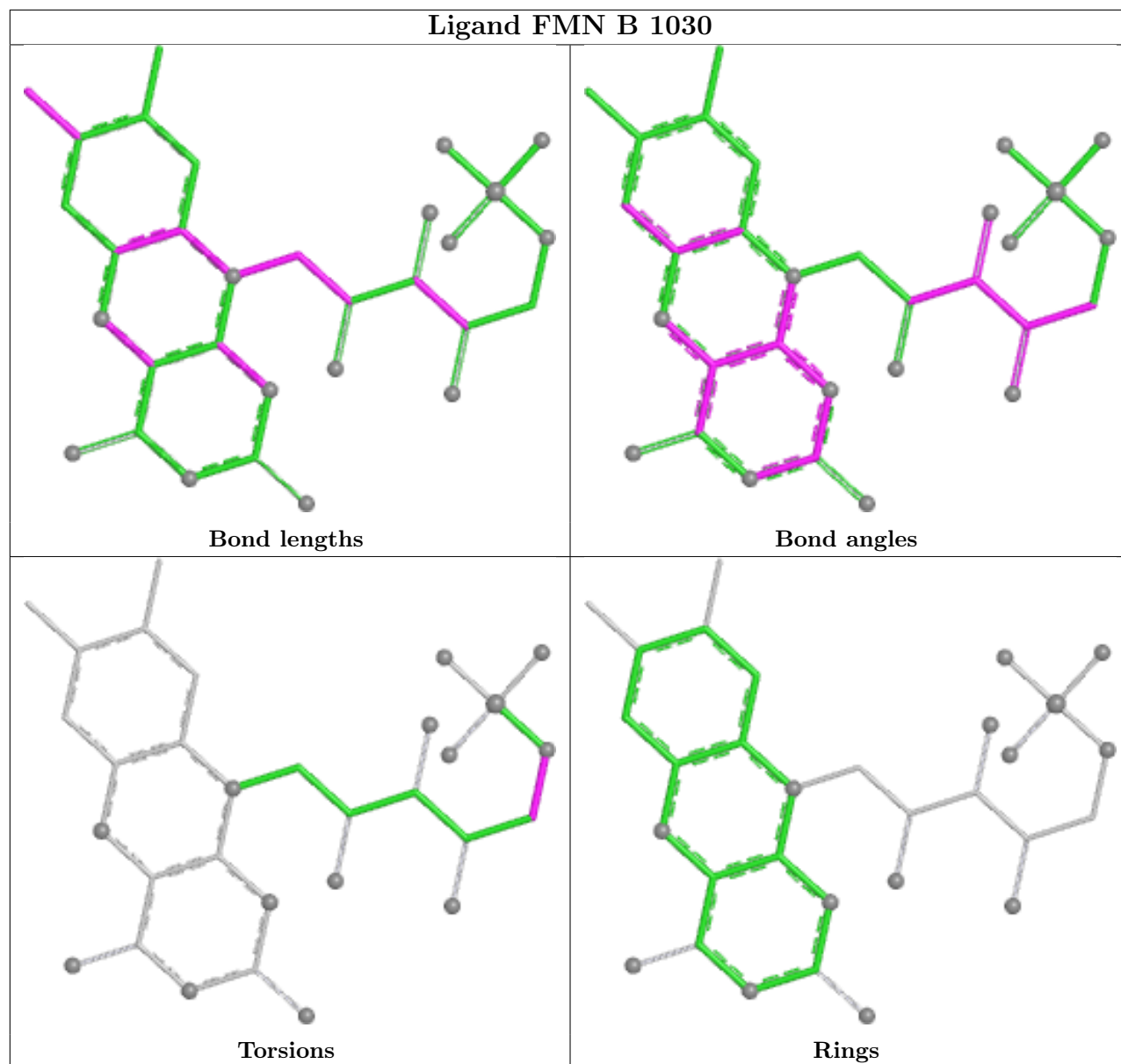
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1026	SF4	1	0
4	A	1031	FAD	1	0
4	C	1031	FAD	2	0
2	B	1026	SF4	1	0

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

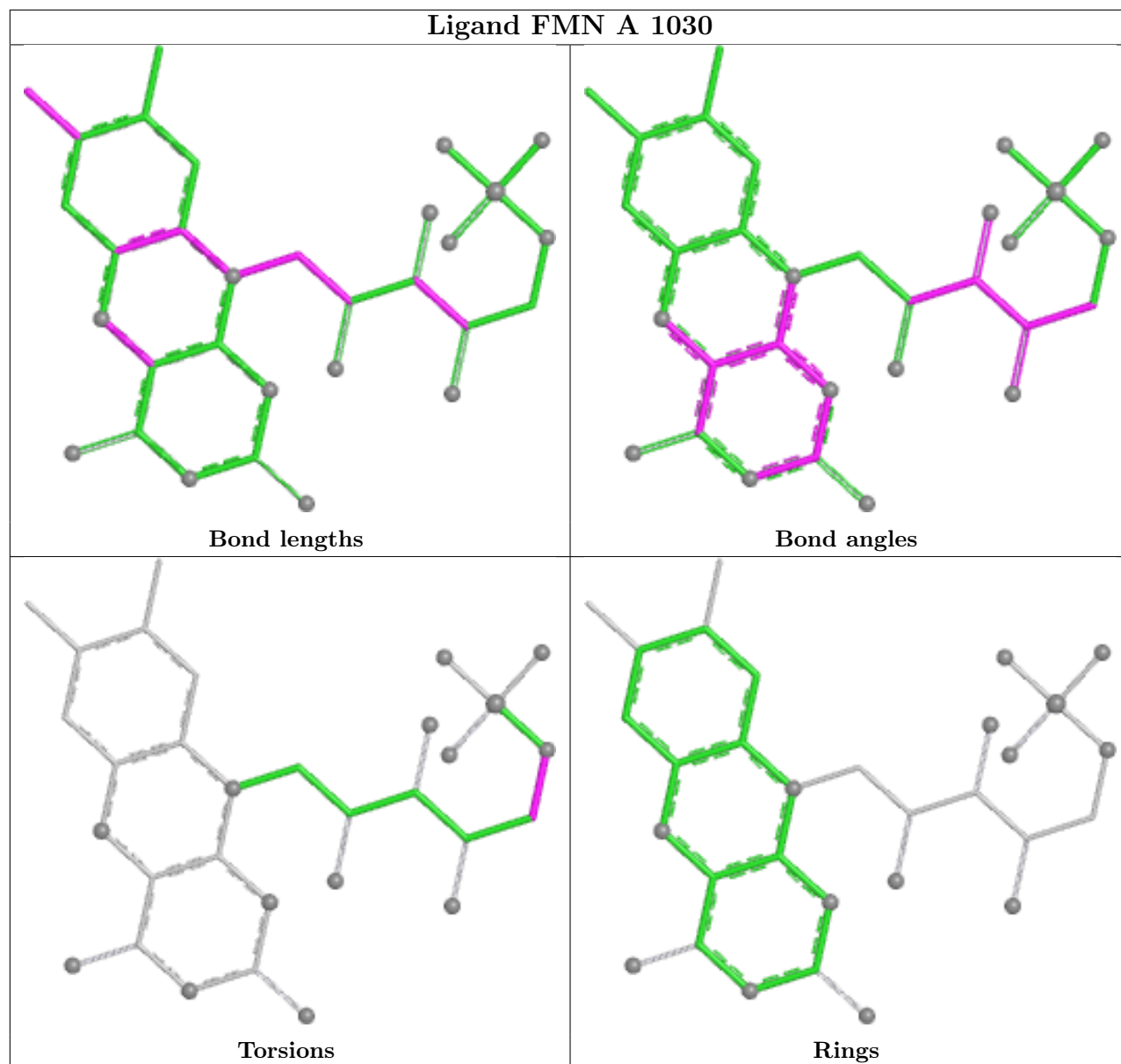




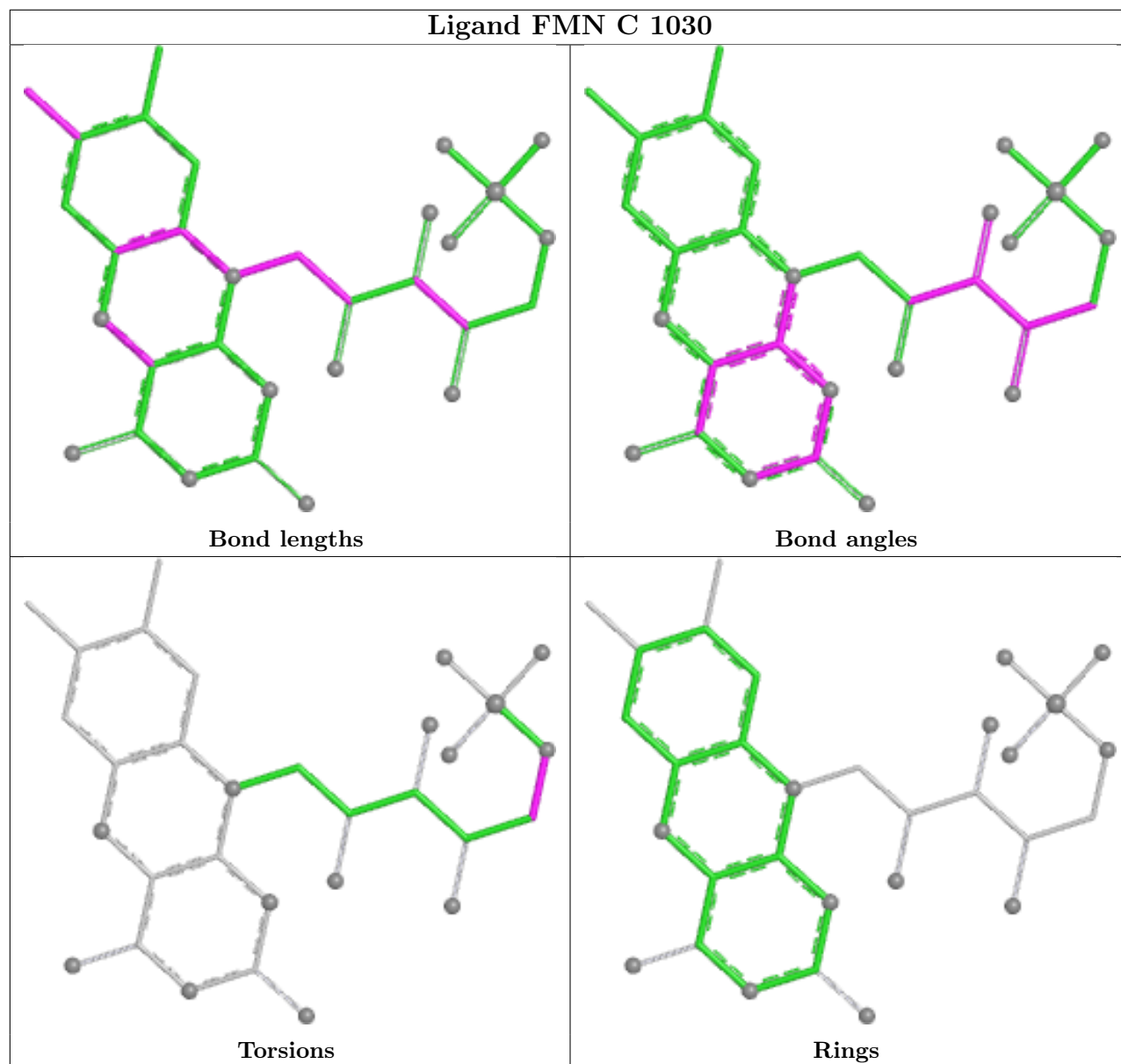
Ligand FMN B 1030



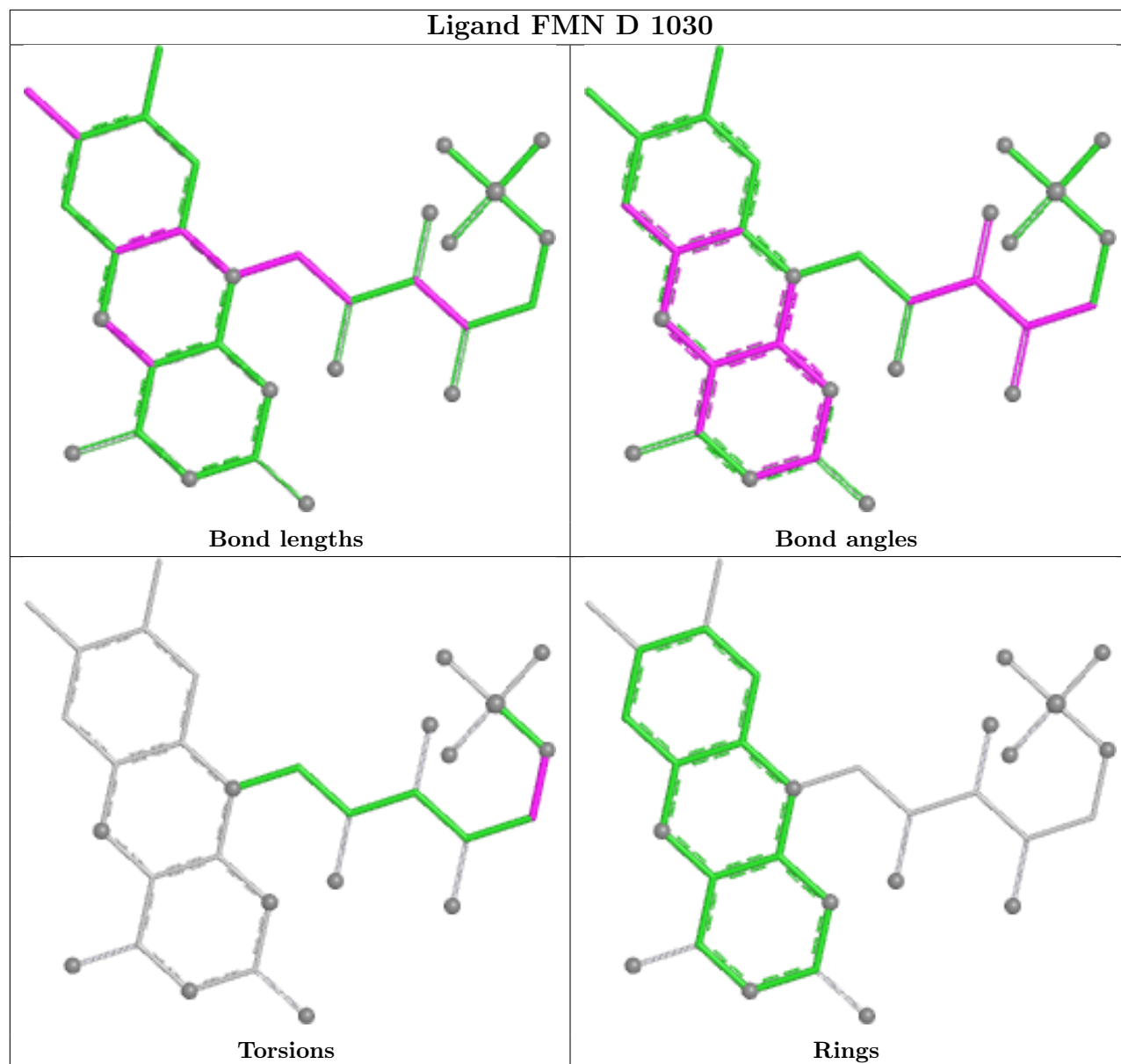
Ligand FMN A 1030

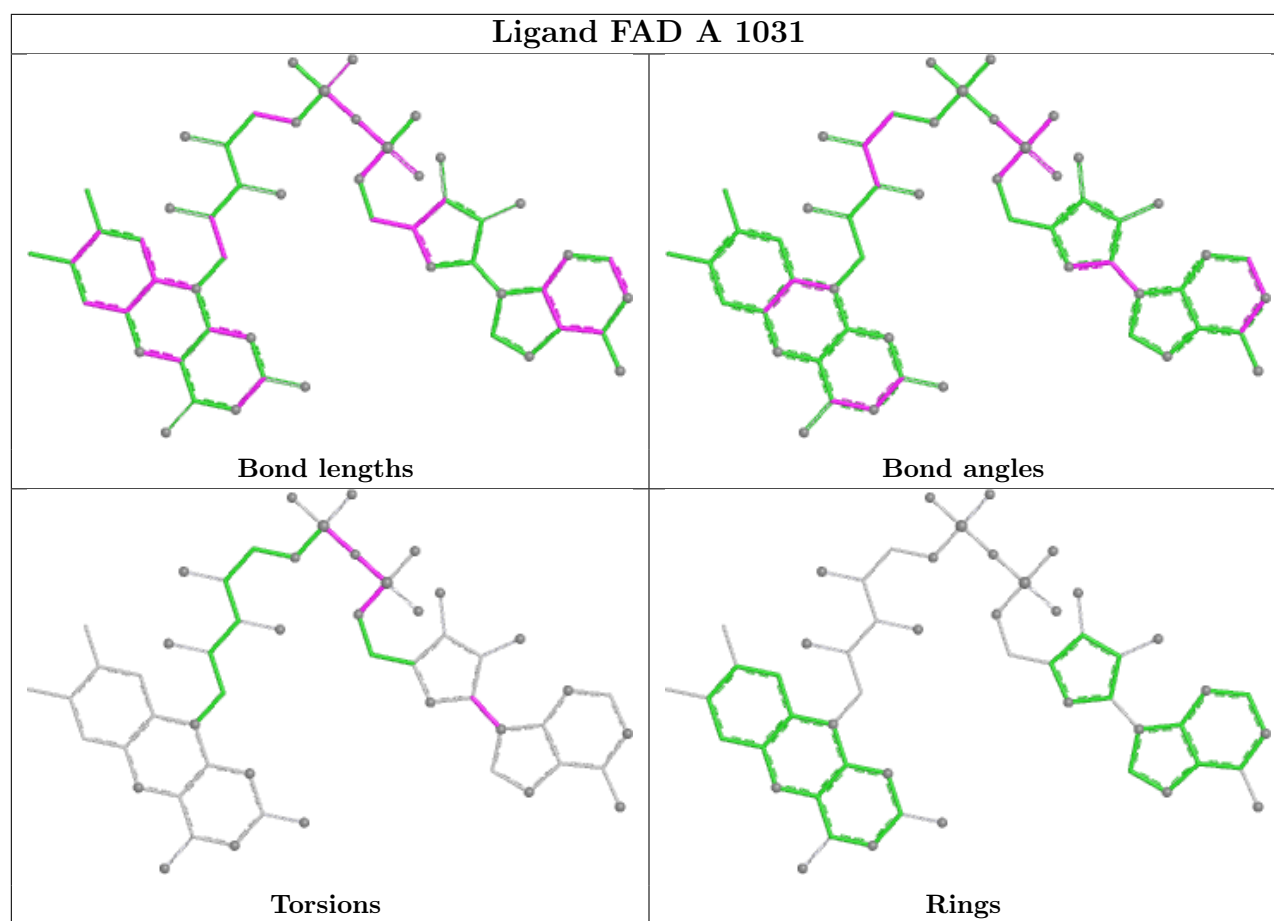


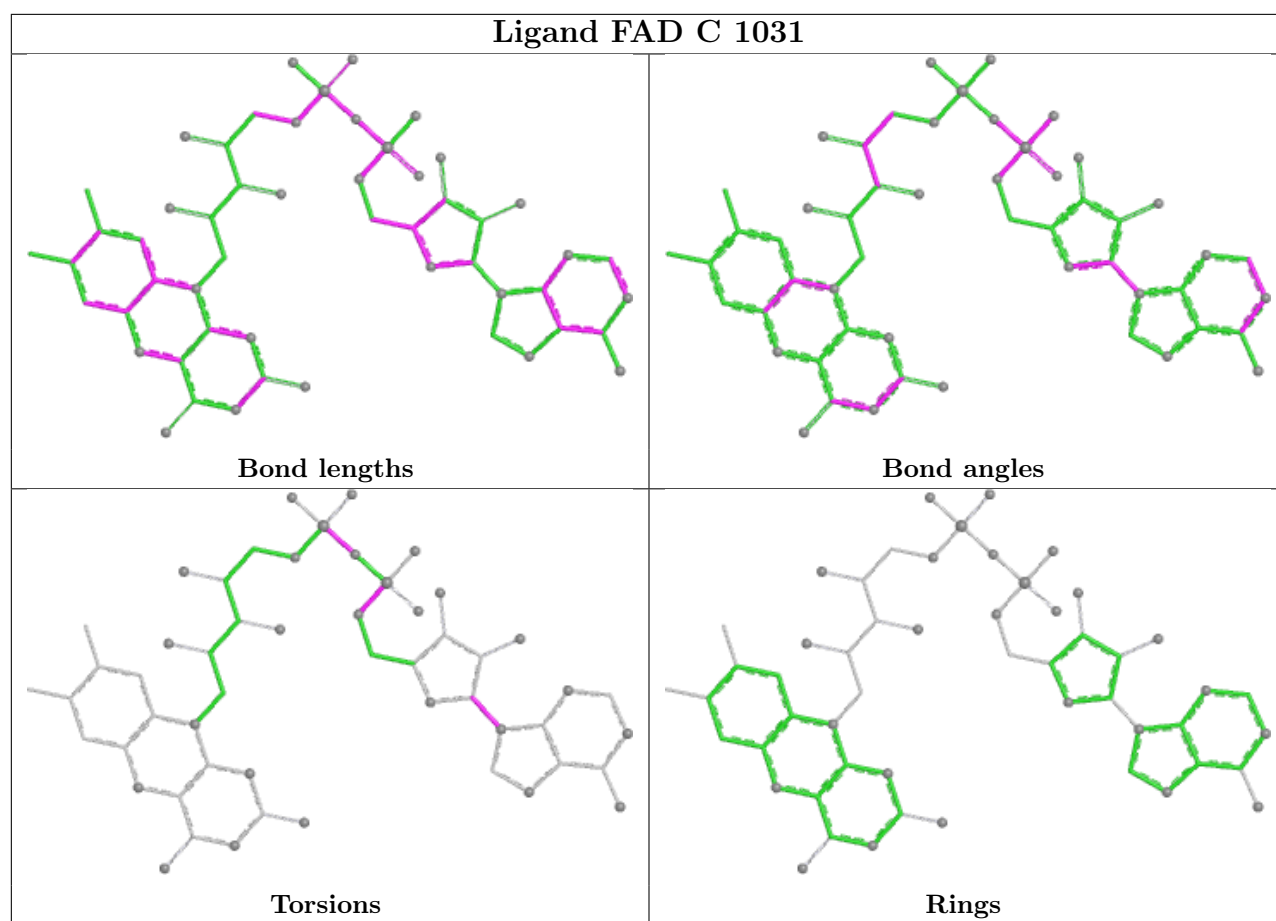
Ligand FMN C 1030



Ligand FMN D 1030







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1005/1025 (98%)	0.32	85 (8%) 16 18	9, 19, 38, 58	4 (0%)
1	B	1005/1025 (98%)	0.33	91 (9%) 15 16	11, 19, 38, 58	5 (0%)
1	C	1010/1025 (98%)	0.37	96 (9%) 14 14	8, 18, 40, 54	11 (1%)
1	D	1014/1025 (98%)	0.33	100 (9%) 13 13	7, 18, 38, 55	7 (0%)
All	All	4034/4100 (98%)	0.34	372 (9%) 14 16	7, 18, 39, 58	27 (0%)

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ALA	11.9
1	A	2	ALA	10.2
1	C	2	ALA	9.9
1	C	682	LEU	9.0
1	B	417	GLY	8.8
1	B	2	ALA	8.4
1	D	417	GLY	8.1
1	C	423	GLU	7.4
1	C	391	LEU	7.4
1	B	367	PHE	7.2
1	D	416	THR	6.9
1	C	324	CYS	6.7
1	C	323	ALA	6.5
1	D	676	GLY	6.5
1	D	901	ASN	6.4
1	A	52	CYS	6.3
1	C	325	HIS	6.2
1	C	1010	PRO	6.1
1	A	51	HIS	6.1
1	A	325	HIS	6.1
1	D	673	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	326	SER	5.9
1	D	52	CYS	5.8
1	C	416	THR	5.7
1	D	367	PHE	5.7
1	B	391	LEU	5.7
1	D	902	ALA	5.5
1	D	679	GLY	5.5
1	A	391	LEU	5.4
1	D	675	MET	5.2
1	B	1017	LEU	5.2
1	C	907	LEU	5.2
1	A	324	CYS	5.2
1	C	322	CYS	5.1
1	C	459	TRP	5.1
1	D	907	LEU	5.1
1	C	320	GLY	5.0
1	A	50	PHE	4.9
1	A	175	CYS	4.9
1	A	901	ASN	4.9
1	D	1009	THR	4.9
1	B	941	ILE	4.9
1	D	391	LEU	4.8
1	A	674	GLY	4.8
1	B	901	ASN	4.7
1	A	417	GLY	4.7
1	C	51	HIS	4.7
1	D	1019	LEU	4.7
1	C	901	ASN	4.7
1	A	367	PHE	4.7
1	D	1010	PRO	4.7
1	C	1017	LEU	4.6
1	A	682	LEU	4.6
1	C	52	CYS	4.6
1	A	673	HIS	4.5
1	D	414	ASP	4.5
1	B	419	TRP	4.4
1	C	908	GLU	4.4
1	B	51	HIS	4.4
1	D	175	CYS	4.4
1	A	426	ILE	4.4
1	C	329	PRO	4.4
1	C	675	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	677	GLU	4.4
1	C	367	PHE	4.3
1	A	416	THR	4.3
1	B	682	LEU	4.3
1	A	870	GLU	4.3
1	C	415	GLU	4.3
1	D	459	TRP	4.3
1	D	689	GLU	4.3
1	D	941	ILE	4.3
1	C	426	ILE	4.2
1	D	22	THR	4.2
1	C	910	LYS	4.2
1	A	322	CYS	4.2
1	B	396	VAL	4.1
1	D	322	CYS	4.1
1	C	175	CYS	4.1
1	D	49	CYS	4.1
1	D	419	TRP	4.1
1	B	52	CYS	4.1
1	D	51	HIS	4.0
1	A	415	GLU	4.0
1	D	857	GLU	4.0
1	A	896	ARG	4.0
1	A	1017	LEU	4.0
1	C	906	PRO	4.0
1	A	419	TRP	4.0
1	B	899	GLU	4.0
1	C	420	ASN	3.9
1	C	419	TRP	3.9
1	D	418	LYS	3.9
1	C	898	LYS	3.9
1	B	867	ARG	3.9
1	B	673	HIS	3.8
1	B	324	CYS	3.8
1	B	900	GLN	3.8
1	C	331	ILE	3.8
1	C	917	PRO	3.8
1	C	872	MET	3.8
1	A	49	CYS	3.8
1	C	868	ILE	3.7
1	C	909	ARG	3.7
1	A	36	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	908	GLU	3.7
1	C	413	GLN	3.7
1	B	459	TRP	3.7
1	B	416	THR	3.7
1	C	422	ASP	3.7
1	D	300	ASP	3.7
1	B	1018	PRO	3.6
1	D	1017	LEU	3.6
1	B	415	GLU	3.6
1	C	870	GLU	3.6
1	C	330	SER	3.6
1	C	867	ARG	3.6
1	D	678	ARG	3.5
1	D	900	GLN	3.5
1	C	904	PHE	3.5
1	B	49	CYS	3.5
1	B	1010	PRO	3.5
1	B	50	PHE	3.4
1	A	680	MET	3.4
1	C	328	LEU	3.4
1	B	409	VAL	3.4
1	C	417	GLY	3.4
1	C	332	ARG	3.4
1	B	414	ASP	3.4
1	D	53	GLU	3.4
1	A	409	VAL	3.4
1	C	421	GLU	3.3
1	C	673	HIS	3.3
1	C	173	ASN	3.3
1	A	328	LEU	3.3
1	D	1018	PRO	3.3
1	D	896	ARG	3.3
1	D	1011	TYR	3.3
1	A	868	ILE	3.3
1	D	293	ILE	3.3
1	D	423	GLU	3.3
1	D	899	GLU	3.3
1	A	414	ASP	3.3
1	A	1009	THR	3.2
1	B	22	THR	3.2
1	C	905	PRO	3.2
1	B	869	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	402	ARG	3.2
1	D	487	ASN	3.2
1	D	295	GLN	3.2
1	C	896	ARG	3.2
1	D	872	MET	3.2
1	C	418	LYS	3.2
1	D	674	GLY	3.2
1	C	1011	TYR	3.1
1	A	407	GLN	3.1
1	C	916	LYS	3.1
1	D	180	GLU	3.1
1	B	681	GLY	3.1
1	C	869	ALA	3.1
1	B	859	HIS	3.1
1	B	296	GLY	3.1
1	A	867	ARG	3.1
1	D	3	PRO	3.0
1	B	443	ARG	3.0
1	D	867	ARG	3.0
1	D	328	LEU	3.0
1	A	1012	GLU	3.0
1	B	1013	PRO	3.0
1	D	1012	GLU	3.0
1	C	871	LEU	3.0
1	B	175	CYS	3.0
1	B	326	SER	3.0
1	A	176	LEU	3.0
1	C	316	SER	2.9
1	D	330	SER	2.9
1	A	458	ARG	2.9
1	D	325	HIS	2.9
1	A	857	GLU	2.9
1	B	180	GLU	2.9
1	C	50	PHE	2.9
1	A	908	GLU	2.9
1	D	273	GLU	2.9
1	A	22	THR	2.9
1	B	328	LEU	2.9
1	B	320	GLY	2.9
1	D	868	ILE	2.9
1	A	696	ARG	2.9
1	C	414	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	680	MET	2.9
1	D	870	GLU	2.9
1	C	395	LYS	2.9
1	D	221	GLU	2.9
1	A	487	ASN	2.9
1	B	410[A]	ARG	2.8
1	D	458	ARG	2.8
1	B	1011	TYR	2.8
1	D	871	LEU	2.8
1	D	363	PHE	2.8
1	C	292	ASP	2.8
1	D	756	ALA	2.8
1	D	873	GLY	2.8
1	A	173	ASN	2.8
1	B	872	MET	2.8
1	A	1016	GLY	2.8
1	C	319	ALA	2.8
1	A	1010	PRO	2.8
1	A	1011	TYR	2.8
1	C	176	LEU	2.7
1	A	11	ASP	2.7
1	A	420	ASN	2.7
1	D	173	ASN	2.7
1	C	327	PRO	2.7
1	D	866	PRO	2.7
1	A	900	GLN	2.7
1	B	295	GLN	2.7
1	D	420	ASN	2.7
1	D	289	LYS	2.7
1	A	422	ASP	2.7
1	D	424	ASP	2.7
1	B	327	PRO	2.7
1	B	908	GLU	2.7
1	B	1012	GLU	2.7
1	C	899	GLU	2.7
1	B	36	LEU	2.7
1	B	897	LEU	2.7
1	A	395	LYS	2.7
1	B	293	ILE	2.7
1	D	910	LYS	2.7
1	D	412	GLU	2.6
1	D	50	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	427	VAL	2.6
1	C	53	GLU	2.6
1	A	1013	PRO	2.6
1	C	1007	ARG	2.6
1	D	239	ASP	2.6
1	B	427	VAL	2.6
1	C	984	ASP	2.6
1	A	871	LEU	2.6
1	B	176	LEU	2.6
1	A	427	VAL	2.6
1	B	395	LYS	2.6
1	B	3	PRO	2.6
1	C	274	GLU	2.6
1	A	681	GLY	2.5
1	A	873	GLY	2.5
1	B	11	ASP	2.5
1	B	407	GLN	2.5
1	A	671	CYS	2.5
1	B	898	LYS	2.5
1	A	872	MET	2.5
1	B	458	ARG	2.5
1	A	3	PRO	2.5
1	C	902	ALA	2.5
1	C	873	GLY	2.5
1	B	316	SER	2.5
1	D	292	ASP	2.5
1	C	393	PRO	2.5
1	D	409	VAL	2.5
1	C	1014	LYS	2.5
1	D	680	MET	2.5
1	C	424	ASP	2.5
1	B	426	ILE	2.5
1	C	409	VAL	2.5
1	B	422	ASP	2.4
1	A	932	LEU	2.4
1	B	408	PHE	2.4
1	B	915	LYS	2.4
1	D	696	ARG	2.4
1	D	917	PRO	2.4
1	B	847	GLN	2.4
1	D	371	ARG	2.4
1	D	394	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	296	GLY	2.4
1	B	672	PRO	2.4
1	B	917	PRO	2.4
1	B	420	ASN	2.4
1	B	910	LYS	2.4
1	B	873	GLY	2.4
1	D	167	ASN	2.4
1	C	897	LEU	2.4
1	A	323	ALA	2.4
1	D	869	ALA	2.4
1	B	856	THR	2.4
1	C	1012	GLU	2.4
1	A	941	ILE	2.4
1	C	862	GLY	2.3
1	C	49	CYS	2.3
1	C	696	ARG	2.3
1	C	1009	THR	2.3
1	D	387	PHE	2.3
1	A	293	ILE	2.3
1	A	180	GLU	2.3
1	B	520	GLU	2.3
1	B	519	PRO	2.3
1	C	1008	THR	2.3
1	C	179	GLN	2.3
1	B	870	GLU	2.3
1	A	909	ARG	2.3
1	C	410[A]	ARG	2.3
1	C	407	GLN	2.3
1	A	897	LEU	2.3
1	B	221	GLU	2.3
1	C	221	GLU	2.3
1	A	239	ASP	2.3
1	B	300	ASP	2.3
1	C	674	GLY	2.3
1	A	885	GLN	2.2
1	C	847	GLN	2.2
1	B	909	ARG	2.2
1	C	36	LEU	2.2
1	D	176	LEU	2.2
1	A	910	LYS	2.2
1	D	407	GLN	2.2
1	D	703	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	428	HIS	2.2
1	A	459	TRP	2.2
1	B	671	CYS	2.2
1	D	898	LYS	2.2
1	B	689	GLU	2.2
1	B	173	ASN	2.2
1	D	315	LYS	2.2
1	D	323	ALA	2.2
1	D	413	GLN	2.2
1	A	264	ASN	2.2
1	A	418	LYS	2.2
1	D	422	ASP	2.1
1	A	421	GLU	2.1
1	A	884	GLU	2.1
1	A	899	GLU	2.1
1	B	700	GLN	2.1
1	C	180	GLU	2.1
1	B	323	ALA	2.1
1	D	517	ALA	2.1
1	A	684	CYS	2.1
1	C	358	ARG	2.1
1	D	932	LEU	2.1
1	A	292	ASP	2.1
1	A	516	SER	2.1
1	D	913	ILE	2.1
1	C	396	VAL	2.1
1	D	671	CYS	2.1
1	A	424	ASP	2.1
1	D	179	GLN	2.1
1	A	332	ARG	2.1
1	B	896	ARG	2.1
1	B	25	HIS	2.1
1	B	325	HIS	2.1
1	D	859	HIS	2.1
1	B	418	LYS	2.1
1	B	756	ALA	2.1
1	A	53	GLU	2.1
1	B	423	GLU	2.1
1	C	321	MET	2.1
1	A	326	SER	2.1
1	B	424	ASP	2.1
1	B	387	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	869	ALA	2.0
1	C	264	ASN	2.0
1	D	847	GLN	2.0
1	C	300	ASP	2.0
1	B	364	ARG	2.0
1	D	682	LEU	2.0
1	A	174	PRO	2.0
1	A	289	LYS	2.0
1	B	329	PRO	2.0
1	C	915	LYS	2.0
1	A	273	GLU	2.0
1	A	847	GLN	2.0
1	D	443	ARG	2.0
1	D	178	SER	2.0
1	D	395	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	A	1029	8/8	0.95	0.09	15,16,18,18	0
2	SF4	B	1029	8/8	0.95	0.08	14,15,17,17	0
2	SF4	A	1028	8/8	0.96	0.08	14,15,16,17	0
2	SF4	A	1026	8/8	0.96	0.07	12,13,15,16	0
2	SF4	B	1026	8/8	0.96	0.08	13,13,15,16	0
2	SF4	B	1028	8/8	0.96	0.07	14,14,16,17	0
2	SF4	A	1027	8/8	0.96	0.07	12,12,14,15	0
2	SF4	C	1026	8/8	0.96	0.07	12,14,15,15	0

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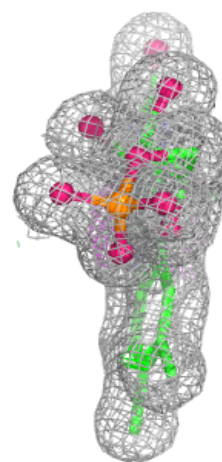
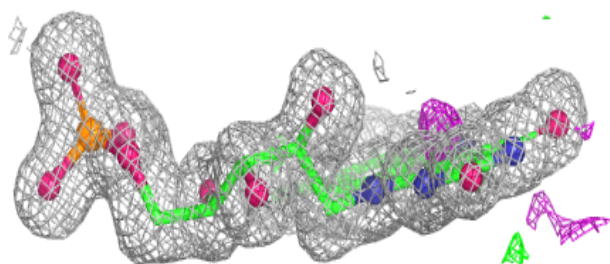
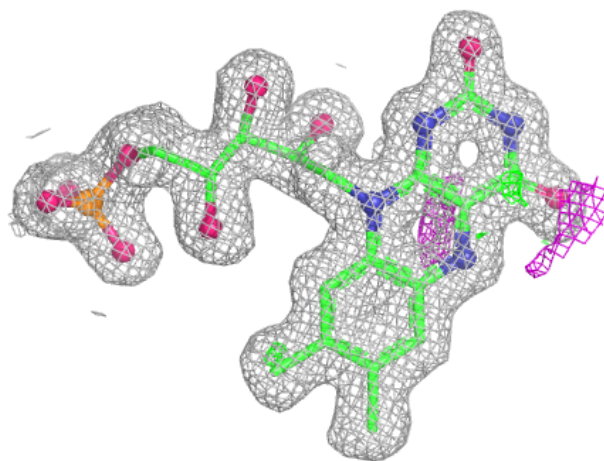
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	C	1028	8/8	0.96	0.07	13,13,15,16	0
2	SF4	C	1029	8/8	0.96	0.07	12,13,15,15	0
2	SF4	D	1029	8/8	0.96	0.08	14,14,16,17	0
3	FMN	A	1030	31/31	0.96	0.06	13,14,16,18	0
4	FAD	A	1031	53/53	0.96	0.06	13,14,16,17	0
4	FAD	B	1031	53/53	0.96	0.06	13,15,17,18	0
4	FAD	C	1031	53/53	0.96	0.06	14,15,17,18	0
4	FAD	D	1031	53/53	0.96	0.06	13,15,16,18	0
2	SF4	C	1027	8/8	0.97	0.07	12,12,14,15	0
3	FMN	B	1030	31/31	0.97	0.06	13,15,17,18	0
3	FMN	C	1030	31/31	0.97	0.06	11,14,15,15	0
3	FMN	D	1030	31/31	0.97	0.06	11,13,14,15	0
2	SF4	D	1026	8/8	0.97	0.07	12,13,15,15	0
2	SF4	D	1027	8/8	0.97	0.07	11,11,14,14	0
2	SF4	D	1028	8/8	0.97	0.07	13,14,16,17	0
2	SF4	B	1027	8/8	0.97	0.07	12,12,15,15	0
5	IUR	A	1034	9/9	0.97	0.12	18,19,22,29	0
5	IUR	B	1034	9/9	0.98	0.10	18,19,21,30	0
5	IUR	C	1034	9/9	0.98	0.10	17,18,20,25	0
5	IUR	D	1034	9/9	0.98	0.10	15,16,19,25	0

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

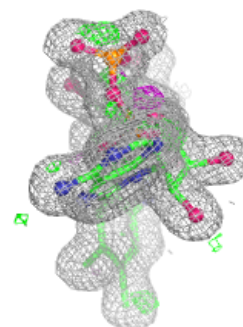
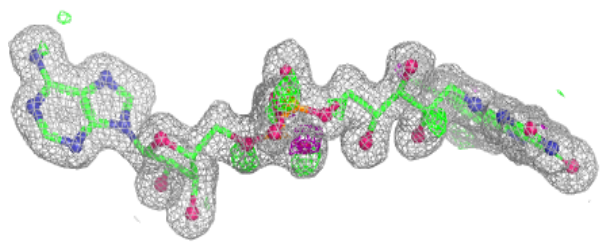
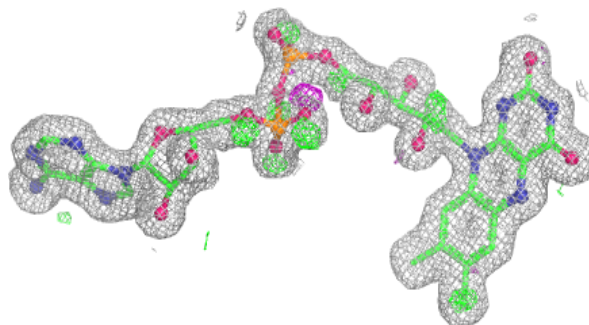
Electron density around FMN A 1030:

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

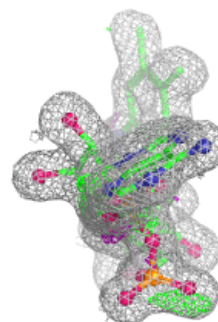
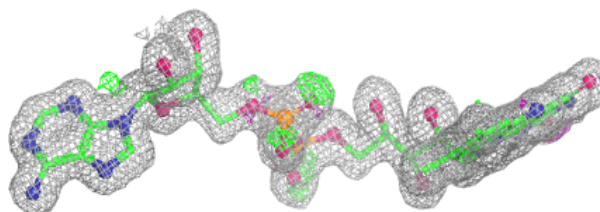
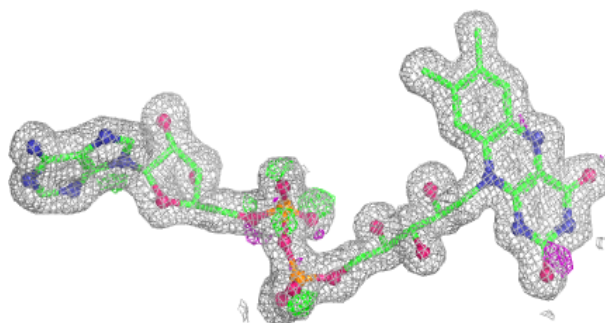


Electron density around FAD A 1031:

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

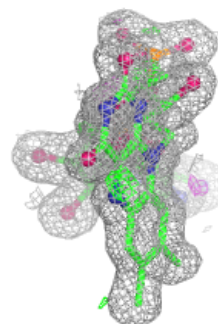
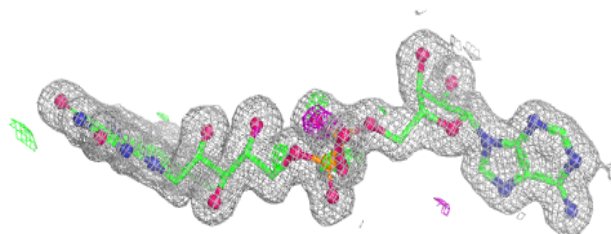
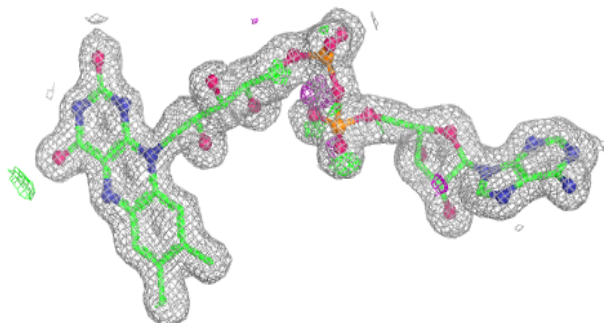
**Electron density around FAD B 1031:**

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

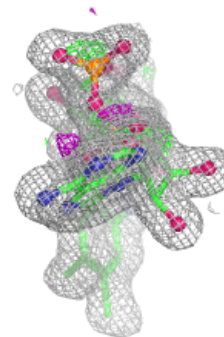
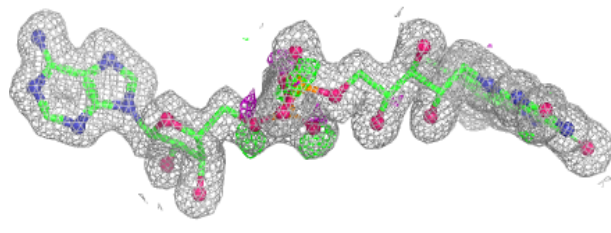
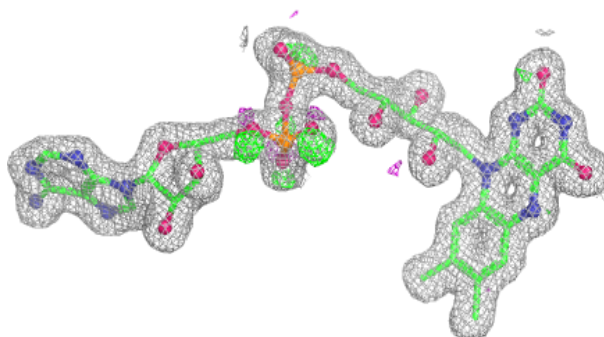


Electron density around FAD C 1031:

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

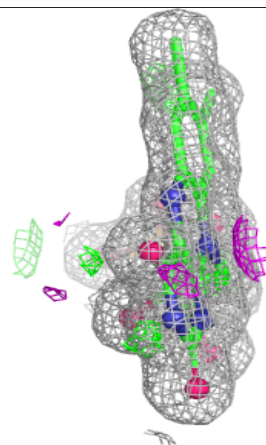
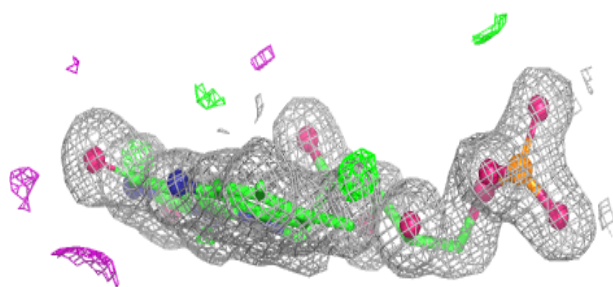
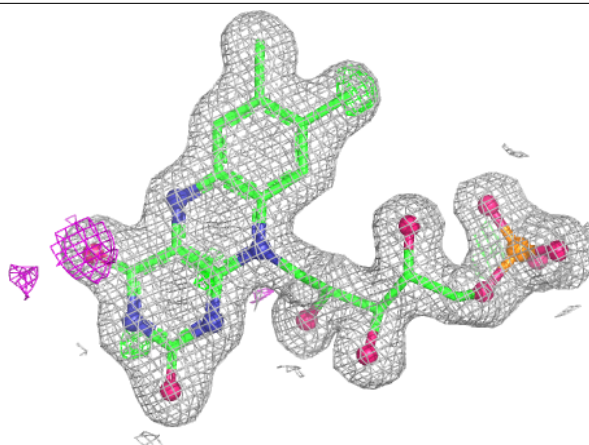
**Electron density around FAD D 1031:**

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



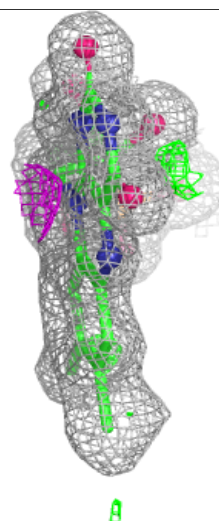
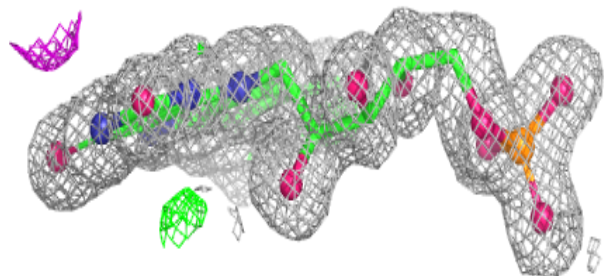
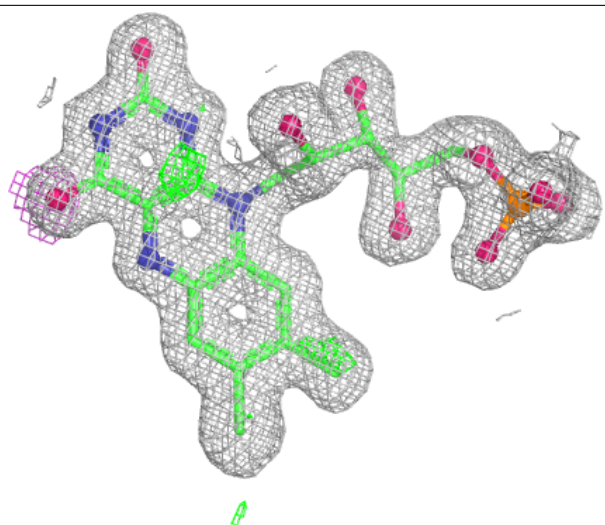
Electron density around FMN B 1030:

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



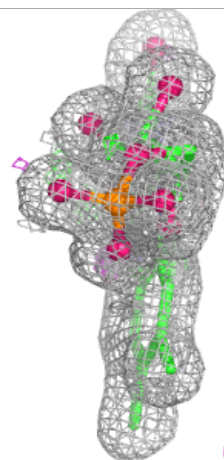
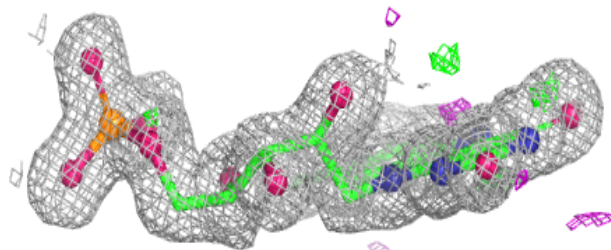
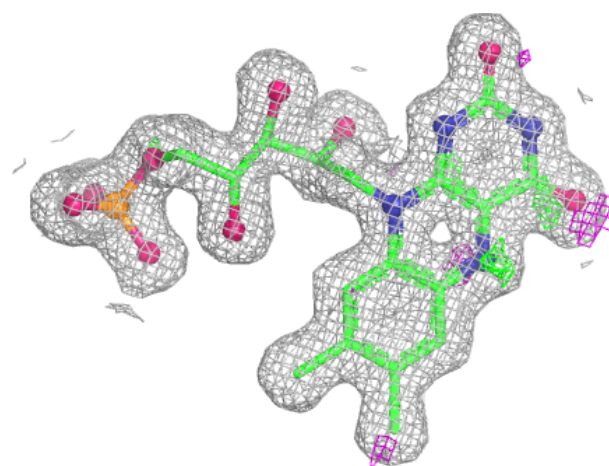
Electron density around FMN C 1030:

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



Electron density around FMN D 1030:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.